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Yucca Mountain Project

Laboratory Research Program to Aid in Developing and Testing the Validity of Conceptual Models for Flow and Transport Through Unsaturated Porous Media

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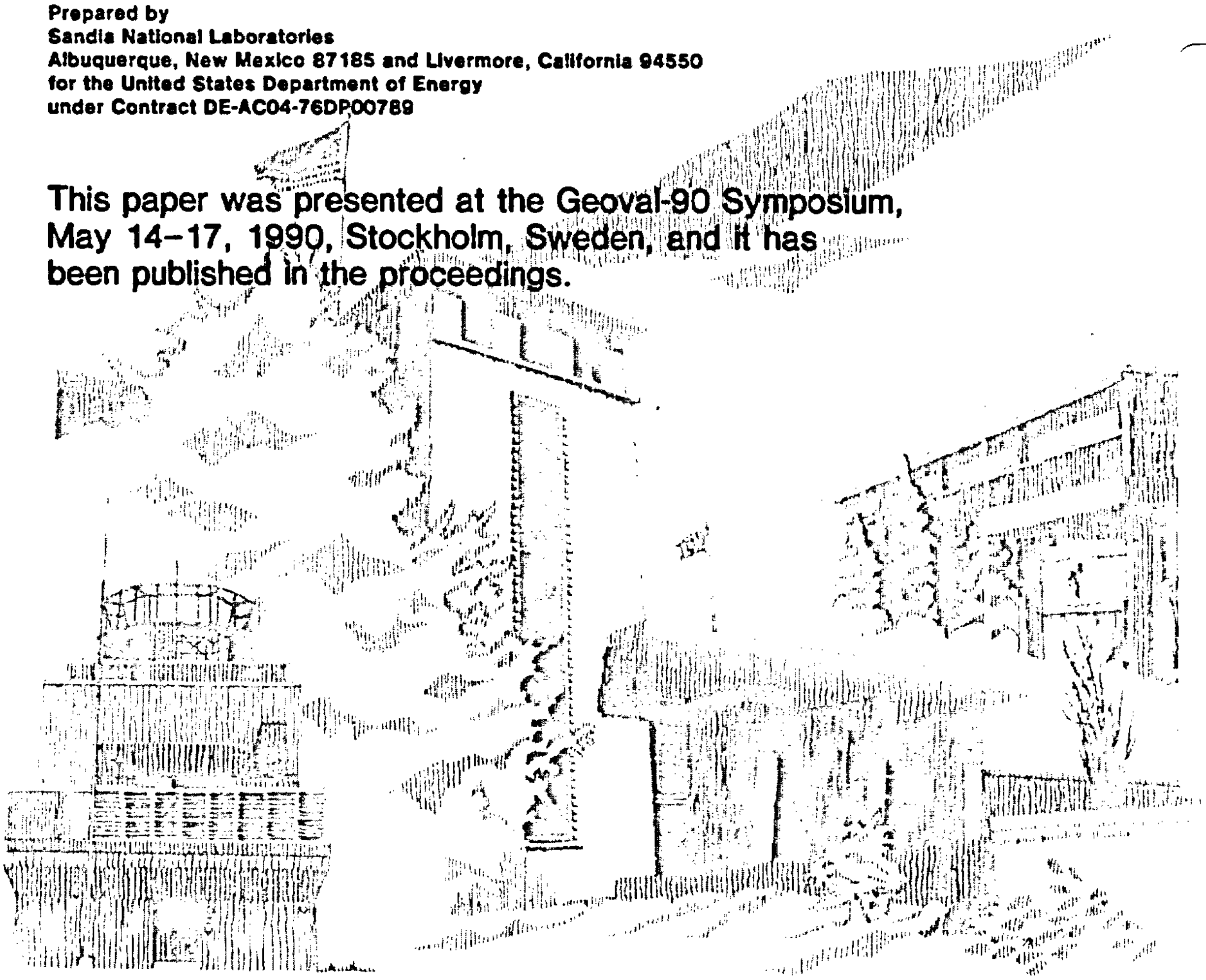

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LABORATORY RESEARCH PROGRAM TO AID IN DEVELOPING AND TESTING THE VALIDITY OF CONCEPTUAL MODELS FOR FLOW AND TRANSPORT THROUGH UNSATURATED POROUS MEDIA*

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ABSTRACT

As part of the Yucca Mountain Project, a laboratory research program is being developed at Sandia National Laboratories that will integrate fundamental physical experimentation with conceptual model formulation and mathematical modeling and aid in subsequent model validation for unsaturated zone water and contaminant transport. Experimental systems are being developed to explore flow and transport processes and assumptions of fundamental importance to various conceptual models. Experimentation will run concurrently in two types of systems: fractured and nonfractured tuffaceous systems; and analogue systems having specific characteristics of the tuff systems but designed to maximize experimental control and resolution of data measurement. Areas in which experimentation currently is directed include infiltration flow instability, water and solute movement in unsaturated fractures, fracture-matrix interaction, and scaling laws to define effective large-scale properties for heterogeneous, fractured media.

*This work was performed under the auspices of the U.S. Department of Energy, Office of Civilian Radioactive Waste Management, Yucca Mountain Project, under contract DE-AC04-76DP00789. This document was prepared under Quality Assurance Level III and WBS 1.2.1.4.6.

INTRODUCTION

The U.S. Department of Energy is investigating a prospective site for a high-level nuclear waste repository located in unsaturated volcanic ash (tuff) deposits hundreds of meters thick at Yucca Mountain, Nevada. As part of this investigation, the ability of the natural system to restrict water movement and to retard the migration of radionuclides if released must be assessed. While this assessment will be made with respect to specific regulations formulated by the U.S. Nuclear Regulatory Commission and the Environmental Protection Agency, the analysis must be made with a sound scientific understanding of the flow and transport processes that occur at the site. Because there always will be uncertainty with respect to the flow and transport processes, our modeling procedures, and the temporal and spatial variation of model parameters, the final assessment will have to be cast in terms of probability. To develop this general understanding, we must systematically

1. identify all processes by which radionuclides could migrate through the rock formation to the accessible environment;
2. 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;
3. bound various processes in terms of system parameters such as initial conditions, boundary conditions, and distribution of properties in both time and space; and
4. provide informational needs for site characterization so that the probability of occurrence for each process can be assessed and appropriate model parameters measured.

Fundamental questions concerning flow and transport in unsaturated porous media can be addressed in part through controlled laboratory experimentation. A laboratory research program is being developed at Sandia National Laboratories for the Yucca Mountain Project that will integrate fundamental physical experimentation with conceptual model formulation and mathematical modeling and aid in testing the validity of models at the meter scale. The laboratory program is part of a broader effort currently being planned that will address the validity of conceptual models used in calculation of groundwater travel time and radionuclide transport through the unsaturated zone at Yucca Mountain. Questions raised in modeling exercises and field studies will be used to direct laboratory experimentation. In general, research in the laboratory is prioritized with respect to understanding flow processes which could cause the site to fail to meet regulatory requirements (i.e., decrease water or radionuclide travel time), testing key assumptions in models for processes considered to be important, and developing new conceptual models as found to be necessary. The research program stresses fundamental research and in this sense will have broad applicability within the general field of flow and transport through unsaturated porous media.

In this paper, the laboratory research program is outlined. The general approach for laboratory experimentation will be presented followed by an outline of several areas of research where studies are currently underway. The program is designed to be flexible. Future studies will be defined as the broader validation effort develops and key informational needs are determined that require a further understanding of flow and transport mechanisms.

APPROACH AND METHODS FOR LABORATORY RESEARCH PROGRAM

Laboratory studies test our understanding of basic processes. Simple qualitative experimentation demonstrating a process is necessary as a first step toward understanding. The approach for the laboratory research program, however, emphasizes systematic quantitative experimentation, conceptual modeling, and model validation (invalidation) exercises directed to achieve fundamental understanding.

Two types of experimental systems will be used. The first is in tuffaceous systems and thus contains all the natural complexity of the rock. Rock types will vary from bedded nonwelded to nonbedded nonwelded, partially welded and welded tuff with and without fractures. Experimental samples will be 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 (i.e., ability to systematically vary system parameters) and resolution of data measurement. To allow systematic variation of hydraulic properties, the analogue systems will be composed of unconsolidated sand, glass beads, porous glass beads, or "rocks" fabricated to specification (e.g., ceramics, sintered glass, or sintered metal). Rough-walled fractures will be simulated with roughened glass plates or fabricated rocks held together at different spacings. Experimentation in both types of systems will run concurrently, with experimentation in analogues driven by what we know about or discover from work in tuff systems and vice versa.

The experimental systems will strive to acquire high-resolution temporal and spatial data to allow the possibility of identifying additional flow and transport mechanisms. In experiments where full three-dimensional data acquisition is required, tomographic techniques using either x-ray or gamma-ray transmission, nuclear magnetic resonance, positron emission, or other methods will be developed and applied. Most of these methods, however, are limited in the size of system to which they can be applied. For many of the questions we are currently investigating, experiments on the scale of a meter are required. To obtain high-quality data at the meter-scale, two-dimensional experiments are conducted in extensive (1x1m) but thin (0.01m) slabs of material. Data measurement techniques for thin slabs include optical, x-ray, and gamma-ray transmission techniques. For many experiments we will concentrate on the first two as they are rapid and can be used as "field" measurement techniques while the gamma-ray densitometer is much slower and is primarily a point measurement technique.

Analogue systems will be designed to take full advantage of optical techniques. Optical techniques for visualizing moisture content make use of the fact that transmission of light through translucent media, such as silica sand or glass beads, increases with an increase in moisture content. By illuminating the back of a thin slab of media, the moisture content integrated over the thickness of the slab is visualized as light intensity that varies from point to point at the front of the slab (see Plate 1). Intensity fields can be recorded up to 30 times a second and digitized into an array of 512 x 512 or more points using video imaging technology (see Plate 2). Currently the optical technique is being used qualitatively to determine "relative" moisture content (one location is wetter or drier relative to another). To further develop the technique, we are developing calibration methods and comparing the optical technique with a standard gamma-ray densitometer. An adaption of the technique will also be used to visualize transient dye concentration in steady-state flow fields (see Plate 3). Calibration methods to allow quantitative measurement of concentration are currently in development. Preliminary results indicate the optical technique is also useful in visualizing packing-induced heterogeneity and thus it may be possible to use it to characterize heterogeneity as well (see Plate 4).

For opaque tuffaceous systems, x-rays replace light and their attenuation is used to measure moisture content in extensive thin slabs. X-ray fluorescing film placed on the back side of the slab transforms the x-ray intensity field into a visible light intensity field which again is visualized, recorded, and digitized using video imaging technology. For situations that do not require high spatial and temporal resolution, a standard gamma-ray densitometer is used.

In experimental design, concepts of dimensional analysis, scaling, and similitude are developed and applied to increase understanding and generalize results [1, 2, 3, 4]. For systems where these concepts are applicable, once a physical experiment is conducted or a solution of the dimensionless form of the governing equation has been calculated for one porous medium, the results apply immediately to all similar porous media and flow systems through scaling relations. Systematic exploration of dimensionless parameter space allows the efficient characterization of system response for all possibilities of the dimensional parameters. The concept of similar porous media can also be exploited to allow experimentation in porous media similar to the one of primary interest. This can minimize the experimental difficulties of working with some porous materials where the time scale of the flow process is either too short or too long to make measurement practical.

CURRENT STUDIES

A number of studies, in various stages of planning or completion, are underway to aid in the development of the laboratory research program. These studies are being used not only to develop techniques but to increase our understanding of several flow and transport processes and to challenge several key assumptions embodied in many currently accepted conceptual models. The studies can be grouped into four main areas of research: infiltration flow instability; water and solute movement in unsaturated fractures; fracture/matrix interaction; and scaling laws to define effective large-scale properties for heterogeneous, fractured media.

1. Infiltration flow instability

Most conceptual models assume that infiltration flows are essentially stable with any irregularity in the flow field caused by spatial variability in hydraulic properties, initial conditions, or boundary conditions. Yet, gravity-driven instability of an infiltration flow or "wetting front instability" can cause the flat wetting front moving downward through an unsaturated porous medium to break into fingers which move vertically, bypassing a large portion of the vadose zone (see Plate 5). Wetting front instability within porous media has been demonstrated in both laboratory and field settings and has been shown to have a dramatic effect on water and solute transport [5, 6, 7, 8, 9]. The development of a two-zone moisture content field consisting of high moisture content finger cores surrounded by lower moisture content fringe regions and the persistence of this structure from infiltration cycle to infiltration cycle (see Plate 6) has been demonstrated and explained with a simple theory based on hysteresis in the moisture characteristic relations [10]. The dependence of finger properties on system parameters for initially dry, coarse, nearly uniform sand has been determined through dimensional analysis and experimentation [11, 12]. Stability criteria and relations for finger width or diameter have been formulated through linear stability analysis and compared to experimental data showing remarkably good agreement for homogeneous media where the analysis applies [12, 13].

Generalization of the results obtained from these previous theoretical and experimental studies suggests many situations, such as an increase in conductivity with depth, unsaturated infiltration from a boundary held at less than saturation, and redistribution following an infiltration event, can cause a wetting front to become unstable and form persistent fingers. Because all of these situations potentially occur at Yucca Mountain, the process of wetting front instability must be understood and bounded. To accomplish this, several complicating factors that may stabilize most situations must be explored. The most important of these factors are pore size distribution, contact angle (wettability), heterogeneity, and initial moisture content. A series of experiments to investigate the effects of these factors is currently underway in a meter-scale slab chamber using optical techniques to follow the evolution of the moisture content fields in silica sands. The grain size distribution of the sand and thus the pore size distribution of the media are being varied systematically (see Plate 7). Similitude theory applied to finger properties is used to design the grain size distributions. Several preliminary experiments in horizontally microlayered sand systems suggest that fingers widen and perhaps are suppressed as the amplitude and spatial frequency of the property oscillation between layers increase (see Plate 8). A series of experiments where microlayering is systematically varied is planned as are experiments where the effects of contact angle and initial moisture content will be systematically explored.

Invasion percolation theory modified to include contact angle, buoyancy, multiple neck pore filling facilitation, and initial moisture content is being used to build a conceptual model which incorporates the essentials of the pore scale mechanism for finger formation (see Plate 9). Combination of experimentation and modeling should allow the bounding of gravity-driven fingering in porous media and thus the ability to assess its occurrence at Yucca Mountain. Our current work investigating flow through rough-walled fractures (2 below) has demonstrated that gravity-driven fingers may occur in vertical fractures as well.

2. Water and solute movement in unsaturated fractures

Many of the units of tuff composing both the saturated and unsaturated zones at Yucca Mountain are considered to be highly fractured [14]. Therefore, an understanding of the effects of fractures on water and solute transport within these zones is crucial. In the extreme of very low permeability matrix, such as in highly welded, vitric tuff, or for matrix which is near saturation, the effect of the matrix on flow and transport through a conducting fracture will be of second order. As a first step toward understanding the more difficult problem where the influence of the matrix on flow through the fracture cannot be neglected, we will study unsaturated flow within a fracture in impermeable media.

Little is known concerning the distribution of water and air in an unsaturated fracture and its influence on flow and transport through the fracture. In both analogue and welded tuff systems the effects of fracture surface roughness and orientation in the gravity field on the unsaturated fracture flow field structure and solute transport will be studied systematically. In particular, gravity-driven instability causing the formation of downward-moving fingers within the fracture should occur in nonhorizontal unsaturated fractures. Preliminary analogue systems consist of two roughened glass plates held together to form a simulated fracture (see Plate 10). Six different roughnesses are being used, and the angle of the fracture plane with respect to gravity is varied. The structure of transient and steady-state flow fields in the glass fractures is recorded photographically or on video and analyzed using digital image analysis. The use of dye pulses in the water supplied to the fracture may allow the characterization of solute transport through these systems as well and will be explored in future studies. Subsequent studies will be made in molds of natural fractures, natural fractures in welded tuff, and fabricated, fractally generated fractures machined into surfaces.

3. Fracture-matrix interaction studies

In fractured, permeable rock formations, the movement of water and solutes between fractures and porous matrix (fracture-matrix interaction) can have a profound influence on the rate at which water and solutes will migrate through the formation. Models of flow through fractured rocks are based on assumptions concerning the fluid and solute transfer between fractures and adjacent porous matrix. Basic research will be performed to understand fracture-matrix interaction (for both water and solute) and challenge our current assumptions concerning the process.

The influence of flow field structure within unsaturated fractures on fracture-matrix interaction will be studied. The influence of gravity-driven instability to cause fingers within a fracture that may persist and greatly influence fracture-matrix interaction will also be considered. We will begin with a simulated fracture, one side of which will be impermeable and clear (glass) and the other side will be porous (ceramic, sintered glass beads or tuff). Such a system will allow us to document carefully the structure of water contained in the fracture while tensiometers installed in the porous side will monitor the transient pressure field.

The physics of fluid and dissolved contaminant transfer between a fracture and the surrounding porous matrix in the presence of a fracture coating or alteration zone will also be explored. Porous media composing the matrix will be fabricated by sintering packs of glass beads. After homogeneous matrix blocks have been made, material will be added to a side of the block to constitute a coating. The thickness of the coating material and its properties will be varied. To understand altered surface chemical properties of a fracture coating requires the systematic variation of the surface chemical properties. Technology exists to alter the surface properties of glass through a number of processes developed for chromatographic analysis of chemical solutions. These techniques may be applied to the fabricated coating layers to allow a systematic exploration of geochemical processes.

4. Scaling laws to define effective large-scale hydraulic properties for heterogeneous, fractured media

Experimentation and subsequent modeling of water movement in a small unsaturated core of tuff have shown the matrix properties of tuff to be highly variable on the centimeter scale [15, 16]. In addition, fractures and microfractures are present in many tuff formations. The definition of equivalent or effective properties on the scale of a meter to tens of meters which embody these smaller scale heterogeneities is essential for repository-scale calculations of water and radionuclide transport. To aid in the formulation and testing of scaling laws for equivalent media property models from the centimeter through the meter scale, we will conduct experimental studies in both analogue and tuff systems. These studies must subsequently be augmented with in situ field experiments of varying scale to extend the relationships to the field.

In analogue systems, porous media with different heterogeneity structure and with and without high permeability fractures will be generated in sand and fabricated rock material. Transient infiltration experiments will be conducted in extensive slab systems composed of these materials and the moisture content within the flow field will be recorded in time using either optical or x-ray techniques and video/digital imaging. Boundary conditions around the edge of the slab will be controlled using porous pressure plates to supply either known pressure or flux. Steady-state moisture flow with transient solute transport experiments will also be conducted. Data will allow the evaluation of equivalent porous media concepts in well parameterized systems.

In tuff systems, thin slabs of tuff up to 1 m square will be cut and ground smooth. Impermeable material will be contact cemented to the sides of the slabs and porous pressure plates will be installed around the edges of the slabs to impose known boundary conditions. Because most slabs will contain naturally occurring fractures, their influence on the developing flow field can be evaluated. Transient infiltration experiments will be conducted and moisture contents within the flow field will be recorded in time using x-ray techniques and video/digital imaging. By cutting slabs along the principal axes of visual bedding and supplying water to a small hole in the center of the slab, anisotropy on the scale of the experiment can be evaluated. Transient solute transport experiments will also be conducted using x-ray absorbing solute or radioactive tracers.

CONCLUSION

Conceptual models applied to predict long-term transport of water and radionuclides at Yucca Mountain or elsewhere must be evaluated critically. Conceptual model formulation begins by making simplifying assumptions. For a model to accurately predict physical system response, the physics of the major processes that occur for the range of parameter space, physical scale and boundary conditions within which the model will be applied must be represented adequately. The goal of the laboratory research program being developed at Sandia National Laboratories is to acquire the fundamental scientific understanding of flow and transport processes that may occur in the unsaturated zone at Yucca Mountain and thereby assist in developing and testing the validity of our conceptual models for performance assessment.

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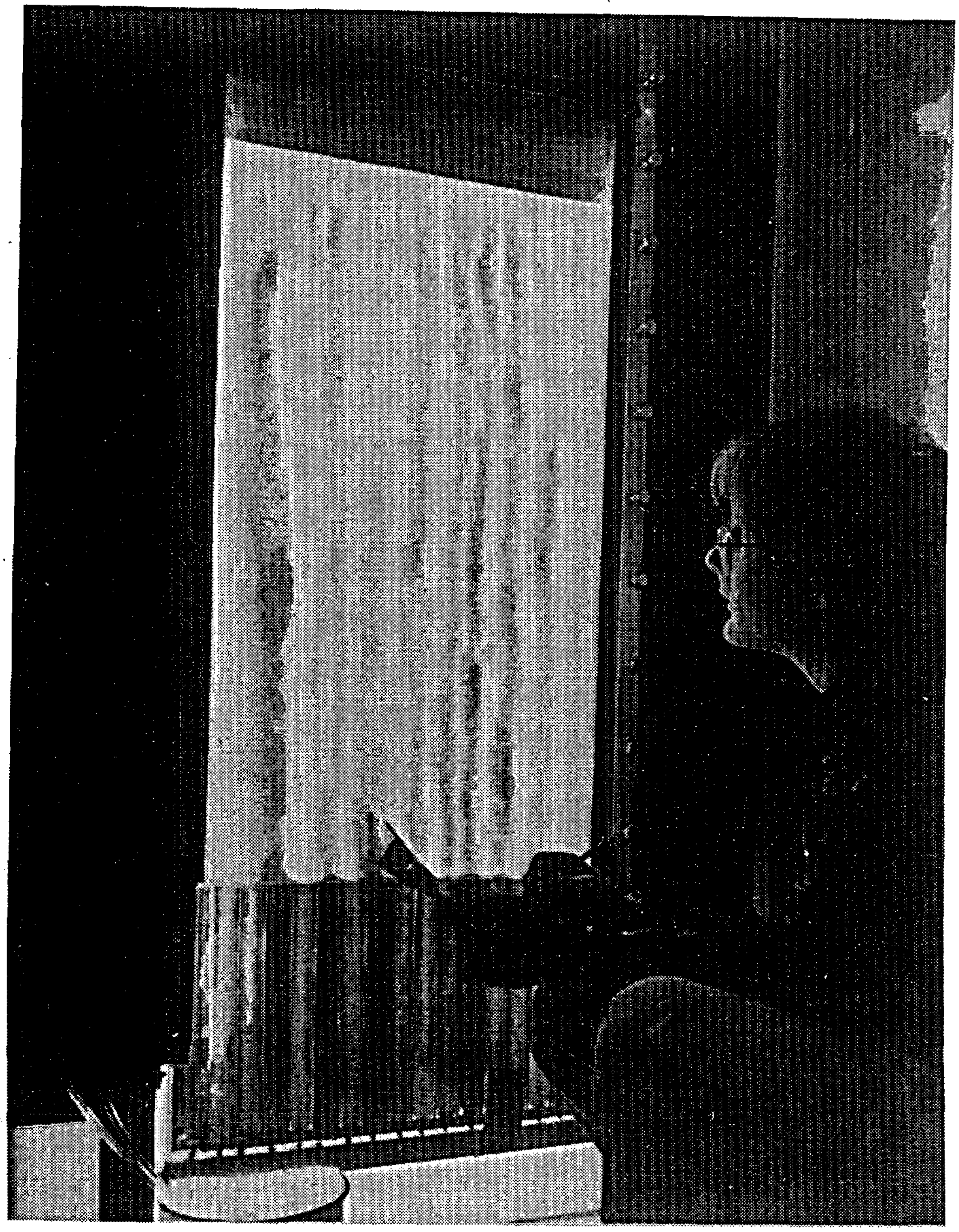

Plate 1. Laboratory apparatus developed for rapid visualization of moisture content in thin slabs of porous media: Moisture content within the thin slab of sand (1-cm-thick, 50-cm-wide, 130-cm-tall) is visualized using an optical technique that measures the transmission of light through translucent media (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, Geoscience Analysis Div. 6315, Sandia National Laboratories]

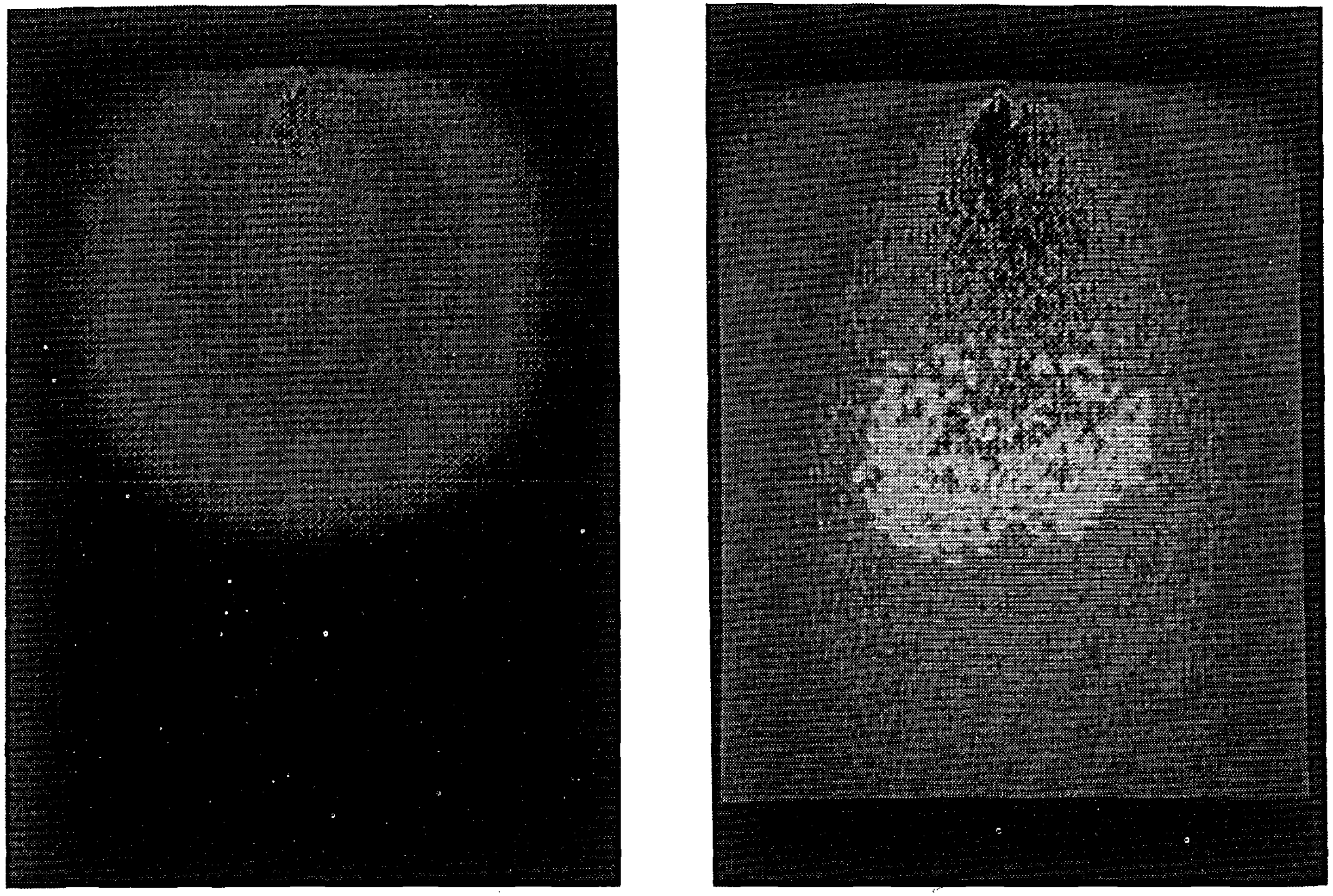

Plate 2. Two-dimensional, transient moisture content field: The optical technique is used to record the moisture content field at 12 min (left) and the steady-state field at 24 hr (right) generated from a buried point source in a thin slab of sand (1-cm-thick, 25-cm-wide, 40-cm-tall). The light intensity 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 contents with red near saturation. [R.J. Glass, Geoscience Analysis Div. 6315, Sandia National Laboratories]

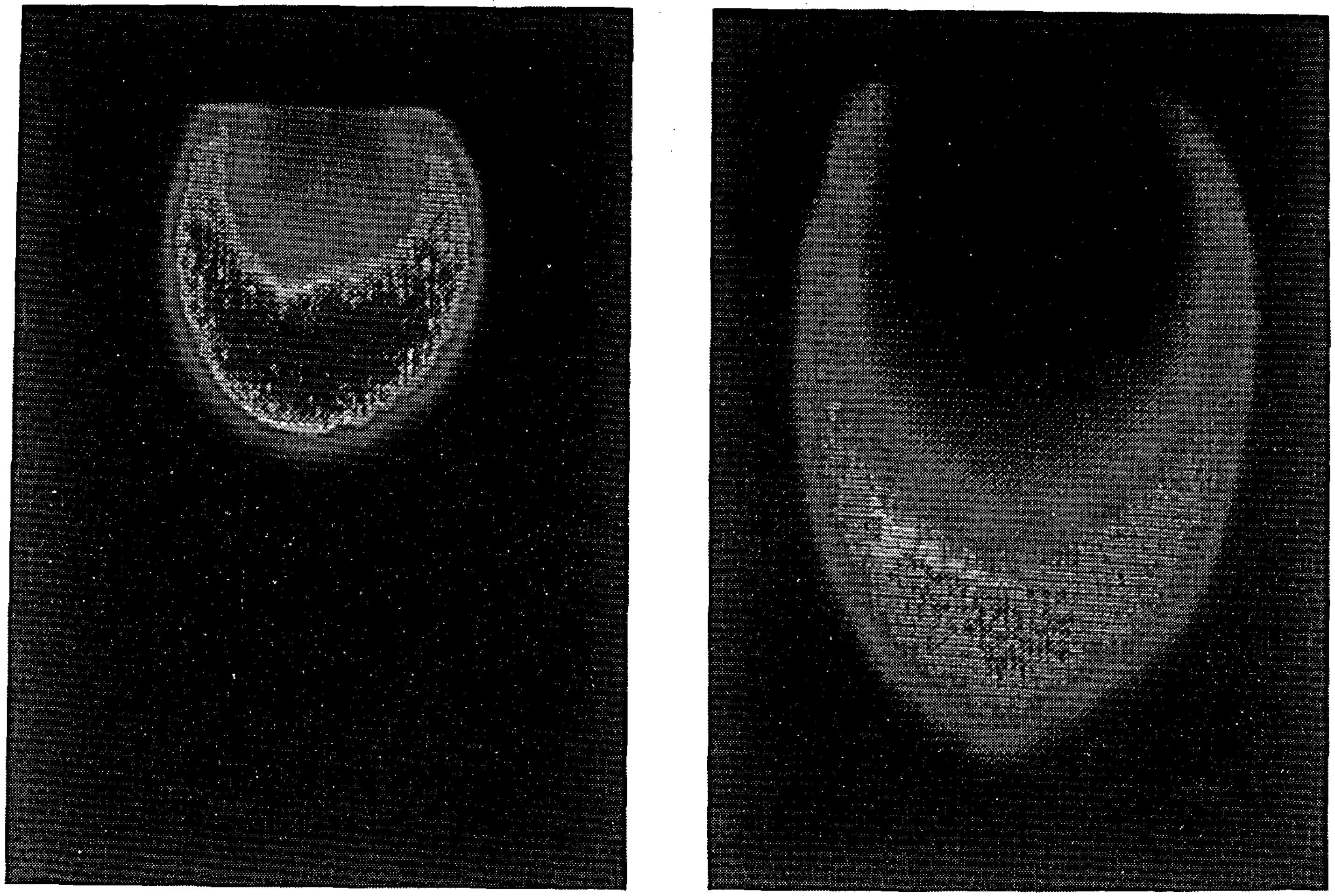

Plate 3. Two-dimensional, transient solute concentration field: The optical technique is used to record the transient solute concentration field at 6 min (left) and 18 min (right) generated from a pulse of dye in the water supply of the steady-state flow field shown in Plate 2. The light intensity field 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, Geoscience Analysis Div. 6315, Sandia National Laboratories]

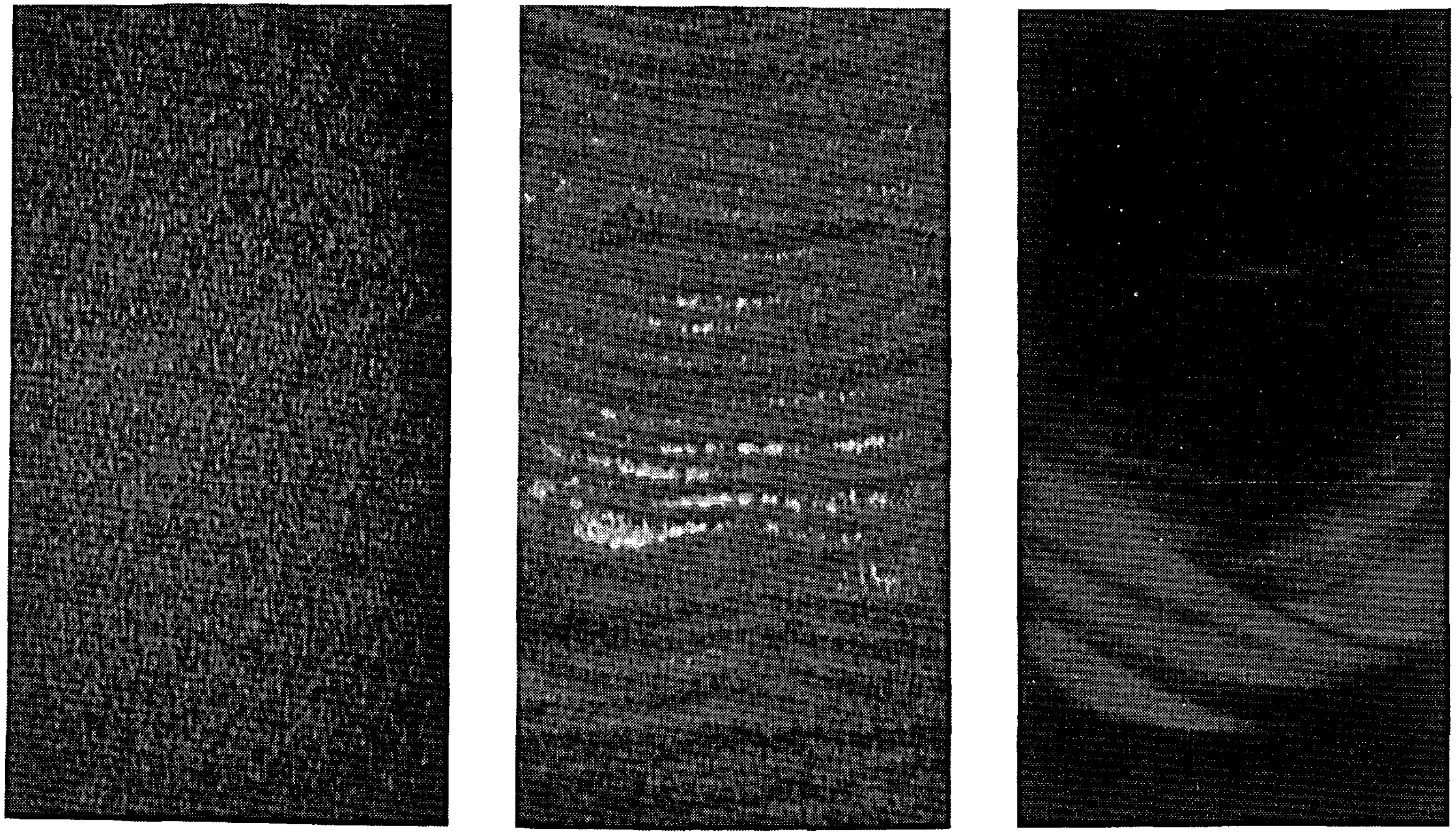

Plate 4. Visualization of heterogeneity structure: Variations in porosity can be visualized using the optical technique in thin slabs of porous media (slab 1-cm-thick, 25-cm-wide, 40-cm-tall). The slab on the left was created using the chamber-filling technique developed to generate homogeneous slabs. 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, Geoscience Analysis Div. 6315, Sandia National Laboratories]

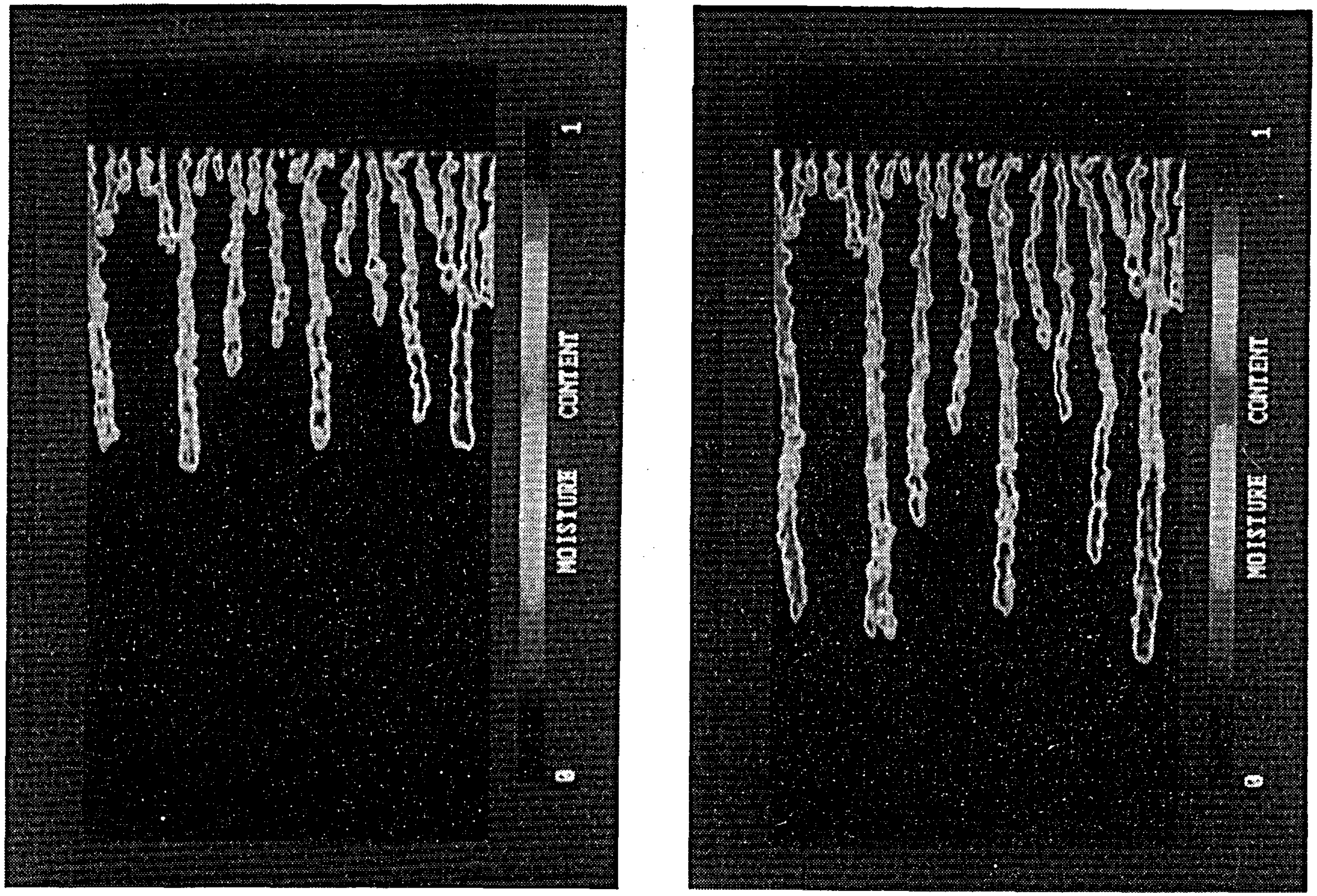

Plate 5. Infiltration flow instability: Infiltration into an unsaturated porous layer can be unstable when the ratio of the total flux into the layer to the saturated conductivity of the layer (R_S) is less than 1. The downward growth of fingers in an initially dry porous medium is shown here in a sequence of two images using the optical technique. The total flux through the system is controlled by a thin top layer of lower conductivity (dark rectangle on top) which uniformly supplies water to the underlying layer at an R_S of 0.1. Fingers form in the higher conductivity medium directly beneath the top layer. The dimensions of the higher conductivity medium are 45 cm wide, 76 cm high and 1 cm thick (into the plane of visualization). If the thickness of the medium is less than the minimum finger width, a two-dimensional flow field is forced as is the case here. [R.J. Glass, Geoscience Analysis Div. 6315, Sandia National Laboratories]

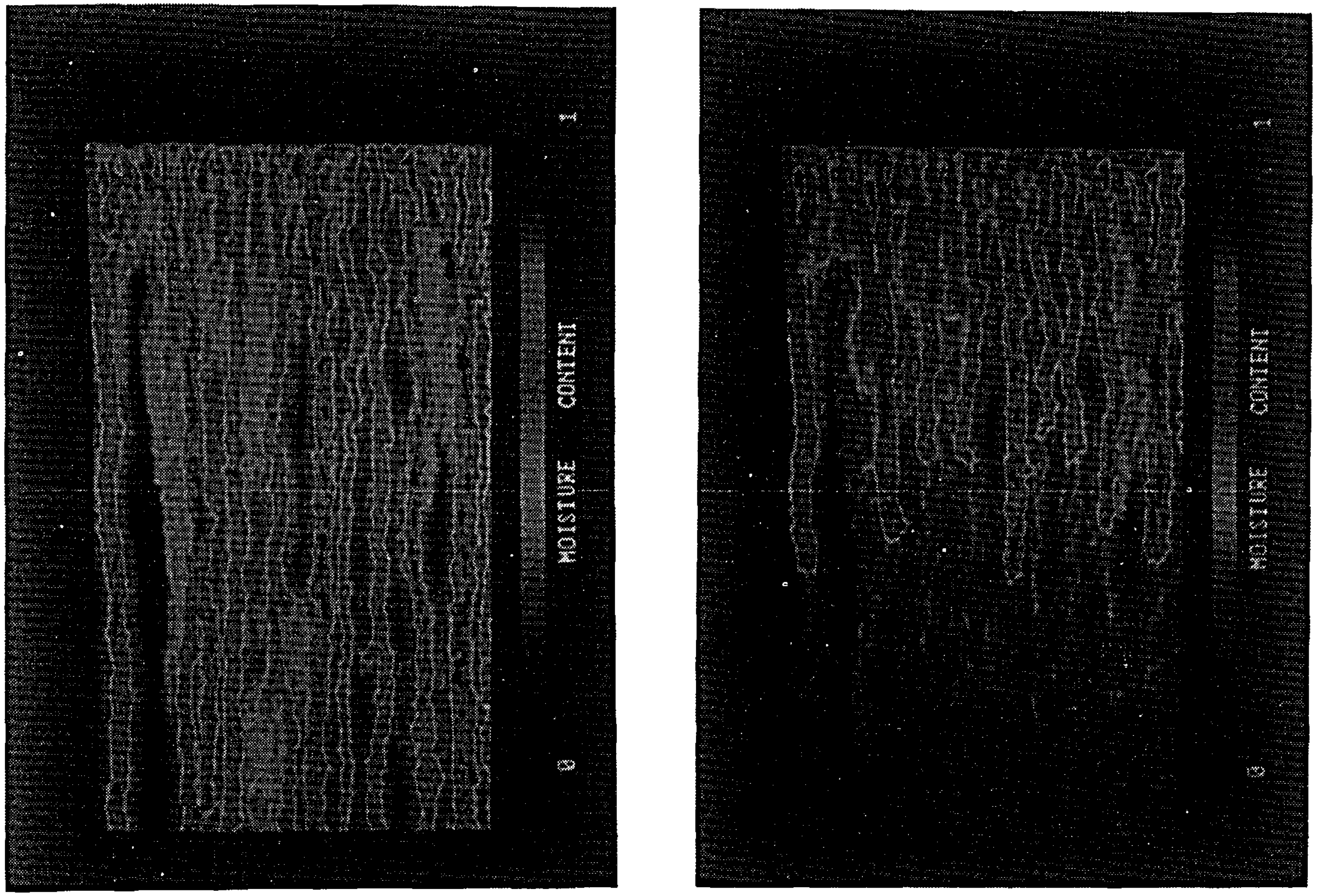

Plate 6. Core-fringe structure development and persistence: Fourteen days after the onset of infiltration shown in Plate 5, finger core regions within less saturated fringe regions continue to conduct almost all of the flow (left). Following a 24-hr interruption of infiltration, a subsequent infiltration event demonstrates continued persistence of the core-fringe region structure (right). The two-zone moisture content structure has been shown to persist until either complete saturation or drying of the layer occurs. [R.J. Glass, Geoscience Analysis Div. 6315, Sandia National Laboratories]

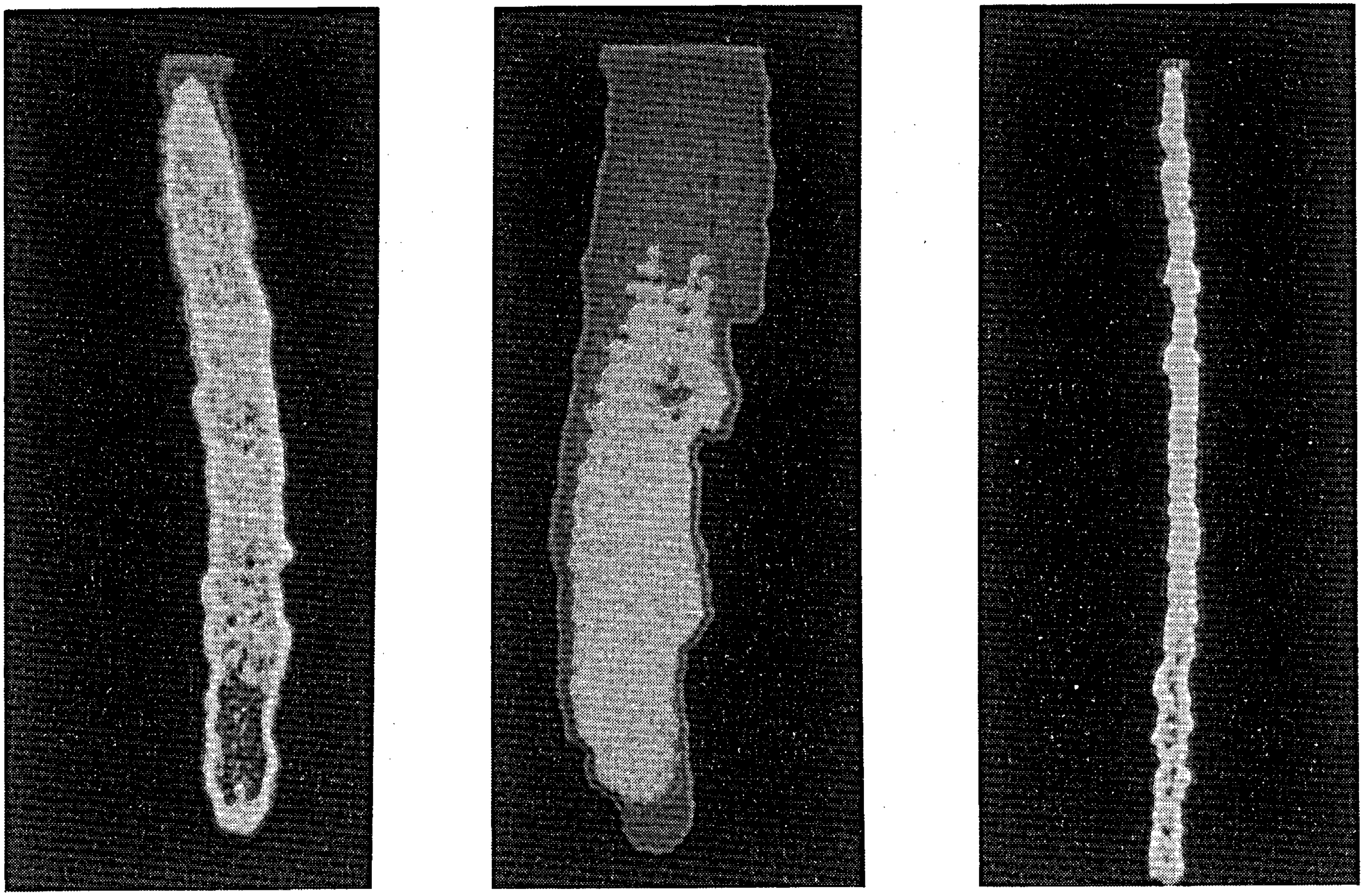

Plate 7. Application of similitude theory to scale finger width: Linear stability analysis, dimensional analysis, and experimentation have yielded formulations for average finger width as a function of system parameters given by the saturated hydraulic conductivity, saturated moisture content, sorptivity, initial moisture content, and the flow into the finger. Similitude theory applied to finger width yields a scaled form containing the microscopic length scale, m (equivalent to the mean grain size). For a family of similar media, finger width is found to scale with m such that finger width increases as the medium texture becomes finer (for the same scaled flow rate into the finger). Experiments to test the theory where the flow rate into the finger and the texture of the sand are varied (m spanning an order of magnitude) are underway. The left and middle plates show the increase in finger width with a fourfold increase in flow into a finger ($m = 0.252$ mm). The plate on the right has the same flow feeding the finger as in the middle and the same scaled flow as in the left; the medium, however, is much coarser ($m = 0.991$ mm). [R.J. Glass, Geoscience Analysis Div. 6315, Sandia National Laboratories]

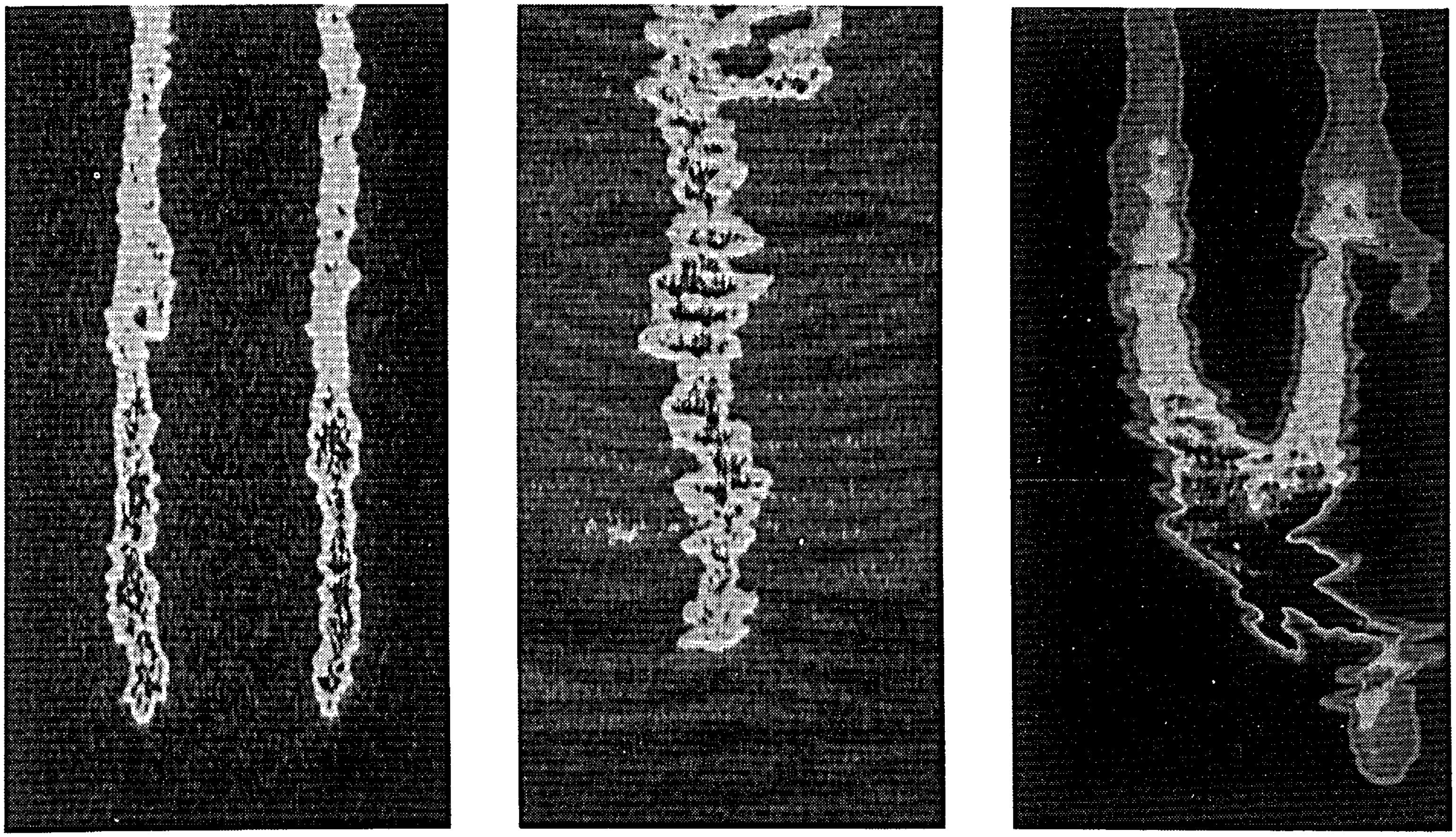

Plate 8. Influence of heterogeneity on finger properties: Heterogeneity fields are those shown in Plate 4. Fingers are generated from two equal strength point sources located 15 cm above the test section. In the homogeneous case (left) the two fingers remain separate. Horizontal microlayering in the middle slab causes merger of the two fingers and a highly variable finger width. The right slab contains a homogeneous zone where fingers remain separate overlying microlayered zones (horizontal on top of crossbedded) where fingers merge and run down-dip of the bedding. [R.J. Glass, Geoscience Analysis Div. 6315, Sandia National Labo~atories]

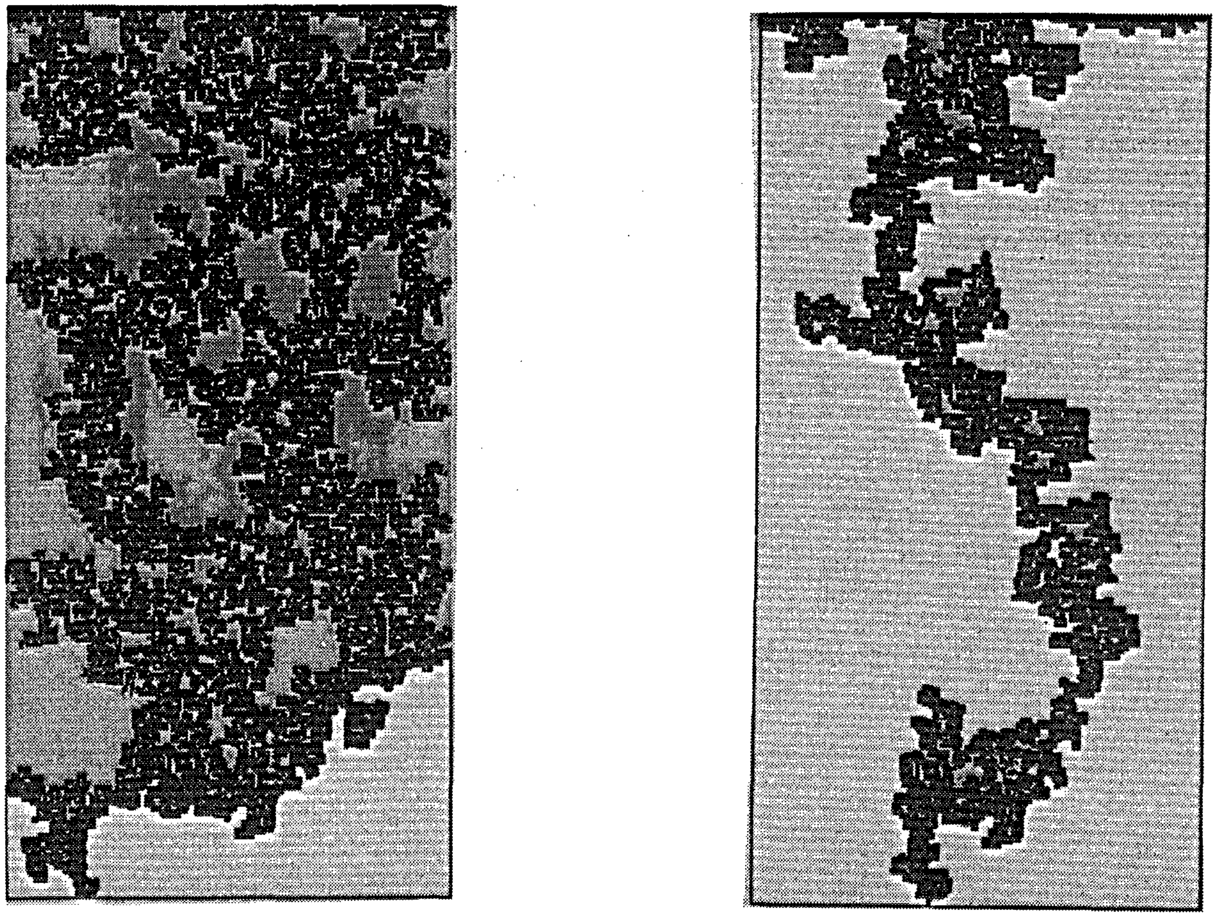

Plate 9. Pore-scale invasion percolation modeling: Two-dimensional networks of pores are generated with radii chosen from a beta distribution. Pores connected to the filling interface are searched to find the pore with the lowest filling potential. This pore is filled, the filled interface is adjusted, and the sequence repeated until the end of the network is reached. Filling potentials are calculated based on pore-filling radii, contact angle, location in the gravity field, and the modification of pore geometry by adjacent-neck-filling facilitation. When the pore network 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, Geoscience Analysis Div. 6315, Sandia National Laboratories]

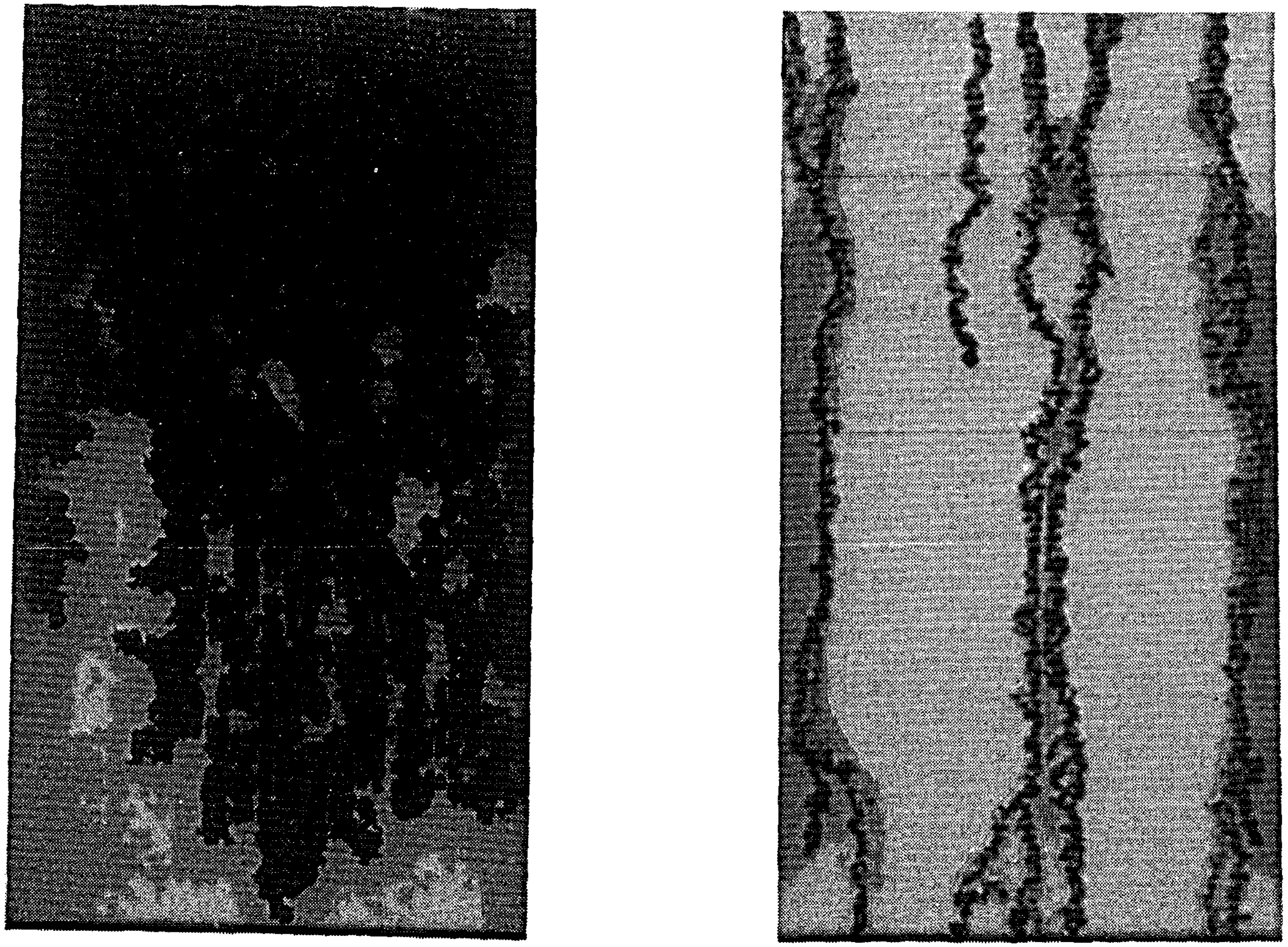

Plate 10. Horizontal and vertical imbibition into transparent analogue fractures: Two roughened glass plates (commercially available obscure glass) are clamped together to form an analogue transparent fracture (30-cm-wide, 60-cm-long). Water imbibes at a constant flow rate supplied through a porous plate 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 shown in Plate 5 where infiltration flow instability in unsaturated porous media occurs and in Plate 9 generated with the pore-scale invasion percolation model. [R.J. Glass, Geoscience Analysis Div. 6315, Sandia National Laboratories]

Appendix

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