SANDIA REPORT

Yucca Mountain Site Characterization Project

Research Program to Develop and Validate Conceptual Models for Flow and Transport Through Unsaturated, Fractured Rock

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RESEARCH PROGRAM TO DEVELOP AND VALIDATE CONCEPTUAL MODELS FOR FLOW AND TRANSPORT THROUGH UNSATURATED, FRACTURED ROCK

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ABSTRACT

As part of the Yucca Mountain Project, our research program to develop and validate conceptual models for flow and transport through unsaturated fractured rock integrates fundamental physical experimentation with conceptual model formulation and mathematical modeling. Our research is directed toward developing and validating macroscopic, continuum-based models and supporting effective property models because of their widespread utility within the context of this project. Success relative to the development and validation of effective property models is predicated on a firm understanding of the basic physics governing flow through fractured media, specifically in the areas of unsaturated flow and transport in a single fracture and fracture-matrix interaction.

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1.0 INTRODUCTION

Mounting concern over the nation's radioactive waste disposal problems has fueled interest in the development of conceptual models for describing water flow and contaminant transport in unsaturated, fractured porous media. Such models will play a key role in the performance assessment of the proposed Yucca Mountain waste repository. Validation of these models within the range of their application for performance assessment requires a more sophisticated understanding of the processes which govern flow and transport within fractured porous media than currently exists.

In support of conceptual model development and validation, a research program has been developed at Sandia National Laboratory for the Yucca Mountain Project to investigate mechanisms and processes that govern flow and transport through unsaturated, fractured rock.[1] The research program integrates fundamental physical experimentation with conceptual model formulation and mathematical modeling. Our approach follows five basic steps:

- identify processes governing water flow and radionuclide transport through fractured porous media;
- develop basic scientific understanding of these processes through fundamental conceptual and mathematical modeling, controlled experimentation, and model validation (invalidation) exercises at both the laboratory and field scales;
- bound the importance or occurrence of various processes in terms of system parameters such as initial conditions, boundary conditions, and distribution of properties in both time and space;
- provide informational needs for site characterization so that the probability of occurrence for each process can be assessed and appropriate model parameters measured; and
- integrate models for important water flow and radionuclide transport processes into performance assessment models.

Fundamental to our approach is systematic physical and numerical experimentation. Physical experimentation takes place in two types of systems: tuffaceous systems containing all the natural complexity of the rock; and analogue systems which are simpler and designed to maximize experimental control and resolution of data measurement (e.g., "rocks" fabricated to specification and roughened glass plates or fabricated rocks held together to form analogue fractures). Relative to tuffaceous experimentation, studies are in progress at both the laboratory and field scale. Numerical experimentation addresses the simulation of physical experiments, the systematic variation of model parameters (sensitivity analysis), and conceptual model simplification.

In both types of experimentation, we stress concepts of dimensional analysis, scaling, and similitude to increase understanding and generalize results.[2,3,4,5,6] For systems to which these concepts are applicable, once a physical experiment is conducted or a solution of the dimensionless form of the governing equation is formulated, the results apply to all similar porous media and flow systems through scaling relations. The concept of similar porous media also is exploited to allow physical experimentation in analogue materials. This can minimize the difficulties of working with some porous materials where the time scale of the process is either too short or too long to make measurement practical.

Questions raised in modeling, laboratory, and field studies are used to direct our research program. In general, research is prioritized with respect to understanding water flow and radionuclide transport processes which could significantly alter our current conceptual models (i.e., significantly decrease or increase water or radionuclide travel times); testing key model assumptions; and developing new conceptual models as necessary. Fundamental research is stressed and in this sense has broad applicability within the general field of flow and transport through fractured porous media.

A number of studies, in various stages of planning or completion, are underway as part of the research program. In this paper, we discuss our general conceptual modeling approach for fractured media and outline our research in two supporting areas: water and nonreactive solute movement in single unsaturated fractures and fracture-matrix interaction.

For the purpose of this paper, we limit our discussion to isothermal flow and, with regard to transport, only consider advection/dispersion processes.

2.0 GENERAL CONCEPTUAL MODELING

Within the context of performance assessment, models for flow and transport through fractured rock will be applied to a myriad of problems (scenarios) at a variety of scales. It is unlikely that a single, all-inclusive, conceptual model can be formulated. For some situations, the assumptions required by a particular conceptual model will be violated and the model cannot be used. The vast majority of scenarios will allow the use of a macroscopic, continuum approach for the formulation and solution of the flow and transport problem. Therefore, the majority of our research is directed toward developing and validating continuum-based models. Application of continuum models to flow and transport through unsaturated, fractured rock has been reviewed in a number of papers.[8,9]

In this approach, isothermal, two phase flow (air/water) through porous media is modeled by application of continuity of mass. Mass flux is given empirically as proportional to the potential gradient, with the proportionality factor denoted as the hydraulic conductivity, a property of the medium. For unsaturated flow, conductivity is a nonlinear function of fluid saturation (possibly hysteretic) and saturation is a nonlinear, hysteretic function of fluid pressure. Fluid potential is a combination of pressure (matric), gravitational, and osmotic potentials. If the gas phase provides negligible resistance to flow of the liquid phase, then the two-phase-flow problem is decoupled, yielding the Richards' equation for liquid water.[10] For many situations within the field of soil physics, the Richards' equation has been shown to adequately model water flow in unsaturated soils.

TUFFACEOUS MATERIALS. A number of tuffaceous rock and fracture samples have been collected for use in the laboratory. Tuffaceous materials have been selected so as to provide samples which are representative of the complex rock systems encountered in the field. Our collection includes samples which range in density from bedded to highly welded tuffs and range in composition from vitric to devitrified as well as zeolitic to non-zeolitic. Our fracture inventory includes tectonic and cooling fractures, single fracture faces as well as mated fracture surfaces. [V.C. Tidwell and R.J. Glass, Div. 6315, Sandia National Laboratories]
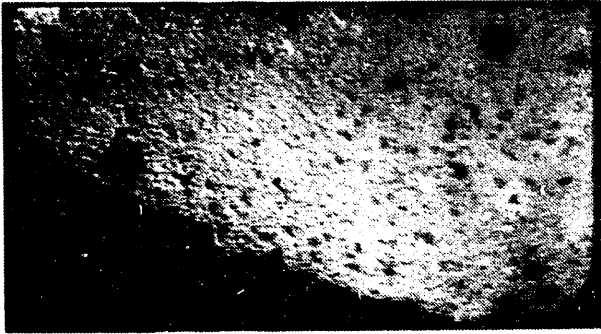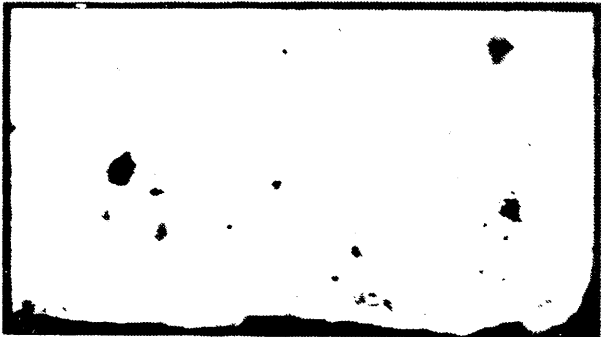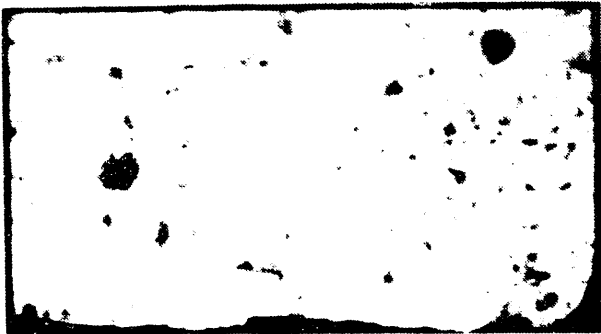
X-RAY ABSORPTION AS A TECHNIQUE FOR MONITORING MOISTURE CONTENT IN POROUS MEDIA. X-ray absorption is being used to monitor moisture and solute concentration fields in heterogeneous, fractured porous media. This technique is of particular interest because it provides a means of obtaining high resolution moisture content and solute concentration data in thin slabs of tuff. X-ray intensity fields are recorded on photographic media, developed, and digitized using video imaging equipment. Shown above is a sequence of x-ray absorption images representing a dry piece of tuff (left), migration of a wetting front in the same piece of tuff (middle), and the moisture content field obtained by subtracting the dry image from the wet image (right). Increasing sample density and hence moisture content is denoted by the blue - green - yellow - red sequence. Quantitative estimates of moisture content and solute concentration are obtained through the use of empirical calibration functions. [V.C. Tidwell and R.J. Class, Div. 6315, Sandia National Laboratories]
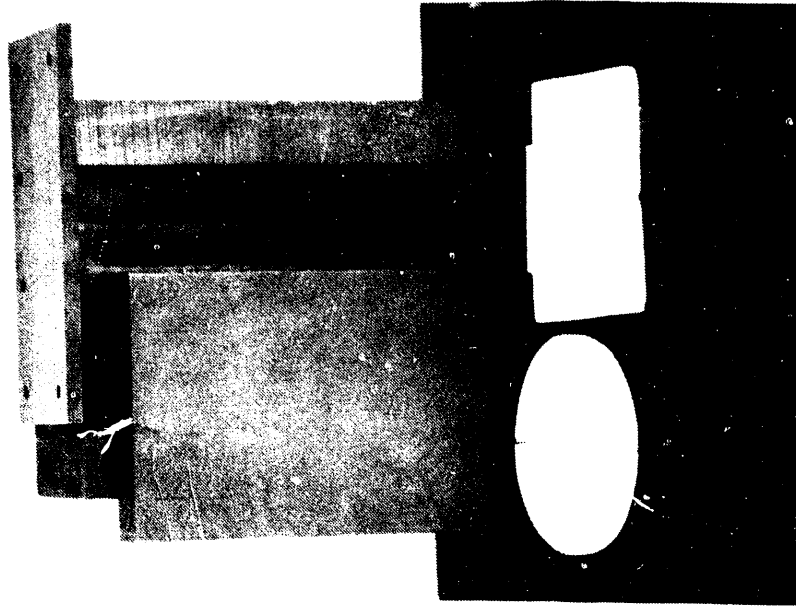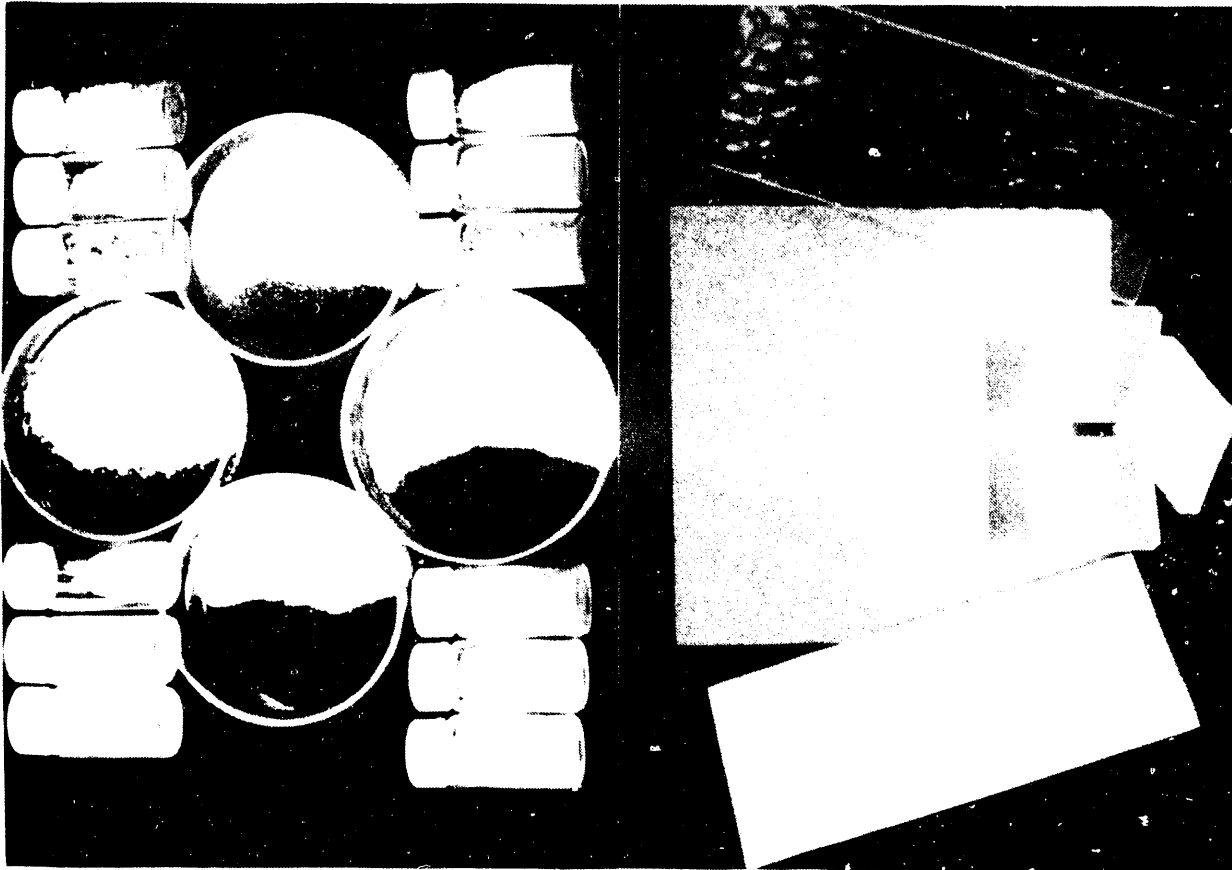
ANALOGUE MATERIALS. Analogue materials play a key role in the experimental program. The use of analogue materials are simpler than tuffaceous materials and thus allow greater experimental control. Analogue material used by the program include a variety of sands and glass beads, fractured and whole sintered glass plates (precision analogue rocks), roughened glass plates (analogue fractures), and fracture molds. [V.C. Tidwell and R.J. Glass, Div. 6315, Sandia National Laboratories]
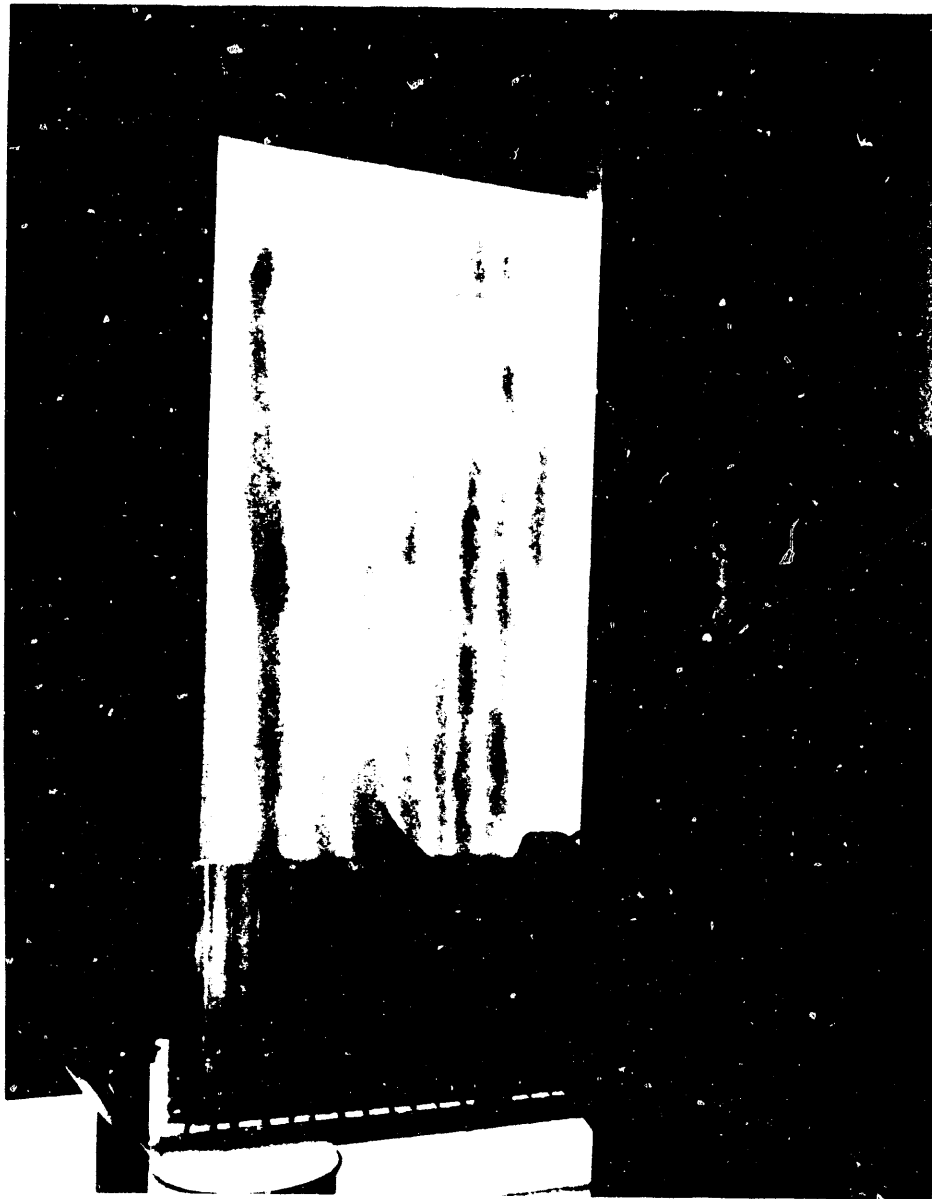
LABORATORY APPARATUS DEVELOPED FOR RAPID VISUALIZATION OF MOISTURE CONTENT IN THIN SLABS OF POROUS MEDIA. Moisture content within thin slabs of sand (1-cm-thick, 50-cm-wide, 130-cm-tall) is visualized using an optical technique that measures the transmission of light through translucent media (the higher the transmission, the higher the moisture content). By illuminating the back of a slab of media, the moisture content distribution integrated over the thickness of the slab is visualized as variations in light intensity at the front of the slab. Using video imaging technology, intensity fields are recorded 30 times a second and digitized into an array of 512x512 points yielding exceptional temporal and spacial resolution. [R.J. Glass, Div. 6315, Sandia National Laboratories]
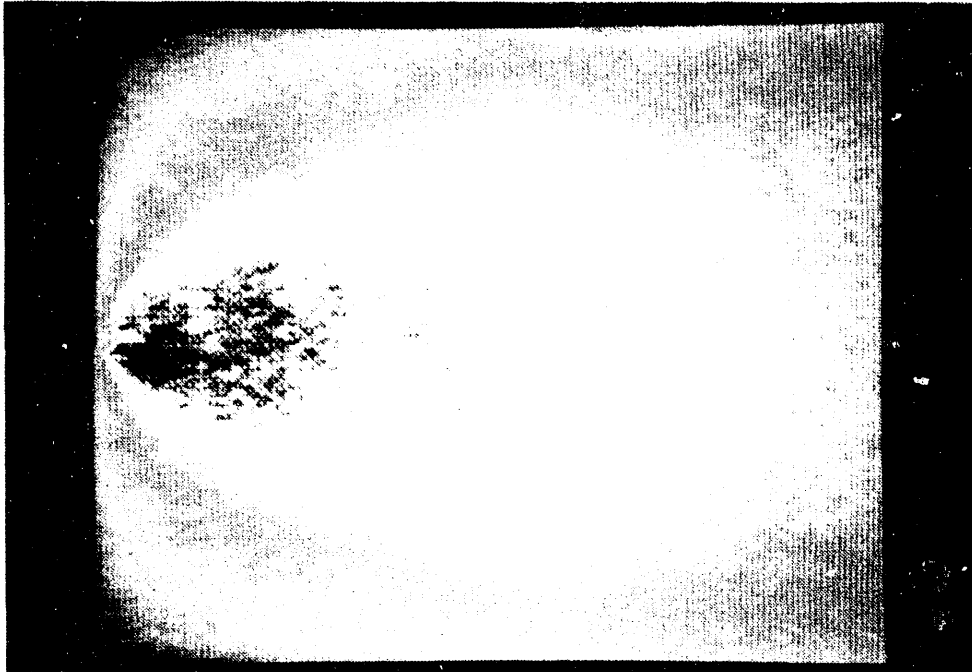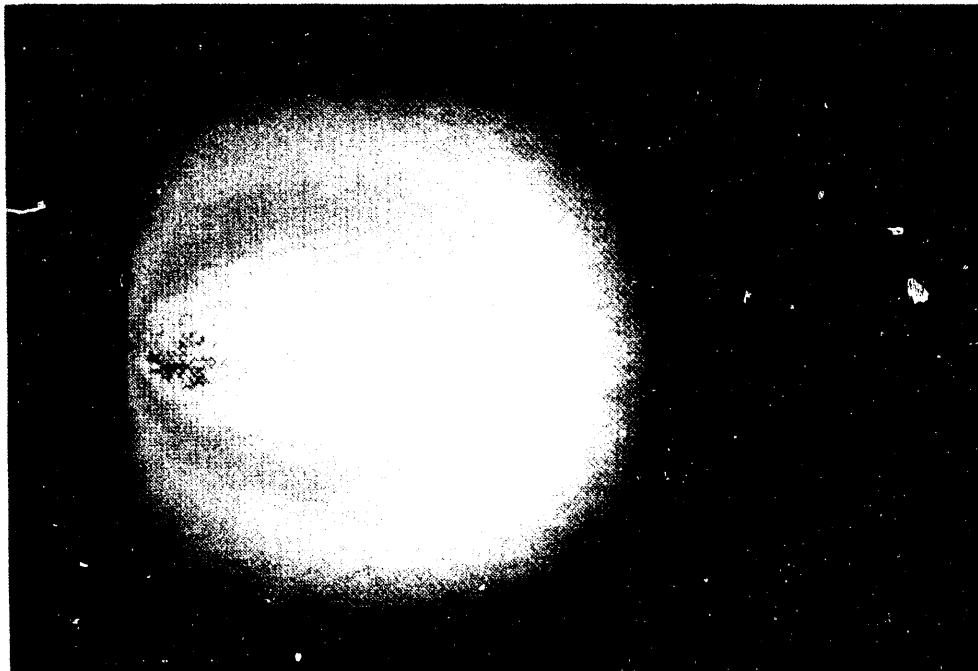
TWO-DIMENSIONAL, TRANSIENT MOISTURE CONTENT FIELDS. The optical technique is used to record the moisture content field at 12 min (left) and the steady-state field at 24 hr (right) generated from a buried point source in a thin slab of sand (1-cm-thick, 25-cm-wide, 40-cm-tall). The light intensity field has been false colored to facilitate visualization of the moisture content with black representing pre-infiltration conditions and the blue-green-yellow-red sequence corresponding to increasing moisture content with red near saturation. [R.J. Glass, Div. 6315, Sandia National Laboratories]
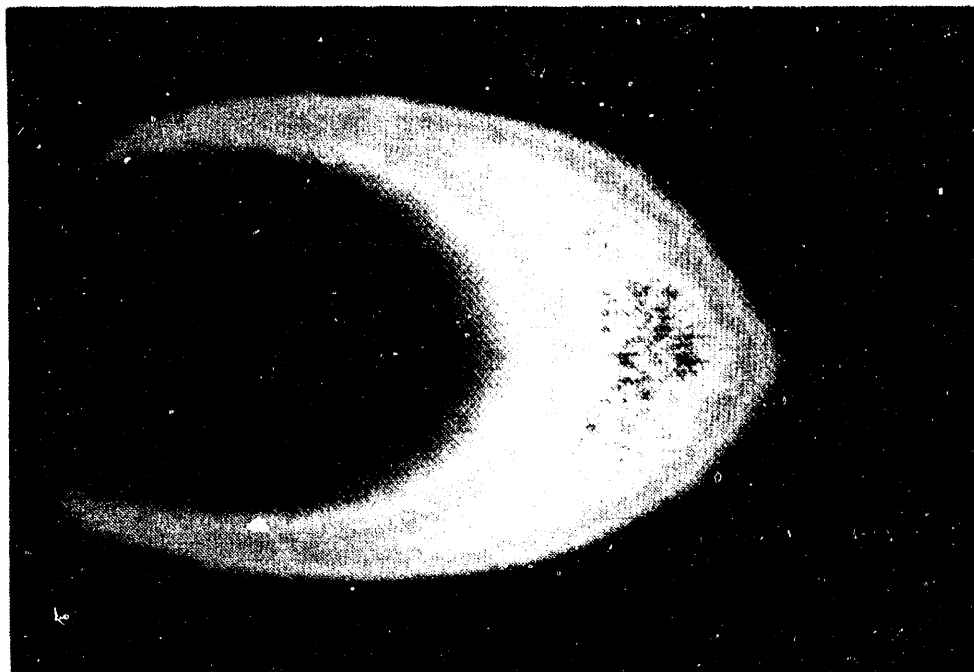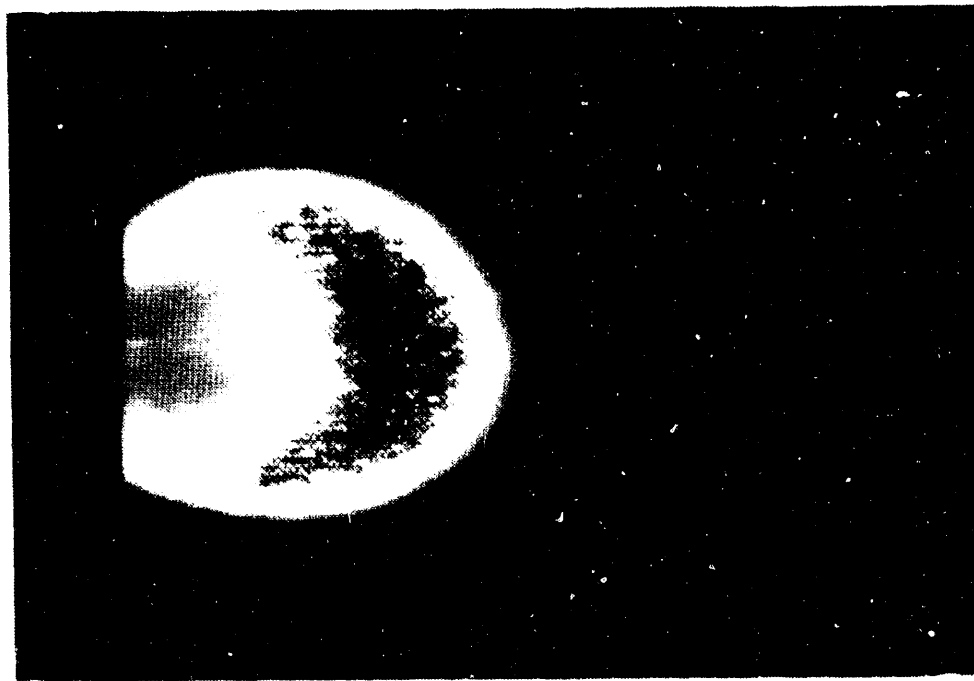
TWO-DIMENSIONAL, TRANSIENT SOLUTE CONCENTRATION FIELDS. The optical technique is used to record the transient solute concentration field at 6 min (left) and 18 min (right) generated from a pulse of dye in the water supply of a steady-state flow field from a buried point source in a thin slab of sand (1-cm-thick, 25-cm-wide, 40-cm-tall). The light intensity field has been false colored to facilitate visualization of the concentration with black representing the pre-pulse, zero concentration conditions and the blue-green-yellow-red sequence corresponding to increasing concentrations with red being the input concentration. [R.J. Glass, Div. 6315, Sandia National Laboratories]
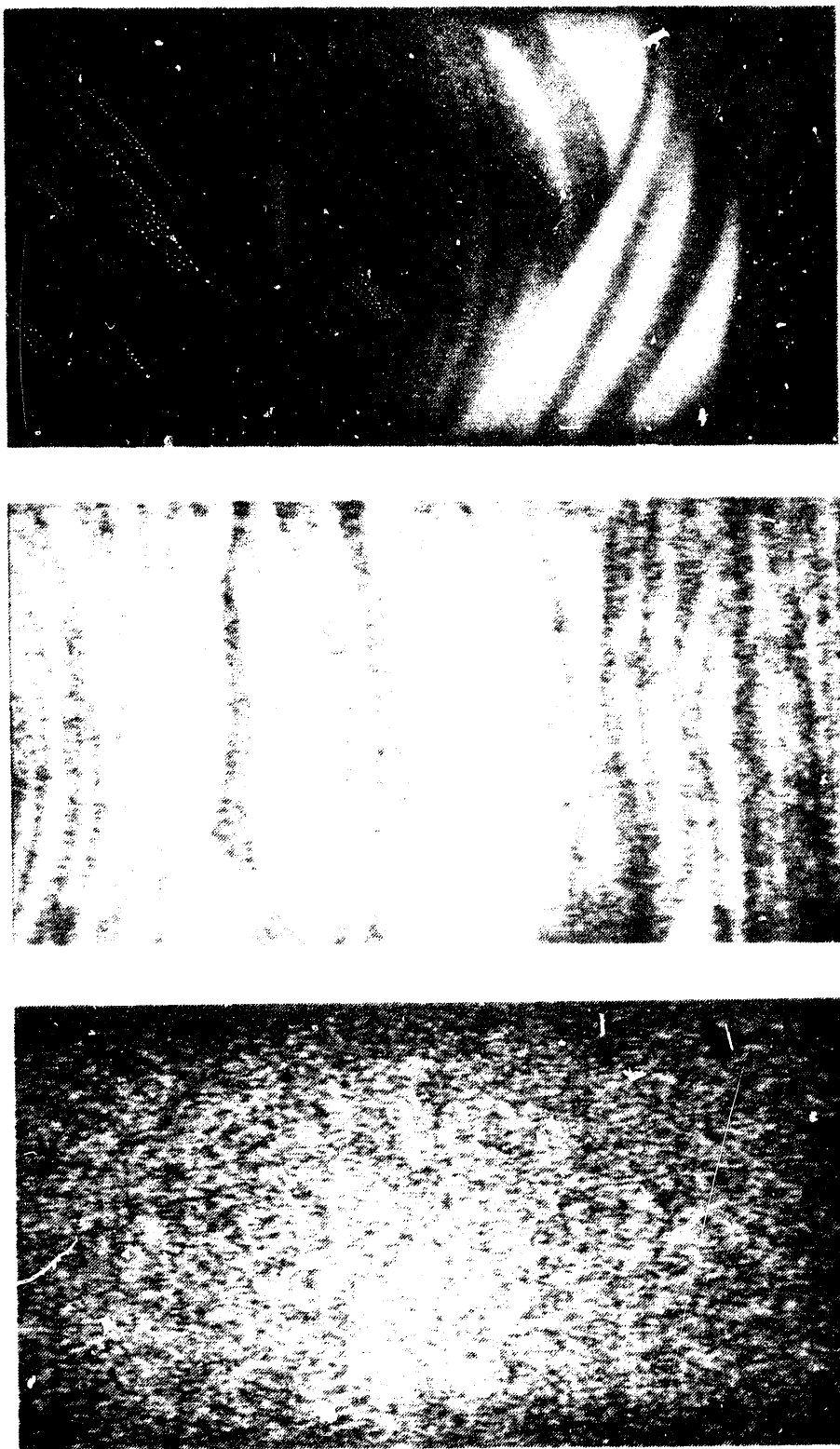
VISUALIZATION OF HETEROGENEITY STRUCTURE. Variations in porosity can be visualized using the optical technique in thin slabs of porous media (slab 1-cm-thick, 25-cm-wide, 40-cm-tall). The slab on the left was created using the chamber-filling technique developed to generate homogeneous slabs. Slabs in the middle and on the right were created using techniques that generate different types of heterogeneity structure. Porosity is indicated by false color with the dark-blue-to-light-blue variation denoting low-to-high porosity. [R.J. Glass, Div. 6315, Sandia National Laboratories]

Using the concept of mass balance, one also can model the transport of solutes through porous media. Nonreactive solute transport results from a combination of advective, dispersive, and diffusive processes. Advective mass flux is given by the mean pore velocity field. Mass flux due to dispersion and diffusion processes is modeled by a gradient law, proportional to the mean concentration gradient. For concentrations where the dilute approximation holds, the combined proportionality factor, denoted as the dispersion coefficient, is considered a property of the medium and a function of the saturation and mean pore water velocity. For many situations in modeling flow of nonreacting tracers in geologic media, the advective mass flux calculated from the velocity fields generated by flow models with average effective hydraulic properties is inadequate. Thus, the details of the velocity distribution are required and must be measured with appropriate experiments.

To apply the continuum approach, we are faced with the standard problem: the determination of macroscopic flow and transport properties at the scale of interest. For problems in which the scale of property measurement is identical to the scale of model application, we may apply the approach with confidence. For problems where our scale of application is different than our scale of measurement, we must make use of intermediate conceptual models, or scaling laws, which define effective properties at the scale of interest. These scaling laws must correctly integrate over the details of the process operating at smaller scales. In unfractured porous media, this integration requires knowledge primarily of the spatial variation of properties. For fractured porous media, this integration also must incorporate the properties of individual fractures and the details of fracture-matrix interaction.

The two-dimensional nature of a fracture yields two distinct effects on steady-state flow and transport, depending on whether flow is in the plane of the fracture or normal to the fracture. Thus, we must consider the definition of flow and transport properties within the fracture as well as the effect of the fracture as a variable-area, pressure-dependent connector to the matrix on the other side. For both steady and transient flows, flow paths in a fractured rock will be controlled by both of these details as well as the variability of matrix properties, variability of fracture properties, and connectivity of the fracture network.

Depending on the problem we wish to solve, we define our continuum (single or multiple) and model effective properties differently. For instance, large-scale modeling of relatively steady-state flow through a fractured media at moderate to high pore pressures may allow the fractures and matrix to be treated as a single composite continuum.[11,12] Here, fractures and the matrix are represented simply as a bimodal pore size distribution. Equivalent properties can be modeled in a variety of ways depending on the connectivity within and between the pore groups composing the fractures and matrix.[13,14,15] In any case, for the approach to be valid, close to equilibrium pressure conditions must exist across all pore groups in a control volume at all times.

For large-scale transient flow conditions, a different approach must be considered. Here, it can be convenient to model the fractured porous media as two interacting, overlapping continua.[16,17] In this dual-porosity approach, interaction between fracture and matrix continua is modeled through a "leakage" term which is a function of a variety of factors such as the gradient between the continua, the ratio between continua properties, matrix-block geometry, and the surface-to-volume ratio of the blocks. Again, equivalent properties for both the fracture and matrix continua must be modeled as well as the leakage or interaction term. Validity of the approach requires, among others, that both the fractures and matrix are sufficiently connected that dual continua can be defined.

In order to develop and validate these and other conceptualizations of the continua as well as to develop effective property models for the conceptualizations, we must understand the details of the flow and transport processes at a scale smaller than the scale of application. The two most important of these are the physics of flow in single fractures and fracture matrix interaction.

3.0 WATER AND SOLUTE MOVEMENT IN A SINGLE UNSATURATED FRACTURE

In order to correctly incorporate the influence of fracture flow into definitions of equivalent hydraulic properties for unsaturated, fractured rock, we must first understand the basic physics of flow and transport in single fractures. For many transient situations, flow within the fracture will be significantly influenced by the surrounding matrix. However, in the extreme of high-flow-rate transients with very low permeability matrix (such as in highly welded,

or zeolitized tuff) or for steady flow through fractured rock near saturation, the effect of the matrix on flow and transport through a conducting fracture will be of second order. For all these situations, the hydraulic properties of a fracture must be determined.

Little is known concerning the distribution of water (referred to as wetted structure) and air in an unsaturated fracture and its influence on flow and transport through the fracture. In addition, fracture-matrix interaction is dependent on the wetted structure within the fracture which connects the matrix on either side of the fracture.

The following questions are being addressed by our current research effort in flow and transport through unsaturated fractures:

- Can macroscale moisture content and relative permeability characteristic curves be defined for individual fractures? Are they a function of scale? Can they be calculated from fracture surface topology (an indirect measure)? How important are air entrapment and hysteresis phenomena?

- Can macroscale solute diffusion/dispersion properties be defined for individual fractures? Can a lumped dispersion coefficient be defined for use in simple one-dimensional models? Is solute dispersion a function of scale? Can a dispersion coefficient be calculated from fracture surface topology?

- Are there any significant differences in flow and transport properties between cooling fractures and tectonic fractures? What types of models for fracture surface topology apply to each?

- Is gravity-driven instability or "fingering" important in nonhorizontal, unsaturated fractures? How does the angle of inclination of the fracture influence finger structure and air entrapment? What are the relative importance of gravity-driven "fingering" and heterogeneity-driven "channeling" on flow field structure and solute transport? Do they act synergistically or antisynergistically?

3.1 Conceptual Modeling

In general, fluid flow through a rough-walled fracture obeys the Navier Stokes equation as long as the aperture of the pore is sufficiently large. A major difficulty arises in the definition of problem geometry, not only in the topology and mating of the fracture surfaces and the effect of lithostatic overburden, but in the determination of which apertures are spanned with each fluid. To yield wetted geometry, the transient Navier Stokes equation for each fluid must be solved. The solution requires proper boundary conditions at the moving water-air interface that incorporate a dynamic contact angle.[18,19] While solution approaches based on cellular automata are in development,[20] this currently is an intractable problem.

Currently, we are using several linked conceptual models to describe fluid flow and solute transport through individual unsaturated fractures, all of which incorporate simplifications that make the problem tractable. Here we briefly outline our modeling approaches for fracture void geometry, unsaturated-fracture wetted-region structure as a function of pressure, and steady flow and solute transport through unsaturated-fracture wetted-region structure. These models are run in series to calculate unsaturated fracture properties of relative permeability, saturation-pressure relation, solute dispersivity, and wetted-region structure.

3.1.1 Modeling of fracture void geometry: The fracture void is modeled by simplifying the geometry to a field of variable apertures within a plane. The plane is divided into a checkerboard and an aperture is defined for each discrete square. To model fracture aperture fields we have two controls: a distribution from which apertures are chosen and the type of spatial structure used to assign apertures within the plane. Currently we have implemented three models to represent spatial structure within the fracture aperture plane: random spatial structure; fractal spatial structure;[21,22] and geostatistical spatial structure.[23]
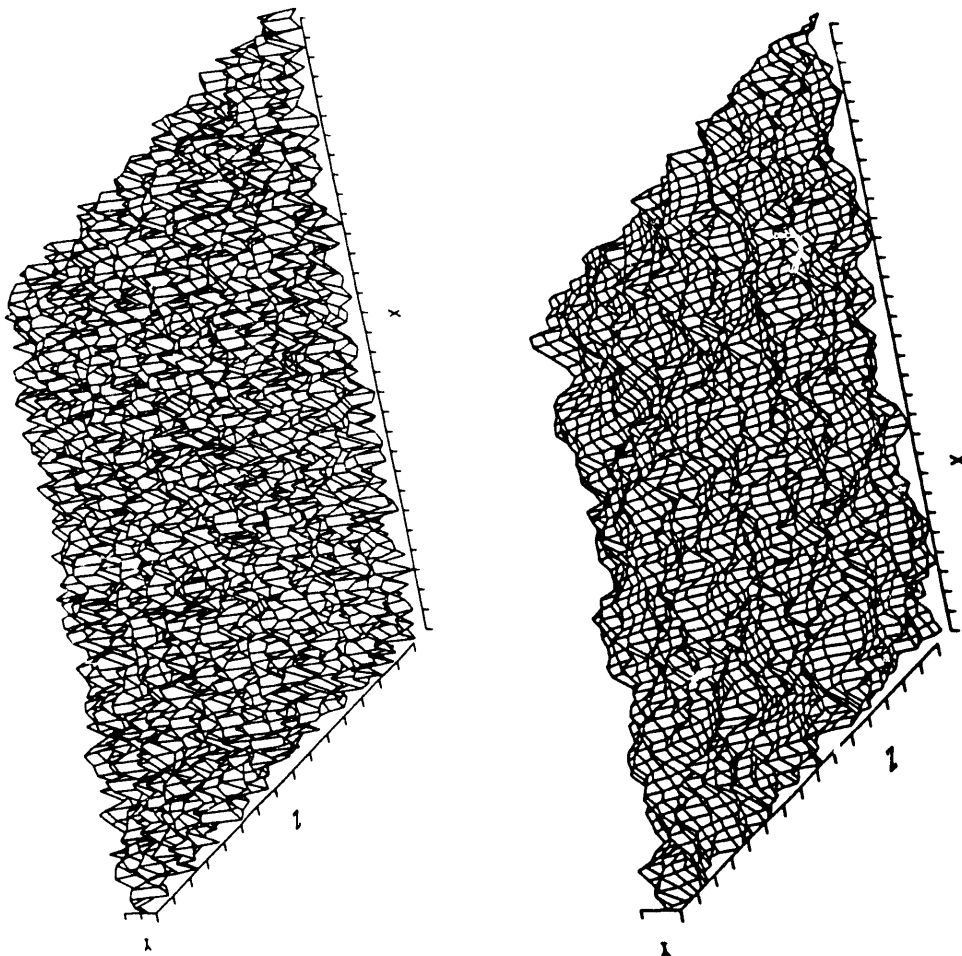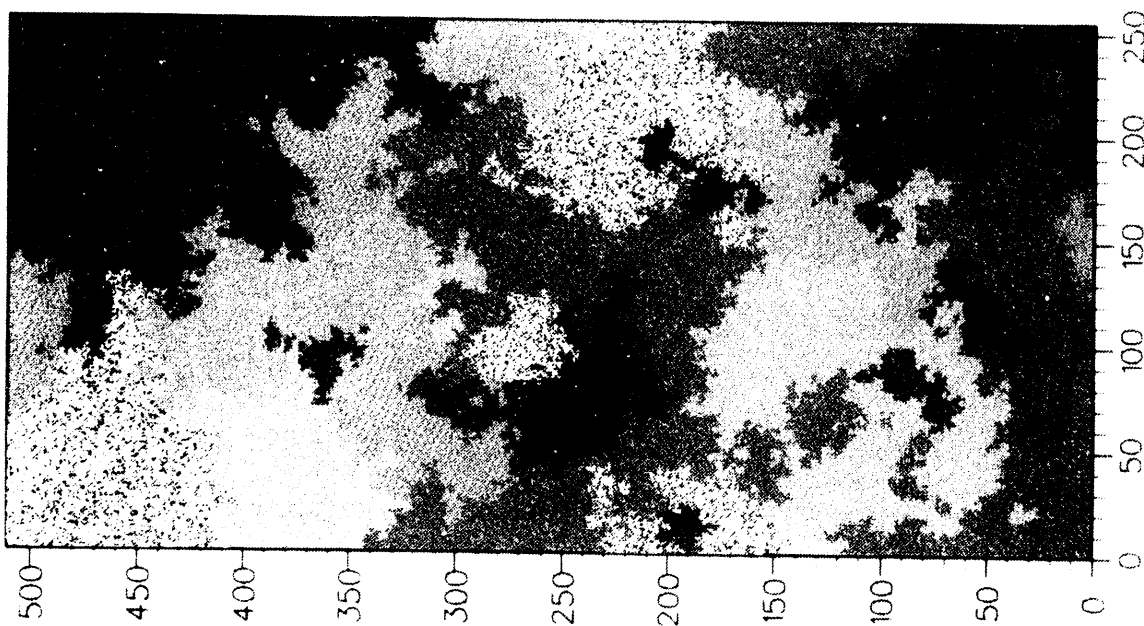
CONCEPTUAL MODELING: Fracture Void Geometry. The fracture void is modeled by simplifying the geometry to a field of variable apertures within a plane. The plane is divided into a checkerboard and an aperture is defined for each discrete square. To model fracture aperture fields we have two controls: a distribution from which apertures are chosen and the type of spatial structure used to assign apertures within the plane. Currently we have implemented , ree models to represent spatial structure within the fracture aperture plane: a) random spatial structure (top right); b) fractal spatial structure (bottom right); and c) geostatistical spatial structure (left). [R.J. Glass, M.E. Thompson, and C.A. Rautman, Div. 6315, Sandia National Laboratories]
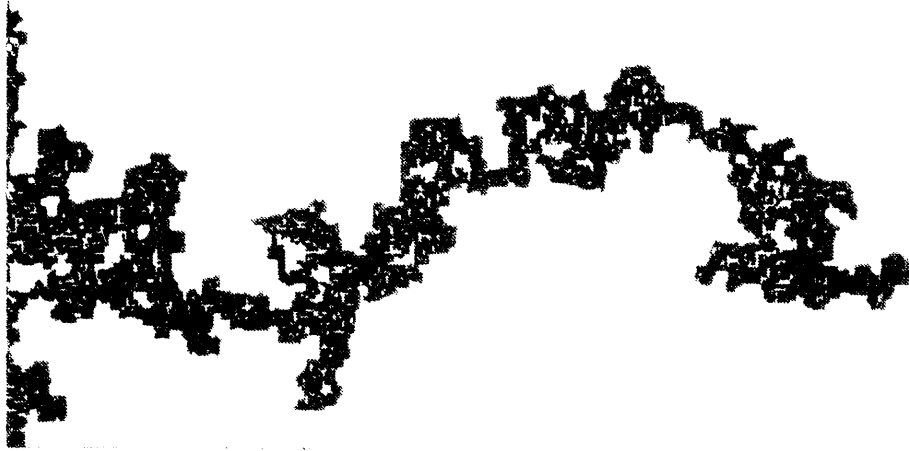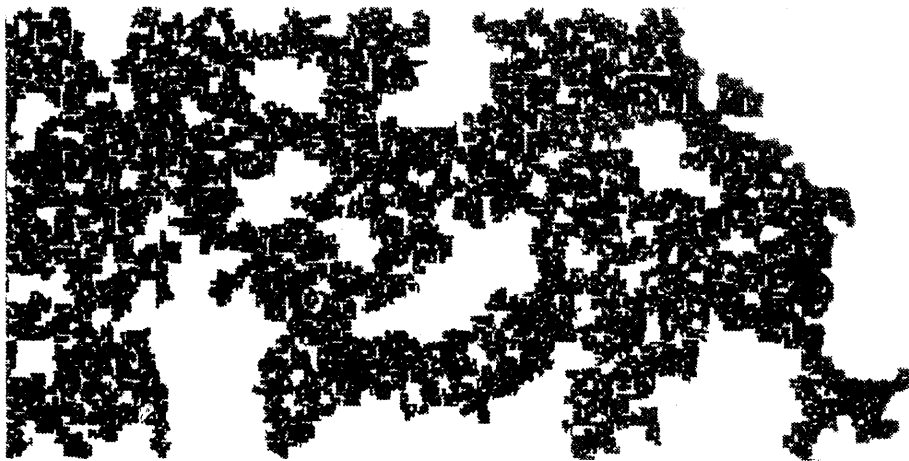
CONCEPTUAL MODELING: Wetted-Region Structure in Unsaturated Fractures. To apply steady flow and transport models to unsaturated fractures, a wetted structure for the aperture field is required as a function of pressure. We are using four approaches to construct the required wetted aperture structures. All the approaches are variations of percolation theory: standard percolation with and without trapping, and invasion percolation with and without trapping. To incorporate the effect of gravity on the wetted-region structure in nonhorizontal fractures, we have modified the invasion percolation models to incorporate a gravity potential. When the fracture is horizontal (left) the interface moves through the network without forming a macroscopic finger (black denotes filled pores, blue are entrapped, red are on the filled interface, and white are unfilled pores beyond the interface). When the same pore network is vertical (right), the downward moving interface breaks into a single finger (network 256 pores wide and 512 pores long. [R.J. Glass, Div. 6315, Sandia National Laboratories]

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3.1.2 Modeling wetted-region structure in unsaturated fractures:

To apply steady flow and transport models to unsaturated fractures, a wetted structure for the aperture field is required as a function of pressure. We are using four approaches to construct the required wetted aperture structures. All the approaches are variations of percolation theory originally proposed by Broadbent and Hammersley[24] for application to pore-scale flow processes in porous media: standard percolation with and without trapping, and invasion percolation with and without trapping.

The standard percolation process conforms to the distribution of fluid within a network under thermodynamic equilibrium. That is, all pores communicate with all pores and no entrapment can occur. For this to be applicable to an unsaturated fracture, we must have very long equilibrium times where each fluid can diffuse through each other until the entire system is in thermodynamic equilibrium. Another situation where the results may be applicable is in finely-rough, rough-walled fractures where water film flow will occur along the walls and thus establish the intercommunication of the water throughout the fracture. For both of these situations, the time scale for the displacement process must be large compared to that for communication processes (either film flow or diffusion). Standard percolation with trapping, first discussed by Dias and Wilkinson,[25] has application to fractures where water enters the fracture from the matrix but communication processes do not exist and air can become entrapped in regions of the fracture.

Invasion-percolation, introduced by Wilkinson and Willemsen,[26] models an imbibition process where the pressure potential within each fluid does not vary in space. This is a reasonable assumption in the limit of infinitesimal flow rate where viscous forces are negligible and the system is dominated by capillary (surface tension) forces. If trapping is included, communication processes either do not exist or displacement takes place on a time scale that is small compared to existing communication processes. Invasion percolation is essentially a simplified form of the pore-scale models developed in the petroleum engineering field.[27,28,29,30] For low-flow situations, invasion percolation should simulate the sequential development of the wetted region within the fracture.

To incorporate the effect of gravity on the wetted-region structure in nonhorizontal fractures, we have modified the invasion percolation models to incorporate a gravity potential.[31] For cases where fingers form, we are adapting conceptual models based on linear stability analysis developed to understand the analogous problem of gravity-driven fingering in porous media.[32,33] Such models are capable of addressing the dynamical relationships for wetted-region structure as a function of system flow rate.

3.1.3 Simplified conceptual models for steady flow and solute transport through the wetted fracture structure:

The steady-state flow of an incompressible fluid through the wetted region of a fracture is modeled by the Reynolds equation, originally developed for lubrication applications. Assumptions required for the derivation of the Reynolds equation are essentially that the cubic law holds locally and that mass is conserved.[35,36] The cubic law is derived for laminar flow between two parallel plates and simply states that the flux is proportional to the product of the pressure gradient and the aperture cubed. A theoretical exploration of this assumption has been performed using perturbation solutions of the Navier Stokes equation.[37]

The flow field solution is used in a solute transport model using a "depth" averaged advective diffusion equation.[38,39,40] Dispersion due to advective field variation is calculated by fitting the solute breakthrough at the end of the fracture to the one-dimensional advective-dispersion model solution. In addition, a solution of the two-region, mobile/immobile advection dispersion model is fit to calculate a different dispersion coefficient and the fractional immobile wetted region.

3.2 Physical Modeling

We have developed a physical modeling or experimental capability that allows us to explore many unsaturated-fracture-flow system parameters (see Table 1). Our experimental apparatus consists of a rotating test stand (RTS), analogue fracture test cells, and digital imaging and processing equipment. The RTS holds within a rigid frame a diffuse light source that backlights a test cell plane and array cameras focused on the test plane. The RTS can be

DIRECTION OF FLOW
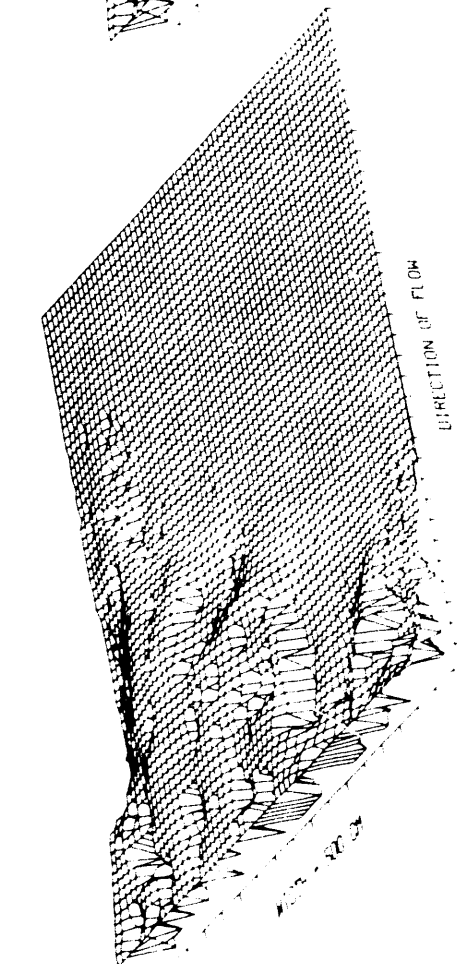
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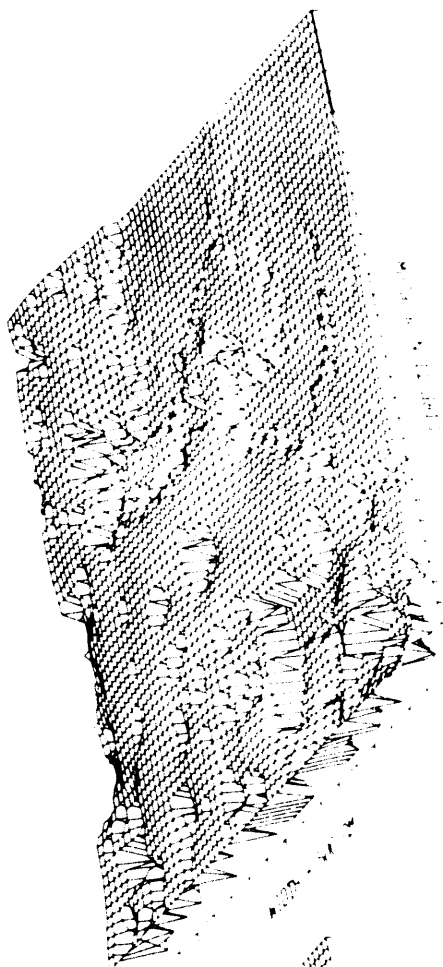
CONCEPTUAL MODELING: Steady Flow and Solute Transport. The steady-state flow of an incompressible fluid (top right) through the wetted region of a fracture (top left) is modeled by the Reynolds equation, originally developed for lubrication applications. Essentially the assumptions require that the cubic law holds locally and that mass is conserved. The cubic law is derived for laminar flow between two parallel plates and simply states that the flux is proportional to the product of the pressure gradient and the aperture cubed.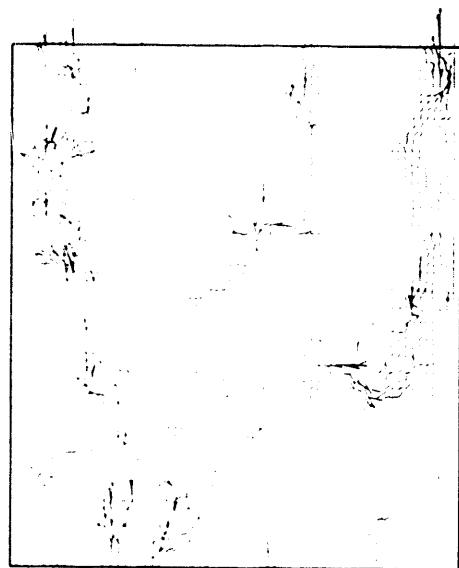 The flow field solution is used in a solute transport model using a "depth" averaged advective diffusion equation (bottom left and right). Dispersion due to advective field variation is calculated by fitting the solute breakthrough at the end of the fracture to the one-dimensional advective-dispersion model solution. [R.J. Glass and M.E. Thompson, Div. 6315, Sandia National Laboratories]

TABLE 1: UNSATURATED FRACTURE FLOW AND TRANSPORT SYSTEM PARAMETERS

1. Physical properties of the fracture
   a. mean topography of roughness/aperture (microscopic length scale)
   b. roughness/aperture distribution about the mean
   c. spatial structure of aperture within fracture plane
   d. distance between fracture walls
   e. microfractures or microporosity at fracture walls

2. Fluid properties (functions of temperature and solute concentration)
   a. surface tension
   b. viscosity
   c. density
   d. contact angle between liquid, gas, and fracture wall (wettability)

3. Composite hydraulic and transport properties
   a. conductivity
   b. fluid characteristic relation
   c. diffusivity
   d. sorptivity
   e. solute dispersivity

4. Isotropy or anisotropy of physical or composite hydrologic and transport properties

5. Heterogeneity of physical or composite hydraulic and transport properties
   a. type
   b. "intensity" or level
   c. length scale of heterogeneity

6. Macroscopic geometry of fracture flow system
   a. macroscopic length scale
   b. orientation in gravity field

7. Initial/boundary conditions
   a. initial saturation
   b. flux or pressure supplied at top of system
   c. air pressure ahead of the wetting front
   d. point or uniform fluid application

rotated through 180 degrees to vary the orientation of the fracture with respect to the gravitational field. The test plane between the light and the cameras can incorporate planar test cells up to 50x100 cm. The analogue fracture test cells are designed to accept exchangeable, translucent, fracture plates (two plates make a fracture) and hold the plates together between two thick outer glass plates with fluid pressure. This pressure system removes long wavelength features from the aperture distributions, and allows us to simulate and vary lithostatic overburden pressure. Top and bottom boundary conditions on the fracture are imposed by narrow pressure plates making use of filter paper. A reed valve within the top plate allows us to switch between two fluids evenly across the fracture for solute transport experiments. Side boundary conditions are either open or closed with side gaskets which may be added or removed during an experiment. Digital images recorded during an experiment (up to 2048x2048 resolution) are analyzed to give wetted and entrapped region structure or transient dye concentrations for transport experiments.

We are making use of several types of fracture plates. Preliminary experimentation focuses on existing, manufactured glass surfaces (e.g., "obscure plate glass") that simulate a fracture and can be modified to explore system parameters of interest (surface topology, microroughness). Microroughness can be induced through sandblasting the surface (the bead size of the blasting material changes the microroughness) or HF etching (exposure time changes microroughness). We also are using fracture plates cast in epoxy and acrylic from naturally occurring fractures. Sol gel coating of the fracture casts to introduce microporosity, simulating microroughness, is being explored. In order to vary fracture aperture distribution and spatial structure systematically, methods also are being explored to fabricate fractures to specification using model-generated aperture distributions.

The aperture field in a particular translucent analogue fracture (glass plate, cast or model-generated fabricated fracture) is characterized by saturating the fracture with dye solution and measuring light transmission on the RTS. Digitization of the image at a number of resolutions yields a series of aperture fields for use in numerical experiments. Numerical simulation at these different resolutions are necessary to determine the resolution required to predict our experiments and thus that required in aperture measurement programs planned as part of site characterization.

3.3 Physical and Numerical Experimentation

Integrated numerical and physical experiments are underway that study the effects of fracture surface roughness (topology) and orientation with respect to gravity on the unsaturated fracture-flow-field structure, hydraulic and transport properties, and scaling behavior of the properties.

Numerical experiments are conducted to determine model parameter sensitivity, to aid in constructing physical experiments, and to compare with physical experiments. Apertures within fracture planes are simulated using random, fractal, or geostatistical models. The appropriateness of the three models for representing spatial structure is being evaluated by measuring and analyzing aperture fields of both cooling and tectonic fractures from existing core and outcrop samples taken from Yucca Mountain. The various percolation models are used to generate a wetted structure as a function of pressure characterized by a saturation and fractal dimensions of wetted, nonwetted, and entrapped regions. Steady-state flow is simulated through the wetted structure and the hydraulic conductivity is calculated. Transport of a pulse of nonreacting solute in the steady flow field is simulated and the breakthrough of the solute at the end of the fracture calculated. The solute concentration break through curve is fit both with a simple one-dimensional solution of the advection dispersion equation to calculate a dispersion coefficient and with a solution to the two-region, mobile/immobile advection dispersion model to calculate a dispersion coefficient and the fractional immobile wetted region.

Physical experiments conducted on the RTS follow a similar sequence. For these experiments, fracture plates will vary within the three types (glass plate, natural fracture casts, and model generated). For a given pair of fracture plates, the transient horizontal water sorption and desorption processes are recorded with digital images under both constant-flow and constant-supply (or extraction) pressure conditions. Knowledge of the flow rate as a function of time in the constant-supply pressure sorption experiments yields the fracture sorptivity. The images

PHYSICAL MODELING: Fracture Flow Experimental Apparatus. We have developed an experimental capability that allows us to explore air/water flow in single fractures. Our experimental apparatus consists of a rotating test stand (RTS), analogue fracture test cells, and a digital-imaging and processing system used in visualizing flow. The RTS is used to vary the orientation of a fracture with respect to the gravitational field (rotation through 180 degrees). A diffuse light source backlights the test plane (fracture) and a CCD camera is focused on the test plane. The analogue fracture test cells are designed to accept exchangeable, translucent, flat fracture plates (two plates make a simulated fracture). The plates are held together between two thick outer-glass plates by fluid pressure. Fracture plates are composed of roughened glass plates or natural fracture casts. Digital images (up to 2048x2048 resolution) are recorded during an experiment and are analyzed to yield wetted and entrapped region structure or give transient dye concentrations for transport experiments. [R.J. Glass and V.C. Tidwell, Div. 6315, Sandia National Laboratories]
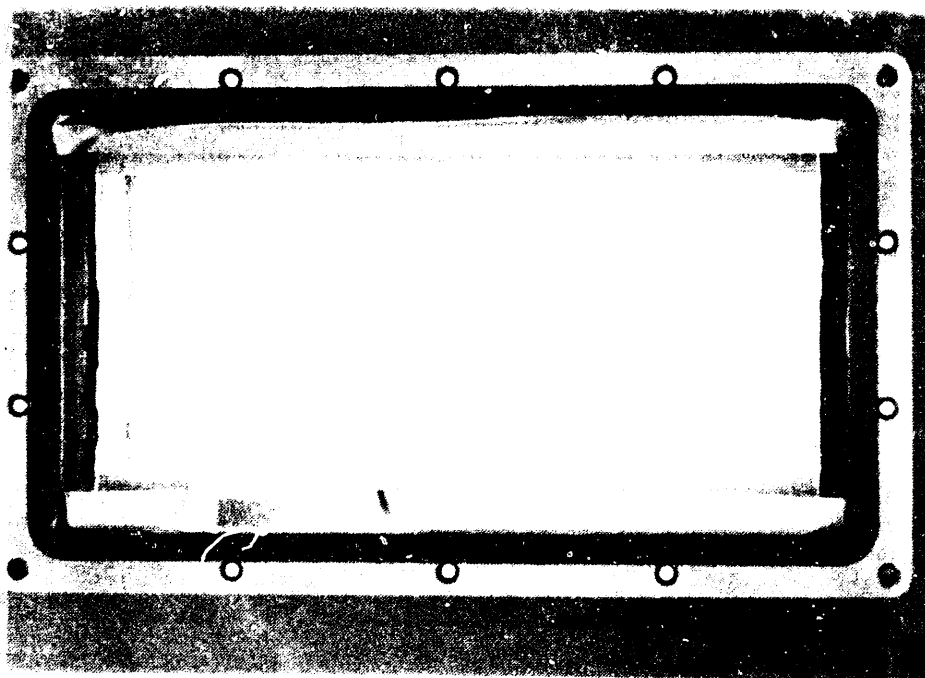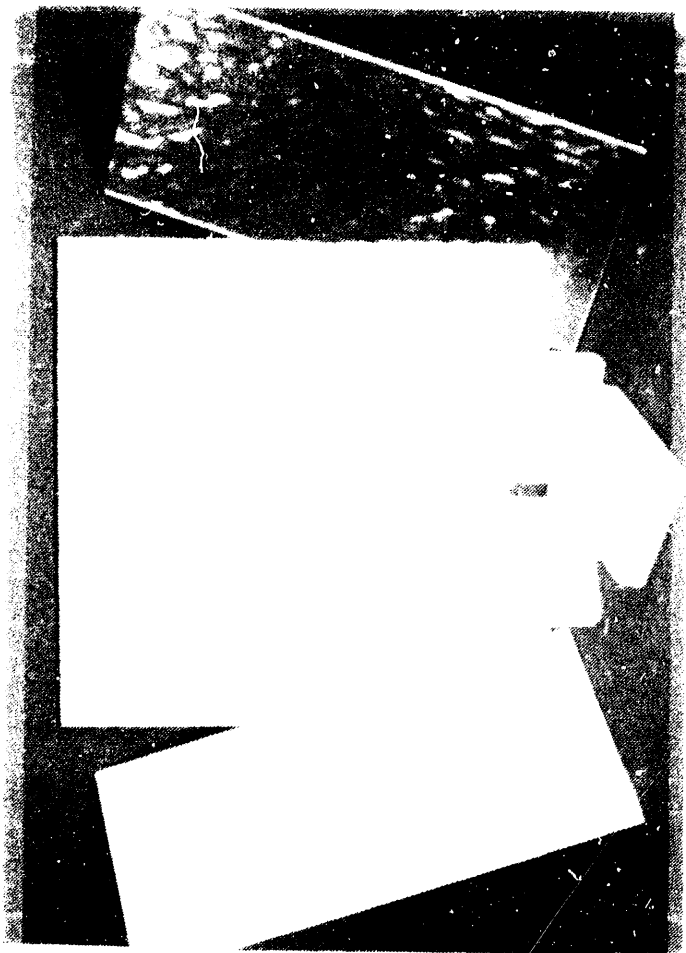
PHYSICAL MODELING: Fracture Plates. Preliminary experimentation focuses on existing, manufactured glass surfaces (e.g., "obscure plate glass") that simulate a fracture and can be modified to explore system parameters of interest (surface topology, microroughness). Microroughness can be induced through sandblasting the surface or HF etching. Natural fractures are cast in epoxy to create a clear replica of the fracture. In order to vary fracture aperture distribution and spatial structure systematically, methods also are being explored to fabricate fractures to specification using model-generated aperture distributions. [R.J. Glass, V.C. Tidwell, and S.R. Brown, Div. 6315, Sandia National Laboratories]
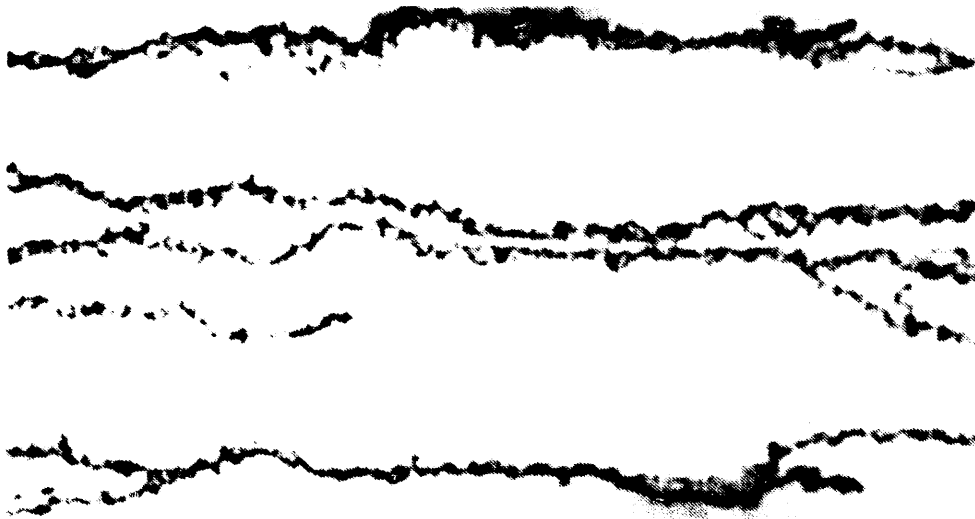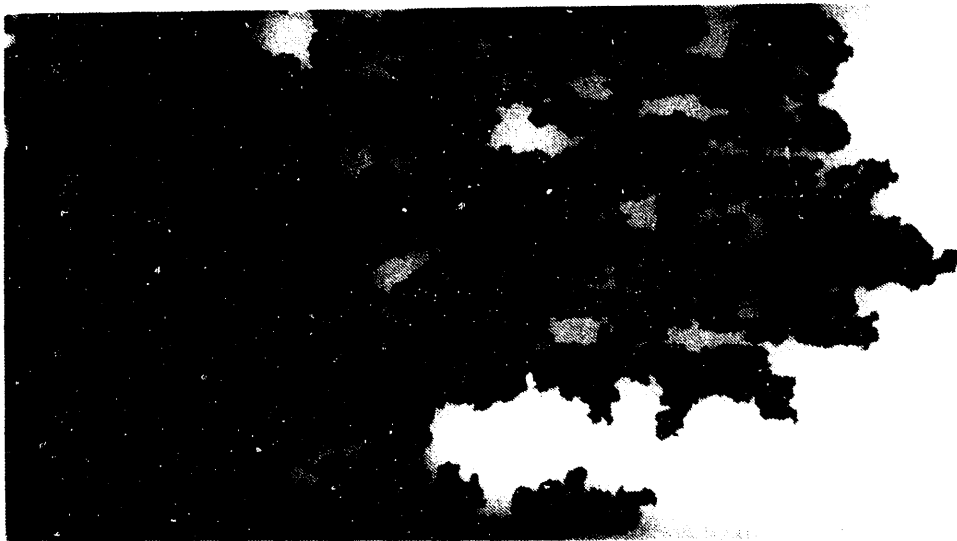
PHYSICAL AND NUMERICAL EXPERIMENTATION: Horizontal and vertical imbibition into transparent analogue fractures. Two roughened glass plates (commercially available obscure glass) are clamped together to form an analogue transparent fracture (30-cm-wide, 60-cm-long). Water imbibes at a constant flow rate supplied through a porous plate at the top of the fracture. The wetted structure is recorded in time both photographically and on video for digital image analysis. The left plate depicts horizontal imbibition and the right plate vertical imbibition where downward moving fingers form. Results of these experiments are qualitatively similar to those where infiltration flow instability in unsaturated porous media occurs and to those generated with the pore-scale invasion percolation model. [R.J. Glass, Div. 6315, Sandia National Laboratories]

from the transient experiments are analyzed and compared with invasion-percolation model predictions using aperture fields measured at different spatial resolutions. This comparison allows us to assess both the ability of the percolation-based models to generate wetted and entrapped aperture structures as a function of total infiltration and the required spatial resolution for aperture field measurement.

Vertical rise and drainage experiments are used to measure hysteretic saturation-pressure relations. Steady-state flows are established with the use of top and bottom pressure plates and monitored at a series of pressures to yield a relative permeability curve. Saturations, wetted-structures, and entrapped-structures at each pressure are measured by analyzing recorded images. At each pressure, a transient dye pulse also is monitored. Light transmission is used to obtain concentration within the flow field as a function of time. Effluent concentration as a function of time also is monitored for evaluation of one-dimensional fracture model transport parameters.

The influence of orientation of the fracture in the gravity field on downward infiltration of water and the formation of gravity-driven fingering is explored as a function of flow rate supplied evenly across the top of the fracture. Fingering flow-field structure is compared with those simulated using invasion-percolation, including gravity, and predicted from linear stability analysis.

Once confidence has been built in a particular set of conceptual models through comparison to physical experimentation, numerical experiments that address issues of property scaling will be conducted.

4.0 FRACTURE-MATRIX INTERACTION

Although unsaturated flow and transport through fractures and porous rock has received increased interest over the last decade, the interaction between the two has received relatively little attention. We define fracture-matrix interaction as the transfer of fluids and solutes between fractures and the porous matrix under either transient or steady flow conditions. The nature and degree of such interaction plays a significant role in the way equivalent hydraulic properties are defined for fractured rock. For example, flow between adjacent matrix blocks will vary radically as a function of pressure and wetting history as pathlines either cross, flow through or circumvent fractures thus impacting the effective permeability of the media.

There are a number of situations where the interaction between fractures and matrix may severely affect flow and transport fields. Two important cases are (1) highly transient flow conditions, especially for infiltrating fluid in an initially dry fracture,[41,42] and (2) steady-state flows normal to fractures where fractures act as variable-area, pressure dependent connectors. Other effects which must be considered include the presence of fracture coatings, air entrapment in the fractures and matrix, and flow fingering and channeling within the fracture plane.

Our research effort concerning the basic physics that govern fracture-matrix interaction addresses the following questions:

-   What impact does fracture-matrix interaction have on flow and transport processes and how does such interaction change as a function of media properties and flow conditions? What is role of scale in the modeling of fracture-matrix interaction?

-   What is the importance of air entrapment in both fractures and in the matrix block, the presence of fracture coatings, and flow channeling and gravity driven fingering in the plane of a fracture on fracture-matrix interaction and how can their effects be modeled?

-   How can fracture-matrix interaction in steady or transient problems be adequately represented within continuum-based models by means of appropriate equivalent property models? Under what conditions can the fractures and porous media be modeled as overlapping continua with their interaction addressed through a "leakage term?" Under what conditions can the effects of fracture-matrix interaction on flow and transport fields be addressed through the composite continuum approach?

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4.1 Conceptual Modeling

The nature and degree to which the fractures and matrix interact dictates how we define the computational continuum and hence the media properties. To aid in our understanding of the basic physics governing fracture-matrix interaction, we are making use of two modeling approaches: pore-scale and discrete, small-scale, continuum modeling.

The pore-scale approach is useful in understanding effects of pore-scale connectivity and network structure on effective property models. Pore-scale modeling is formulated in a fashion similar to that discussed above for the unsaturated fracture studies. Fracture and matrix void structure is assigned according to random, fractal, and geostatistical techniques. Wetted-structures then are defined using percolation-based theories. Steady flow through the wetted-structure is modeled using a resistor network approach and a pore-scale velocity distribution is calculated for use in one-dimensional solute transport models.

A second approach we use is the discrete, small-scale, continuum approach. Here the fractures and matrix are modeled as discrete zones within the continuum characterized by very different properties. This approach essentially treats the fractures as a structured heterogeneity within the matrix. By treating the media in this fashion, fracture-matrix interaction is addressed according to the principles of mass balance at the fracture-matrix interface. Application of this technique requires that continuum-based properties be assigned to individual fractures and matrix blocks.

4.2 Physical Modeling

Physical modeling relies on two experimental systems. The first makes use of tuffaceous materials similar to that encountered at the Yucca Mountain test site. Rock types vary from bedded nonwelded to nonbedded nonwelded, partially welded and welded tuff with fractures. Experimental samples are taken from either Yucca Mountain or natural analogue sites. The second type of experimental system is analogous to the tuff system but simpler, having only certain predetermined attributes of the tuff. These analogue systems are designed to maximize experimental control (enable systematic variation of hydraulic properties) and resolution of data measurement. Thin slabs of sintered glass beads have been found to provide a good analogue for porous rock; however, addition research is being performed to evaluate other types of ceramics and sintered material. Fabrication of fractures is accomplished by mating individual ceramic plates or by inducing the formation of a fracture in a single ceramic plate.

A key element to the physical modeling of flow and transport through fractured media is a means of monitoring moisture and solute content by noninvasive techniques. In sintered or ceramic analogue systems both the moisture and solute transport fields are monitored through the application of optical techniques.[1,43] Alternative techniques are necessary for use in tuff because light cannot be passed through such systems. For thin two-dimensional tuff systems two techniques are currently under investigation: gamma-ray densitometry and x-ray attenuation. For three-dimensional systems, tomographical methods, such as x-ray and gamma-ray transmission, nuclear magnetic resonance, positron emission, and radar and electromagnetic imaging, are being evaluated. With respect to monitoring solute transport in tuffaceous systems, a number of nonreactive tracers are being evaluated according to their potential for detection by the various noninvasive techniques under investigation.

Physical modeling of fracture-matrix interaction primarily relies on two-dimensional systems (three-dimensional investigations will follow at a later time); one which addresses flow normal to the plane of the fracture and the other within the plane of the fracture. For systems aimed at modeling flow normal to the fracture plane, thin slabs of analogue or tuffaceous material cut by a fracture are secured between two glass plates. This system then is incorporated into a test cell similar to that used by the unsaturated fracture program. Investigations involving analogue material are able to make full use of the RTS and video imaging equipment described above whereas
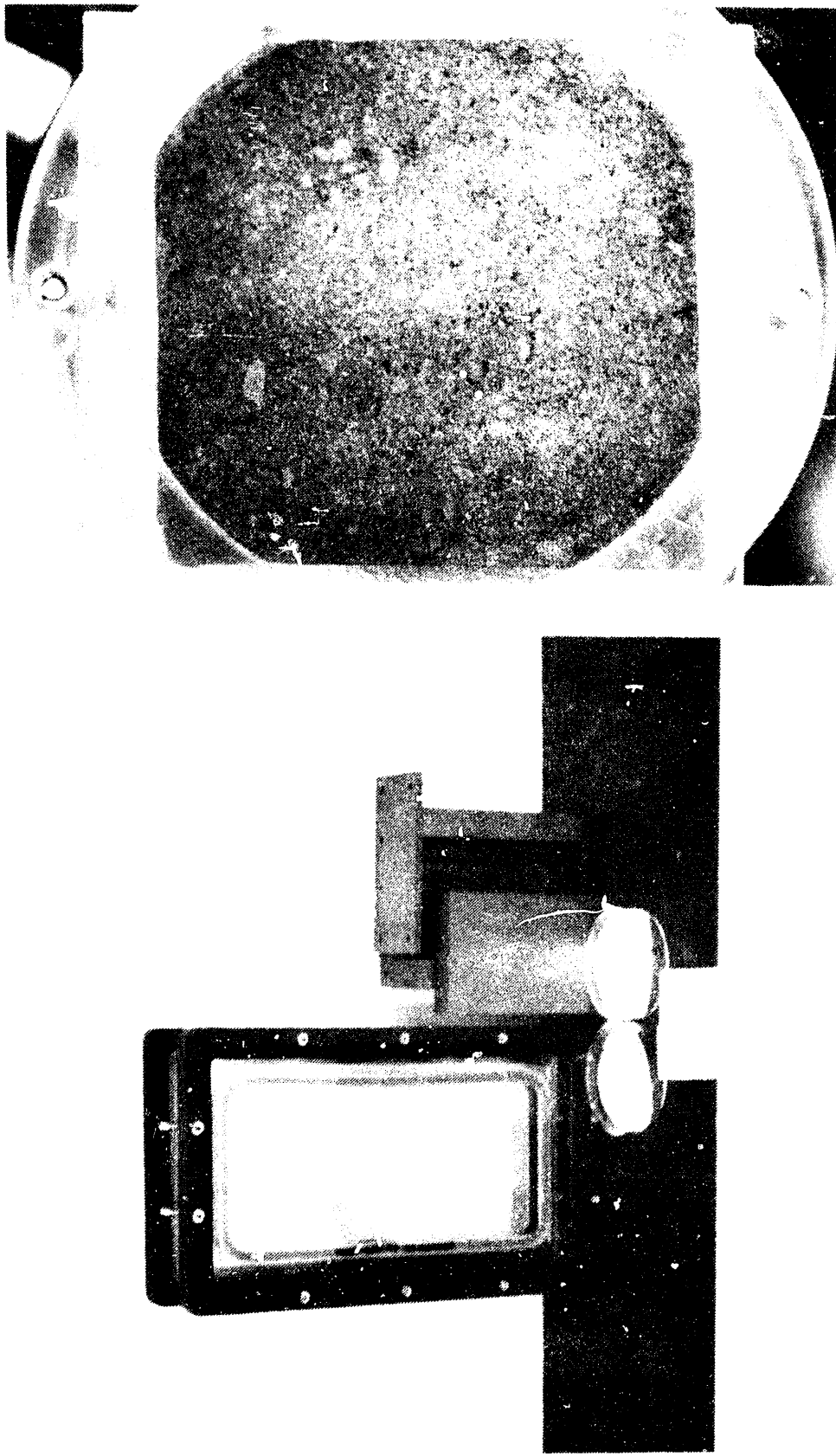
PHYSICAL MODELING: Fracture/Matrix Interaction Experimental Apparatus. We have developed an experimental capability that allows us to explore air/water/solute interaction between fractures and matrix. A variety of test cells have been designed and built which allow the visualization of the transfer of fluids and solutes between fractures and the matrix in both the plane of the fracture and the plane normal to the fracture. Thin slabs of fractured and unfractured tuff or sintered glass plates are secured in a test cell, as shown above, which allows the control of experimental parameters such as initial and boundary conditions, and system geometry. X-ray absorption, transmitted light, or reflected light are then used to monitor changes in the fluid and solute concentration fields. [".C. Tidwell and R.J. Glass, Div. 6315, Sandia National Laboratories]

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tuffaceous test cells are designed to allow direct mounting in both the gamma-ray and x-ray apparatus. The x-ray technique has the further advantage that the resulting exposures may be post-processed with the same equipment and in a similar manner to that of the optical technique.

Modeling of flow and transport in the plane of the fracture is being conducted in a flow cell consisting of an impermeable plate of glass placed on top of a sintered glass plate or the open face of a natural fracture. Boundary conditions are prescribed through the application of thin porous plates equipped with reed valves (to allow introduction of dyes) at the edges of the flow cell. The flow cell is mounted on a table which allows the orientation of the apparatus to vary within the gravity field. The resulting flow and transport fields then can be monitored visually along the plane of the fracture while optical, x-ray, or gamma-ray techniques may be used to monitor flow and transport in the matrix.

Analysis of results obtained by laboratory experimentation will require information concerning hydraulic properties of both the porous media and the fractures. Centrifuge and unit-gradient techniques are of particular interest for measuring hysteretic moisture-suction characteristics, the relative permeability, and dispersion properties of the porous matrix materials. Unit-gradient techniques also are being considered for characterizing fracture properties. Such tests are conducted either on fracture casts or on the fracture itself (matrix is maintained at saturation to avoid interaction).
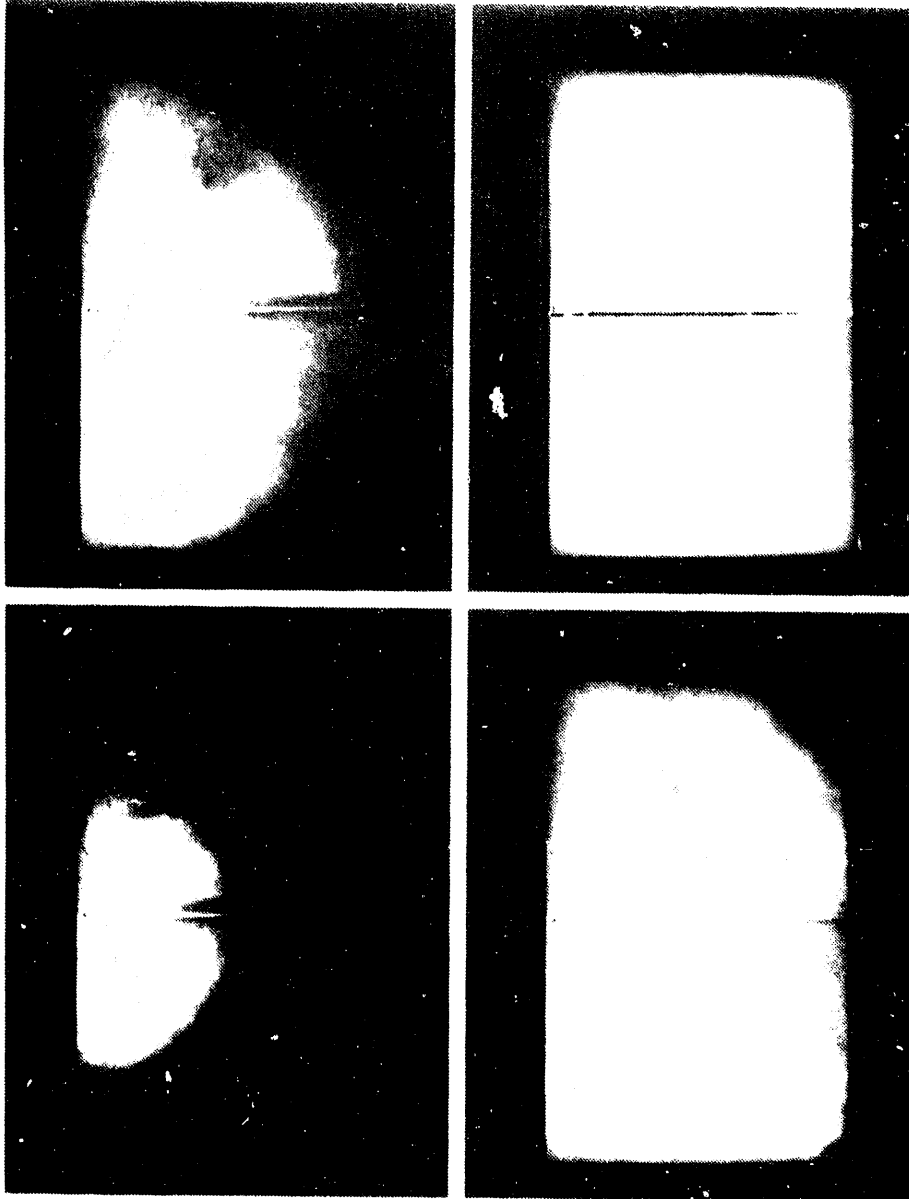
4.3 Physical and Numerical Experimentation

A numerical modeling program has been instituted in an effort to improve our understanding of the processes governing fracture-matrix interaction and to aid in the design and analysis of physical experiments. Both a pore-scale and macroscopic, continuum approach is utilized by this program. Whereas continuum-based models represent the primary analysis tool for our laboratory program, pore-scale modeling is of particular interest because it allows direct analysis of saturation structure as a function of pore pressure and wetting history. With respect to continuum-based models, special attention is given to the means by which the continua and media properties are defined for a particular problem.

Physical experiments are being performed to investigate the nature of fracture-matrix interaction for a number of flow regimes. One such group of studies is focused on the behavior of a wetting front as it percolates through an initially dry fracture. Experimentation involves the use of both analogue and tuffaceous materials in which a constant head or constant flow rate is maintained at the upper boundary of the system while monitoring the outflow rate and the matrix pressure field (by means of tensiometry). Systematic variation of matrix and fracture properties, flow rates, and fracture orientation is incorporated into the testing scheme. Nonreactive dyes also are used to investigate transport processes under transient flow conditions.

Other studies are focusing on matrix-dominated flow and transport subject to steady and transient boundary conditions. Such studies are aimed at investigating the role of fractures as variable-area, pressure-dependent connectors between adjacent matrix blocks. Boundary conditions are established through the use of porous plates at the upper and lower ends of the flow cell. Tests are conducted in both tuffaceous and analogue materials subject to a variety of boundary conditions, fracture orientations, and media properties.

Because of the simplicity of the experimental system, a wide variety of investigations are performed by making a few simple modifications to the base system. For example, the physics of fluid transfer between a fracture and the surrounding porous matrix in the presence of a fracture coating or alteration zone is explored by the application of special materials to the faces of the fabricated fractures (or use of natural fractures with coatings). The chemical and physical properties of these special materials are varied systematically in an attempt to emulate various natural coatings. Other modifications involve efforts to control the circulation of air in the fracture and matrix during testing to investigate the effects of air entrapment on fracture-matrix interaction. The experimental system is also modified to allow the investigation of fracture networks. Such networks consist of a grid of mated sintered glass plates or tuff samples hosting multiple fractures.

PHYSICAL AND NUMERICAL EXPERIMENTATION: Flow Parallel to the Fracture Plane. Of particular importance to modeling flow and transport through fractured porous media is a knowledge of the impact of matrix imbibition on fracture percolation. To investigate relevant conceptual models, an experimental system has been fabricated which allows visualization of the interaction of fluids and solutes between fractures and the matrix in a plane normal to the fracture. The experimental system consists of thin, sintered glass plates mated together to form an analogue fracture. The sintered plates are held together by a test cell which is used in conjunction with the rotating test stand. Moisture content and solute concentration fields are acquired through video imaging of the transmitted light intensity fields. Shown here is the capture of fracture infiltration by the surrounding air dry matrix. Increasing moisuture content is denoted by the blue - green - yellow - red sequence. [V.C. Tidwell and R.J. Glass, Div. 6315, Sandia National Laboratories]

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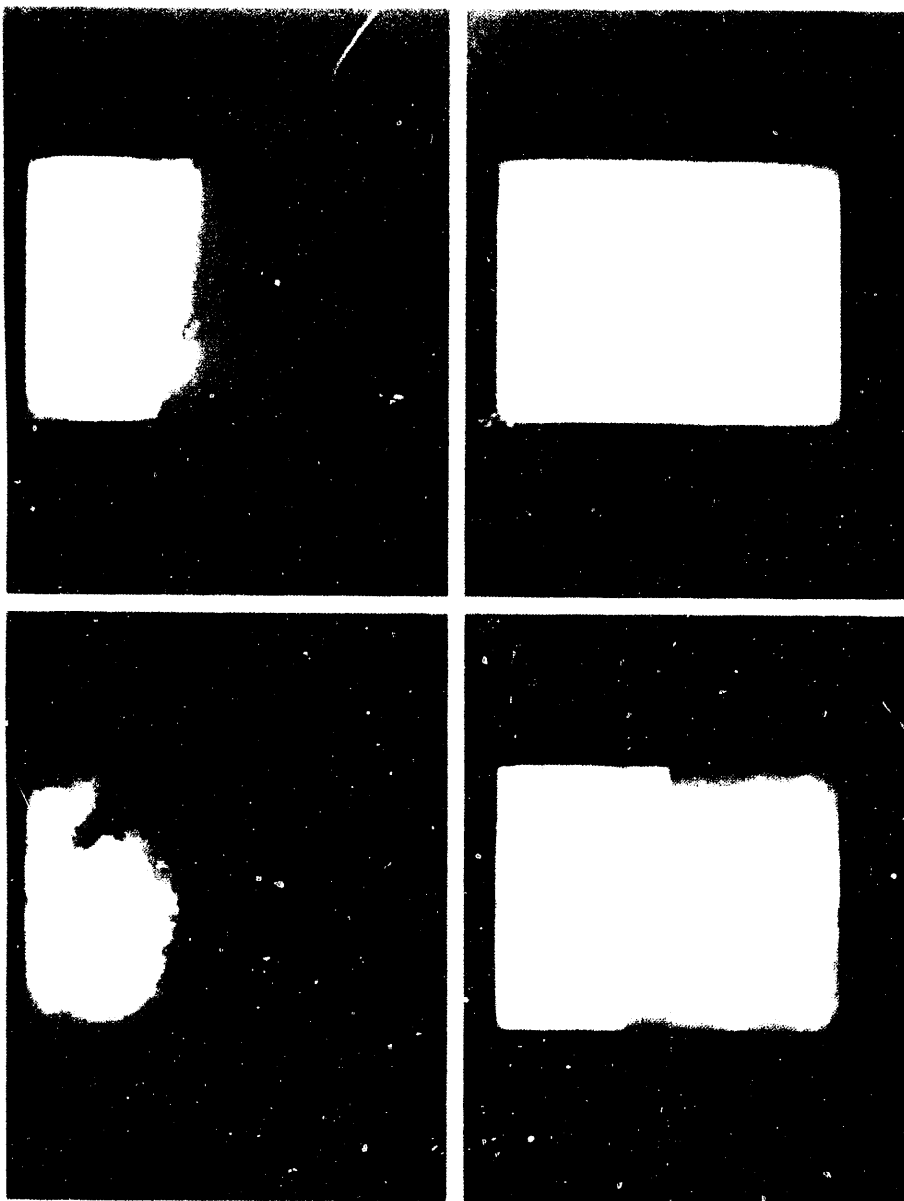
PHYSICAL AND NUMERICAL EXPERIMENTATION: Flow Normal to the Fracture Plane. Also being challenged are assumptions concerning the impact of desaturated fractures on matrix dominated flow and transport. The impact of desaturated fractures is investigated in the plane normal to the fracture by fabricating an analogue fracture through the mating of two thin sintered glass plates. Flow and transport normal to the fracture plane is then induced by controlling the boundary conditions of the test cell which holds the analogue fracture. Transmitted light techniques are applied to monitor the ensuing flow and transport fields which are digitized using video imaging equipment. In this series of images, the impact of a single desaturated fracture on the development of a transient flow field is clearly shown. Increasing moisuture content is denoted by the blue - green - yellow sequence. [V.C. Tidwell and R.J. Glass, Div. 6315, Sandia National Laboratories]

The experiments described to this point primarily focus on systems in which flow is constrained to be vertically down the fracture or normal to the fracture; however, the path of flow along the plane of an unsaturated fracture is also of interest. Therefore, an experimental system has been developed in which the plane of a fracture is simulated by placing an impermeable plate of glass on top of a sintered glass plate or the open face of a natural fracture. A variety of flow and transport studies are being conducted for both steady-state and transient flow conditions within the plane of the fracture to investigate the effect of saturation structure on fracture-matrix interaction. Other tests involve incremental wetting of an initially dry fracture by inducing capillary-driven flow from a saturated matrix. Such tests provide insight into the means by which the contact area between matrix blocks grows with decreasing pore pressure.

For those cases involving steady-state flow and transport studies, effective media properties are measured. Pressure-saturation characteristics as well as relative permeability relationships are established for a range of wetting and drying cycles. Dye concentration in flow-cell effluent also is monitored for evaluation of one-dimensional fracture model transport parameters. Efforts then are made to match various empirical and numerical models to the measured effective parameters.

5.0 CONCLUSION

Given the complex fracture system present in the fractured rock at Yucca Mountain, discrete modeling is not realistic for most performance assessment exercises. In order to make such modeling more tractable, local-scale variability introduced by the fracture network and porous matrix is averaged in a variety of ways through the definition of effective media properties. To define effective media properties, assumptions concerning the nature and degree of fracture-matrix interaction must be made.

The key issue for our research in developing and validating macroscale flow and transport models for fractured media lies in the definition of the continuum and the effective properties thereof at the scale of interest. Our success will be dependent on our understanding of the basic physics governing flow and transport through fractured media and in particular on our understanding of flow and transport in unsaturated fractures and interaction between fractures and matrix. The research in the areas outlined in this paper will provide this required fundamental understanding.

Our next step will be to fold this understanding into credible definitions of equivalent hydraulic property models for use in performance assessment. This step will require the definition of individual fracture variability and networking and the definition of matrix variability. Evaluation of the definitions will require extensive numerical experimentation and field-scale experiments. These and other issues including geochemical processes affecting transport are under consideration within the context of the overall research program.

NOTE

Due to the length constraints on this paper and the fact that the majority of our figures would be photographs, we have not included figures in this paper. Figures will be presented during the oral presentation of the paper. A copy of this paper including the presentation figures may be obtained from the authors.
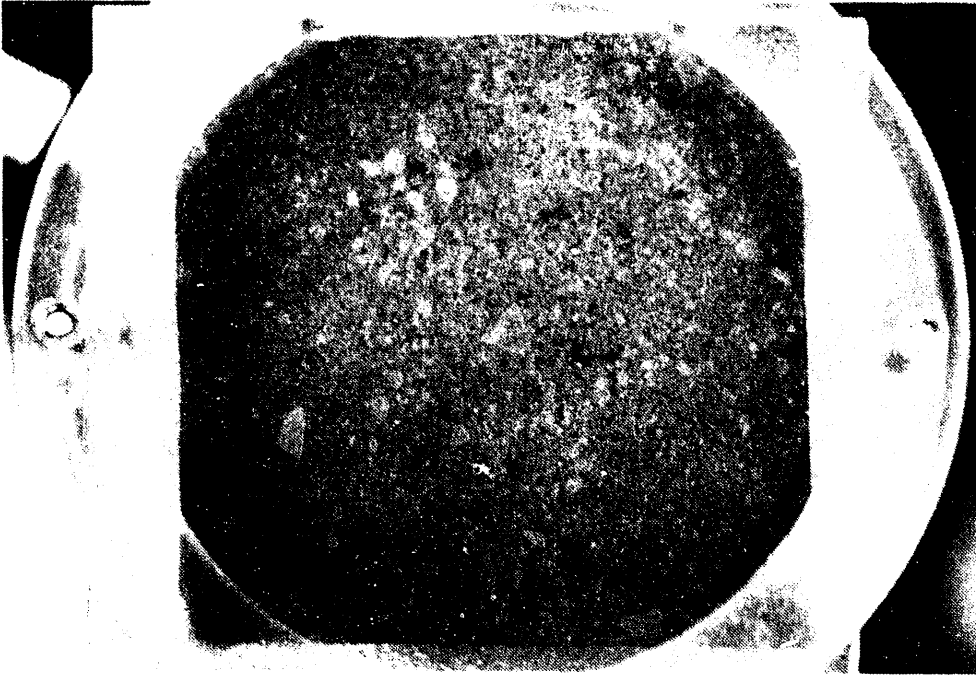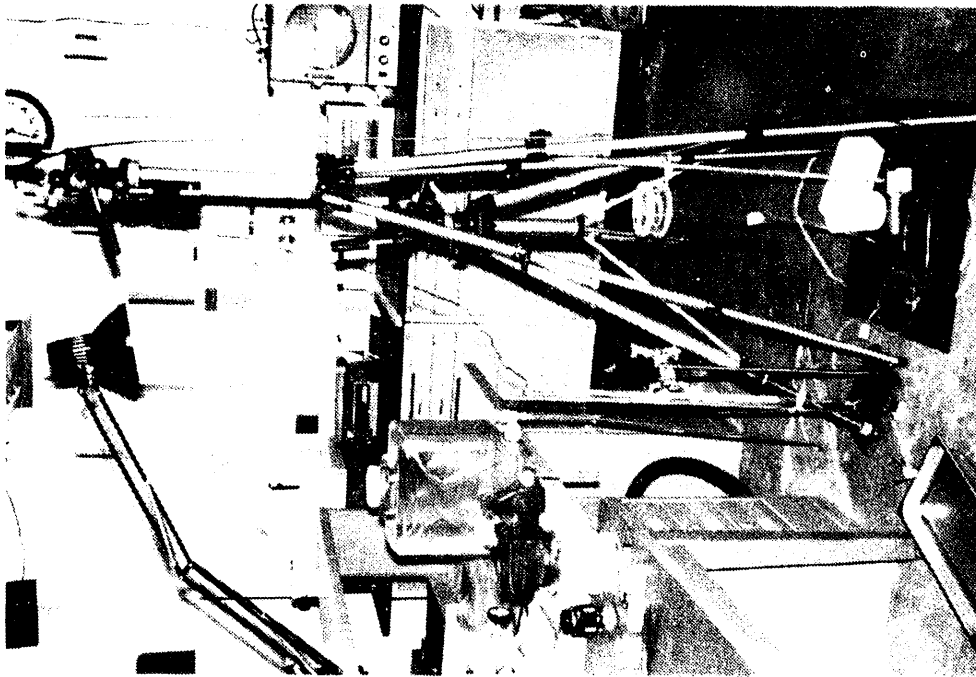
PHYSICAL AND NUMERICAL EXPERIMENTATION: Matrix Induced Wetting and Drying of a Fracture Plane. Inter-matrix block flow and transport occurs at contact points and where water spans the aperture across a fracture. To challenge assumptions concerning inter-matrix block flow and transport an experimental apparatus has been developed to visualize changes in fracture plane wetted structure induced by variations in fluid potential within the matrix. The system consists of a roughen glass plate secured to a smooth plate of tuff or analogue porous material. By sealing the tuff or analogue sample to an extraction plate, variable suction pressures may be applied to the system. [V.C. Tidwell and R.J. Glass, Div. 6315, Sandia National Laboratories]
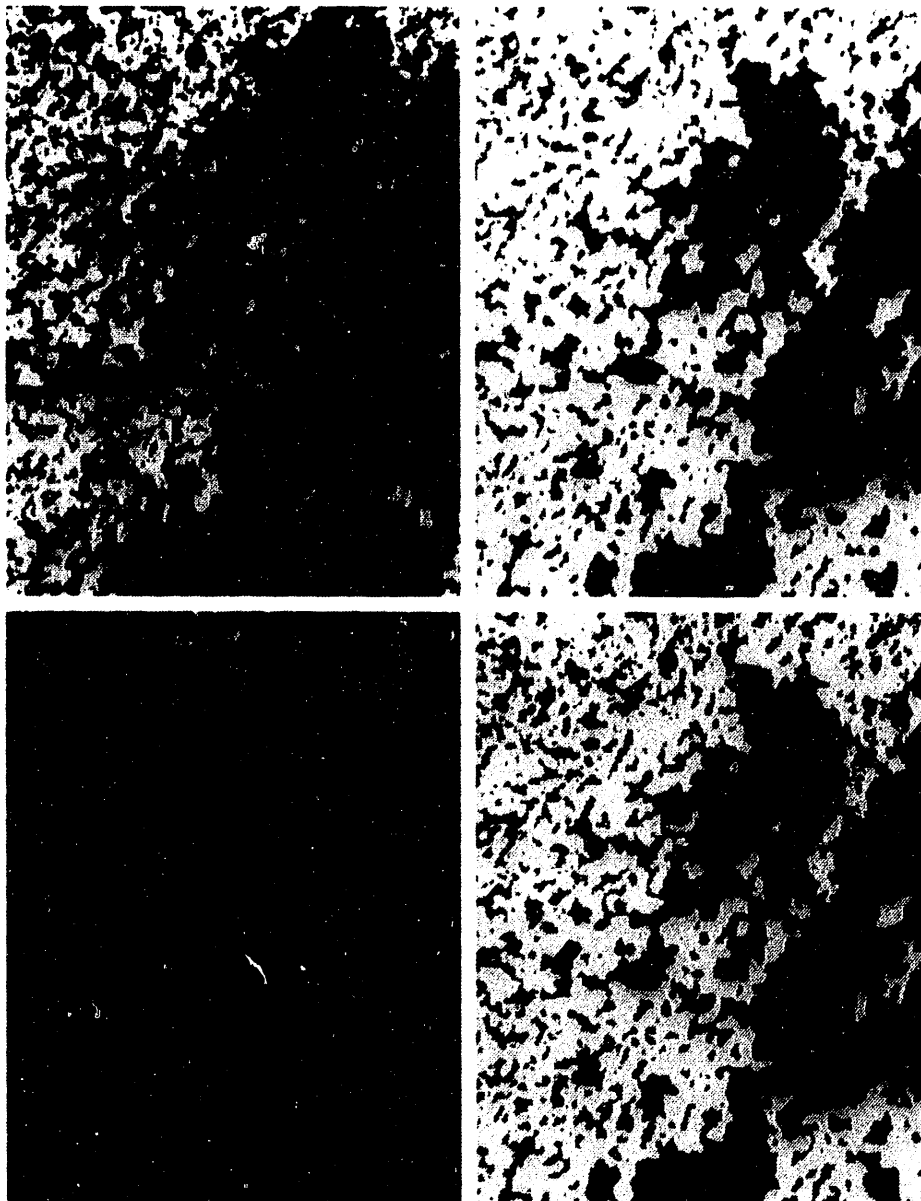
PHYSICAL AND NUMERICAL EXPERIMENTATION: Matrix Induced Wetting and Drying of a Fracture Plane. The wetted structure within the plane of a fracture is monitored by imaging the reflected light intensity field. Shown here is a series of images of the fracture plane when the matrix is subjected to a) 20 cm of suction (top left), b) 10 cm of suction (top right), c) 5 cm of suction (bottom left), and d) 0 cm of suction (lower right). Note that black corresponds to air filled pores while red represents water saturated pores. [V.C. Tidwell and R.J. Glass, Div. 6315, Sandia National Laboratories]

PHYSICAL AND NUMERICAL EXPERIMENTATION: Gravity-Driven Fingering and Fracture/Matrix Interaction. Gravity-driven fingering associated with non-horizontal fractures may significantly limit the transfer of fluids and solutes between the fracture and matrix because of the reduction in wetted area within the fracture. For this reason efforts are being made to evaluate the impact of fingering on fracture/matrix interaction. A vertical fracture has been fabricated by securing a roughened glass plate on the face of a smooth slab of densely-welded tuff. The series of photographs show the development of a flow field generated by a single point source. Note that the generated flow field wets less than 25% of the fracture plane. [R.J. Glass and V.C. Tidwell, Div. 6315, Sandia National Laboratories]

PHYSICAL AND NUMERICAL EXPERIMENTATION: Scaling Studies Conducted in the Laboratory. Meter scale slabs and blocks of tuff are being used to challenge assumptions concerning the scaling of media properties. A minipermeameter is being used to collect air permeability data from slabs and blocks of tuff at a variety of measurement scales. Based on this information effective media properties can be estimated by means of fractal, classical statistical, and geostatistical techniques, as well as through the application of scaling laws. These approaches may then be compared to actual measurements made on the bulk slabs or blocks. [V.C. Tidwell, C.A. Rautman, and R.J. Glass, Div. 6315, Sandia National Laboratories]

PHYSICAL AND NUMERICAL EXPERIMENTATION: Scaling Studies Conducted in the Field. An analogue field site has been selected at NTS for conducting scaling studies. The site is located approximately 20 miles southwest of G Tunnel and was selected because of its similarity to the bedded units of the Calico Hills Formation. Because of the bluff forming attributes of the unit, this field site offers an expansive area to conduct near three-dimensional outcrop studies. The field program will involve investigations utilizing the minipermeameter, as well as the collection and characterization of a number of small core samples. The core samples and minipermeameter data are designed to further expand the work conducted at the laboratory scale. [C.A. Rautman, V.C. Tidwell, and R.J. Glass, Div. 6315, Sandia National Laboratories]

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