PROCEEDINGS

OF

WORKSHOP IV

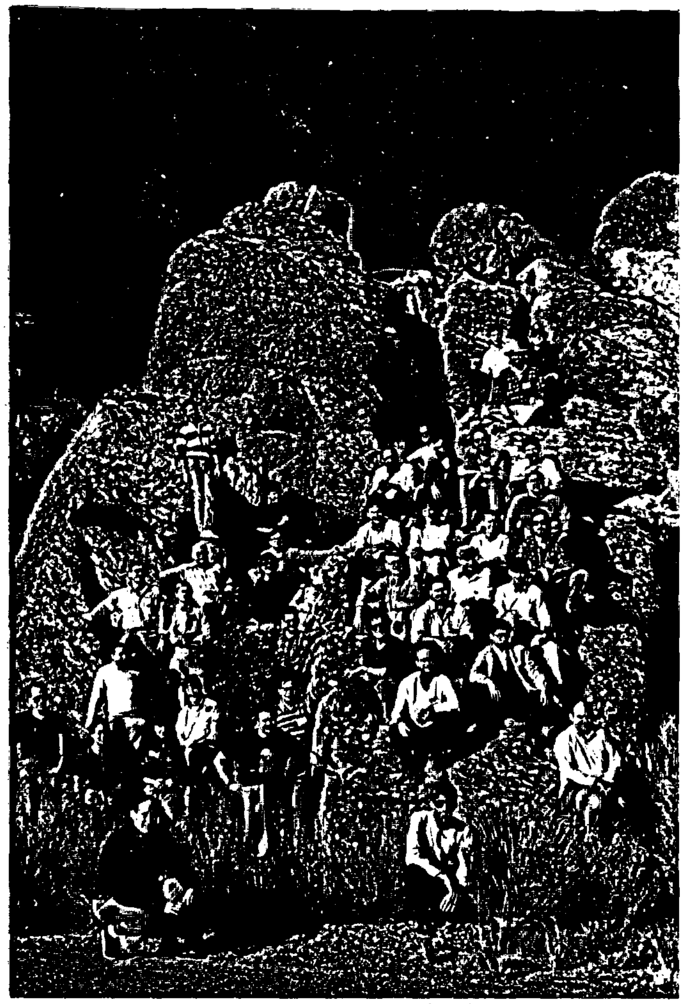
ON

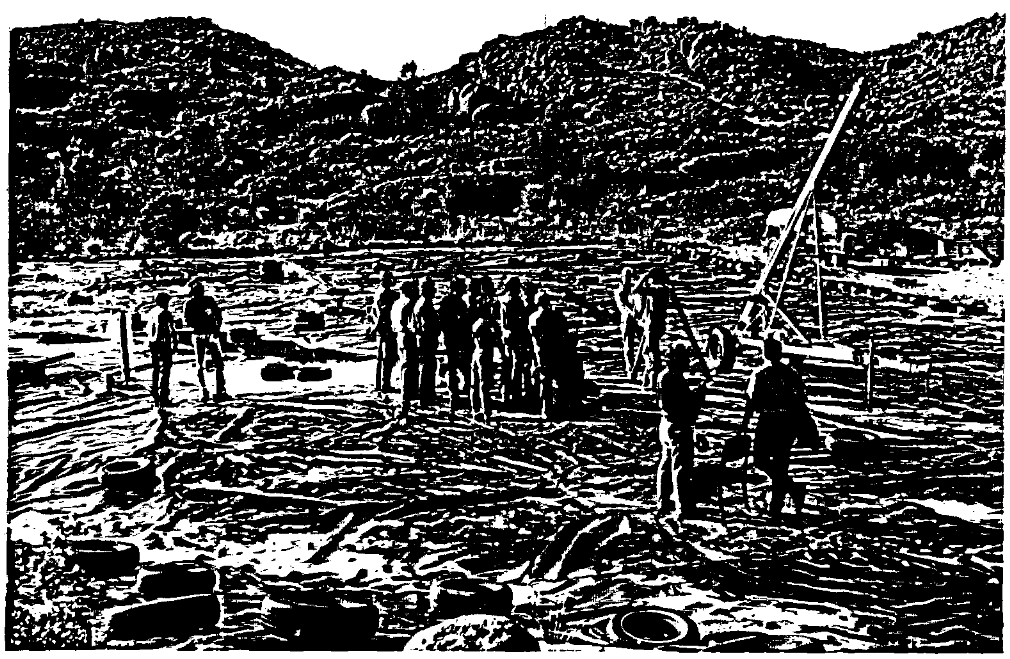
FLOW AND TRANSPORT THROUGH UNSATURATED FRACTURED ROCK -- RELATED TO HIGH-LEVEL RADIOACTIVE WASTE DISPOSAL

SPONSORED BY:

U. S. NUCLEAR REGULATORY COMMISSION
CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
SANDIA NATIONAL LABORATORIES
UNIVERSITY OF ARIZONA (HOST)

DECEMBER 12-15, 1988
TUCSON, ARIZONA





Part of workshop group on field trip to Apache Leap Test Site. Outcrop is slightly welded tuff.

PREFACE

This was the fourth workshop held on this topic since an interest developed in the possible siting of a high-level radioactive waste repository in the unsaturated zone. The first was held in August, 1982, at Rio Rico, near Nogales, Arizona. The second was held near Oracle, Arizona, in January, 1984. The third, in January, 1986, and the fourth, in December, 1988, were held in Tucson. They focused on the technical aspects of water flow and radionuclide transport through unsaturated fractured rock, now the only geologic medium under consideration by the U.S. Department of Energy and the U.S. Nuclear Regulatory Commission for a high-level waste repository.

Prior to 1980, there was little interest in flow and transport through unsaturated fractured rock. Since then, interests have developed not only for high-level radioactive waste concerns but for the disposal of all types for waste. Numerous waste sites are located in fractured rock settings involving an unsaturated zone as a source of contaminants or through which contaminants move to reach the accessible environment. For example, many EPA Superfund Sites require the removal of contaminants from fractured rock, saturated and unsaturated. In some regions, recharge through unsaturated fractured rock to water supply aquifers is an important process.

Technical aspects of flow and transport through unsaturated fractured rock relate to understanding and describing the relevant interrelated processes, assessing and developing characterization and monitoring experimental methods, and flow and transport computer simulations. The most complex systems are two-phase, nonisothermal and combined fracture and matrix flow and transport, with large spatial variability and nonlinear properties. For high-level waste disposal, scales of kilometers and thousands of years are of interest. The extension of research results from the experimental scale to repository scale is critical to repository site characterization.

Workshop IV was sponsored by the U.S. Nuclear Regulatory Commission, Center for Nuclear Waste Regulatory Analyses, Sandia National Laboratories and the University of Arizona. Selected participants were invited to make presentations related to their research in a fashion to generate discussion. General discussion sessions were lead by selected discussants. Speakers and discussants were requested to provide copies of their visual aids and outlines but not manuscripts. The Proceedings include the material supplied by each speaker and discussant for the purpose of providing brief coverage of the topics discussed so that authors can be contacted for additional detail. Tom Nicholson presented questions concerning research needs and requested responses from the participants. In addition to oral responses, some written responses are included in the Proceedings.

The rapid advance of knowledge and number of professionals in flow and transport through unsaturated fractured rock are leading to a recognized scientific subdiscipline, that will likely have applications to many environmental problems.

Dan Evans

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ORGANIZATION AND PROGRAM

Workshop IV -- Flow and Transport Through Unsaturated Fractured Rock -- Related to High-Level Radioactive Waste Disposal

Sponsored by -- Nuclear Regulatory Commission
Center for Nuclear Waste Regulatory Analyses
Sandia National Laboratories
University of Arizona

Date and place -- December 12-15, 1988; Radisson Suite Hotel
6555 E. Speedway, Tucson, AZ
(602) 721-7100

Organizing Committee -- Thomas J. Nicholson, NRC-RES/WMB
Donald L. Chery, NRC-NMSS/TR
John L. Russell, CNWRA
E. J.(Tito) Bonano, Sandia-WMS
Daniel D. Evans, Coordinator
Dept. of Hydrology and Water Resources
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General Scope -- Physical and chemical processes and relevant parameters, experimental methods and results, and modeling

Schedule -- Daytime meetings in Salon B
Evening discussions in Salon A

PROGRAM

Dec.12 12:30 pm Registration (near Salon B) -- <u>FEE $125</u>
Mon pm Field studies; Chm. Dan Evans, University of Arizona
1:15 Introductory remarks
1:30 Dan Evans and Todd Rasmussen
Experimental studies -- Apache Leap Tuff
3:00 Break
3:15 Dwight Hoxie and Alan Flint, USGS
G. Bodvarsson, LBL
Experimental studies -- Yucca Mountain
5:00 Adjourn
6:30-
8:00 Reception - Radisson Hotel, Garden Court

Dec.13
Tues Site visitations
8:00 am to 5:30 pm (leave lobby area at 8:00 am)
Trip to UA research laboratories and field sites
(box lunch provided by Radisson)

Tues pm 7:30-
9:00 Informal discussions -
Leader: L.G. Wilson, U. of Arizona, Methods for the vadose zone, ASTM project
Leader: S. Crestana, U. of California at Davis, Gamma- and X-ray tomography studies

Dec. 14
Wed am Physical Aspects; Chm. Tom Nicholson, Nuclear Regulatory Com.

8:00	Rien van Genuchten, U.S. Salinity Laboratory Solute movement in dual-porosity media
8:45	Douglas Smith, University of New Mexico Pore characteristics of tuff
9:15	Art Warrick, University of Arizona Scaling of matric hydrologic properties
9:45	Discussion
10:00	Break
10:30	Jane Long, Lawrence Berkeley Laboratory Seismic/hydrologic analyses
11:00	Scott Tyler, Desert Research Institute Applications of fractal mathematics to parameter estimation
11:30	Discussion
12:00	Lunch

Wed pm Geochemical Aspects; Chm. Randy Bassett, University of Arizona

1:30	Don Langmuir, Colorado School of Mines Predicting the mobilities of anionic tracers and radionuclides: What do we need to know?
2:00	Bill Murphy, Center for Nuclear Waste Reg. Analyses Surface reactions versus diffusion transport in mineral dissolution and growth kinetics
2:30	Randy Bassett, University of Arizona Chemical sampling and mass transfer
3:00	Break
3:30	Al Yang, U.S. Geological Survey Monitoring of gas movement in a borehole completed in the unsaturated zone at Yucca Mt.
4:00	James Kumhansl, Sandia National Laboratories Site selection criteria and preliminary results from the Valles Caldera natural analog study
4:30	Discussion
5:00	Adjourn
7:30 -9:00	Informal discussion - Leader: Jim Yeh, University of Arizona, Strategies for flow and transport estimations

Dec 15

Thur am Modeling Aspects; Chm. Art Warrick, University of Arizona

8:00	Karsten Pruess, Lawrence Berkeley Laboratory Current issues in the modeling of nonisothermal multiphase flows in fractured media
8:45	Scott Sinnock, Sandia National Laboratories Quantifying uncertainty in modeling unsaturated flow
9:15	Bryan Travis, Los Alamos National Laboratory Simulating flow and transport over a range of length scales
9:45	Discussion
10:00	Break
10.30	Rachid Ababou, Princeton University Unsaturated flow in spatially variable and anisotropic media
11:00	Todd Rasmussen, University of Arizona Variably saturated fracture flow modeling using the boundary integral method
11:30	Discussion
12:00	Lunch

Thur pm Research needs; Chm. John Russell, Center for Nuclear Waste Regulatory Analyses

Discussion leaders

1:30	Don Chery, NRC Licensing perspective
	Tom Nicholson, NRC Research questions
	Joe Wang, LBL Summary of research needs from previous sessions
3:00	Break
	David Galliegos, Sandia Performance assessment considerations
	Dick Codell Questions dealing with near-field phenonena
	Dan Evans Data needs
5:00	End of Workshop

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Laboratory and Field Studies at the Apache Leap Tuff Site

Daniel D. Evans and Todd C. Rasmussen

Department of Hydrology & Water Resources

A series of experiments have been conducted which focus on obtaining characterization data sets of the physical, hydraulic, pneumatic and thermal properties of unsaturated fractured rock at a field site in tuff near Superior, Arizona. One of the studies focuses on data sets collected from an abandoned road tunnel constructed in welded tuff. Also, geochemical sampling of sulfate distribution caused by nearby smelter emissions during a fifty year period may provide information about travel times in the unsaturated tuff. An additional study focusing on the causes of air flow through fractures is ongoing. A study of precipitation inputs and the resultant runoff, evaporation, and infiltration is being conducted on a 2 ha watershed in the slightly welded tuff. Rock blocks with an embedded fracture are also being studied in the laboratory to determine the hydraulic properties of fractures under unsaturated conditions. Finally, a heater experiment is being planned to evaluate the effect of a subsurface heat source on fluid and solute migration in an unsaturated fractured rock.

This presentation focuses on properties of slightly welded tuff at 105 locations in nine inclined boreholes at one field site. A 30 m by 50 m plastic cover has been placed over the site to control surface hydraulic boundary conditions. Core samples removed from the boreholes at three meter intervals are used to estimate properties in the laboratory. Both laboratory and field parameter estimates are available in the form of a draft data package. Physical properties include the bulk and skeletal densities, effective porosity, pore surface area, and pore size distribution. Laboratory hydraulic properties include the saturated and unsaturated hydraulic conductivity, and the moisture characteristic curve. Measured pneumatic properties are the oven-dry and relative air permeability. Saturated and unsaturated thermal conductivity are also measured.

Field measurements are obtained for intervals corresponding to the same three meter interval used for collecting core samples. Results for field experiments include the saturated hydraulic conductivity and the ambient air permeability. Water content measurements as a function of time before and after a water imbibition experiment in four of the nine boreholes are also available. Borehole temperatures are also monitored, providing a time series of the thermal response of the subsurface to annual surface temperature changes.

Differences between laboratory and field measured parameters are of interest because laboratory methods are often used to estimate field scale parameters. Measurements such as saturated hydraulic conductivity, pneumatic permeability and thermal conductivity are often obtained on core segments and then used to predict field behavior. Using the Apache Leap data sets, it is shown that field saturated hydraulic conductivities are generally similar to laboratory measurements for the same interval, except for increases in field estimates due to the influence of fractures. Pneumatic permeabilities demonstrate the same influence of fractures, and also demonstrate the influence of matric suction on the relative saturation of the rock matrix which causes a reduction in field pneumatic permeability when compared to laboratory oven-dried samples. Finally, field estimates of thermal diffusivity based on the propagation of seasonal heat with depth compare favorably to laboratory estimates using measurements of core thermal conductivity.

An additional comparison has been made between laboratory permeabilities calculated using water as well as air. Comparisons between the two indicate that computed oven-dry air permeabilities are higher than saturated water permeabilities. The ratio of the two permeabilities is used to calculate a pore size assuming the slip-flow, or Klinkenberg, phenomenon. The Klinkenberg pore size compares favorably with mercury intrusion pore sizes for the samples. The effect of field hydraulic testing has been to increase the relative saturation of the matrix during the injection phase of the testing. Subsequent drainage has caused a progressive decrease in the water content of the rock matrix. At the same time, the pneumatic permeability of rock intervals are increasing from very low values observed immediately following flooding.

Ongoing experiments are being conducted to determine the cross-borehole air permeability of the fractured rock. Parameters estimated from such tests will be representative of a larger volume than interval and laboratory core tests. Air will be injected under low pressure at a central borehole and pressure changes will be monitored in packed-off intervals in surrounding boreholes at distances from 5 m to over 15 m. The influence of open boreholes will be minimized by isolating all open intervals with packers. The use of air-phase tracers for determining travel times between boreholes will also be examined. Helium gas has been used at the site to provide breakthrough curves between boreholes.

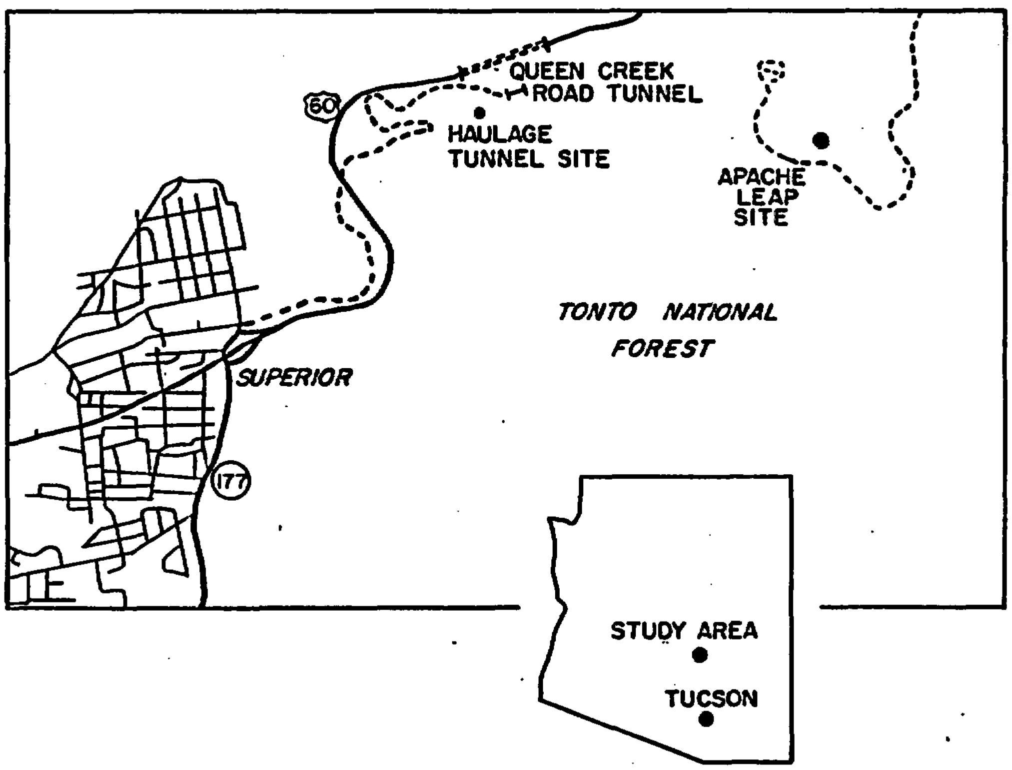


Figure 1: Location of field sites near Superior, Arizona.

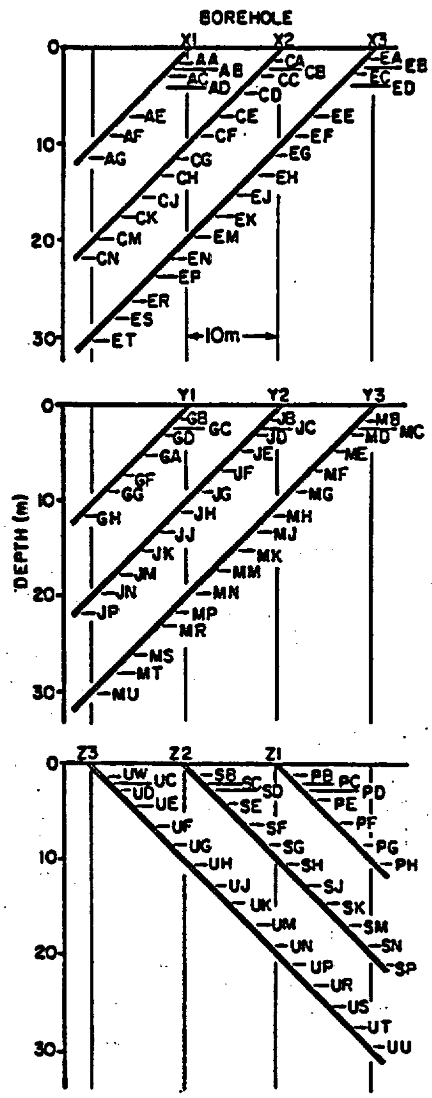


Figure 2: Core sample locations and designations.

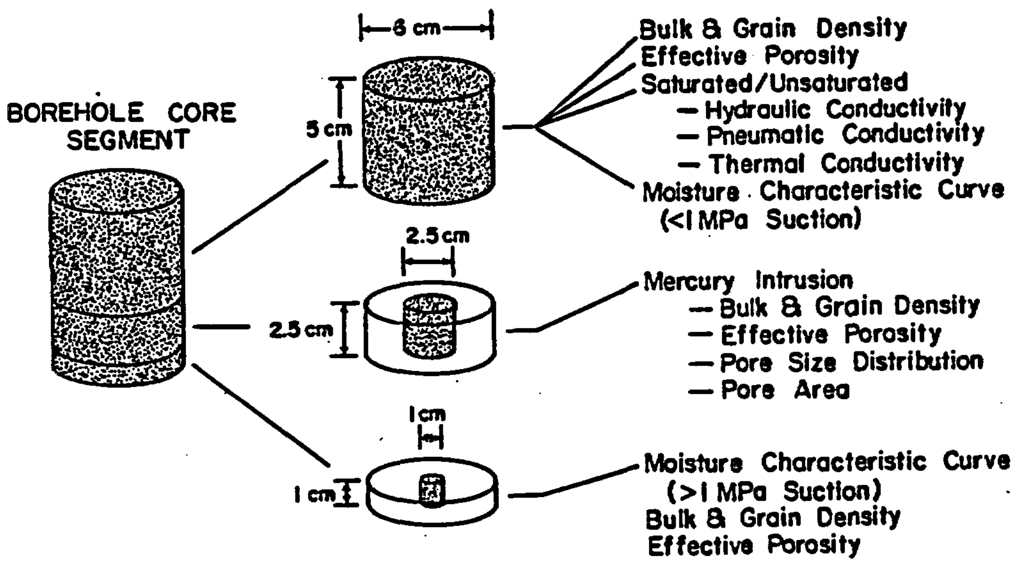


Figure 3: Core sample dimensions and measurements for segment.

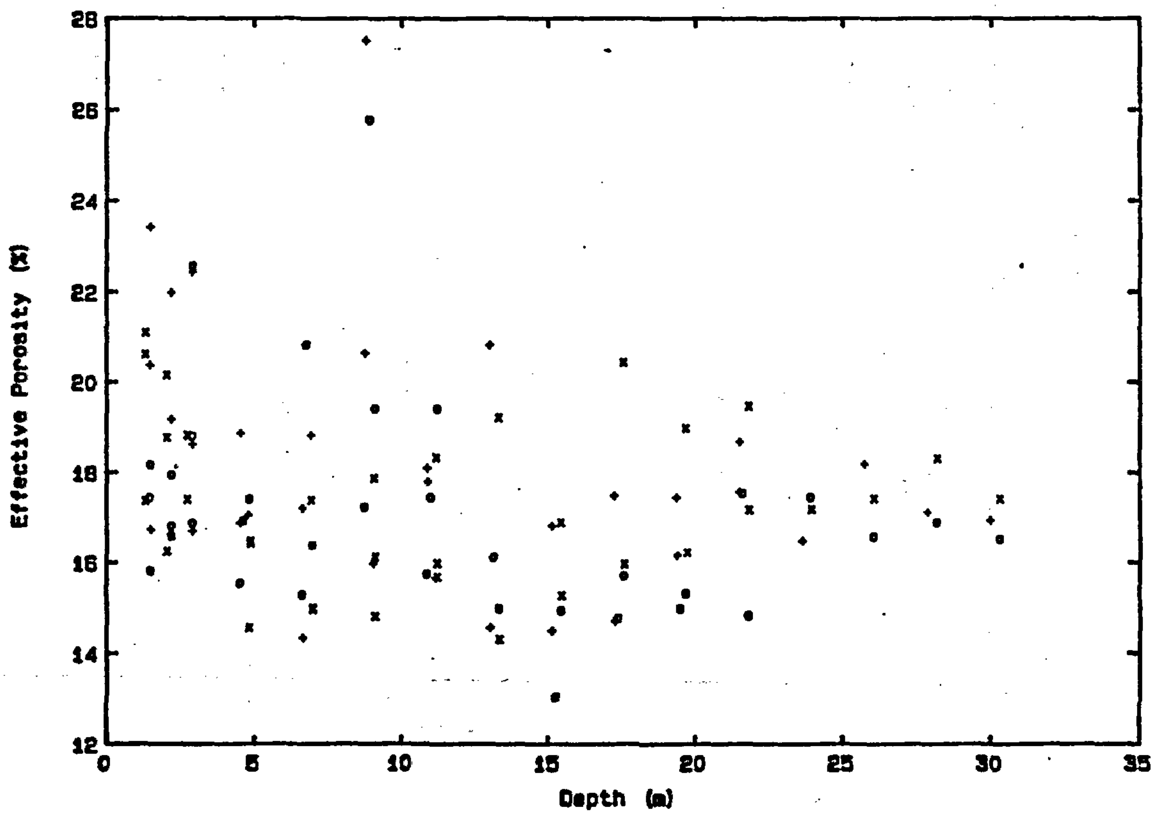


Figure 4: Effective porosity estimated from large Apache Leap tuff core segments.

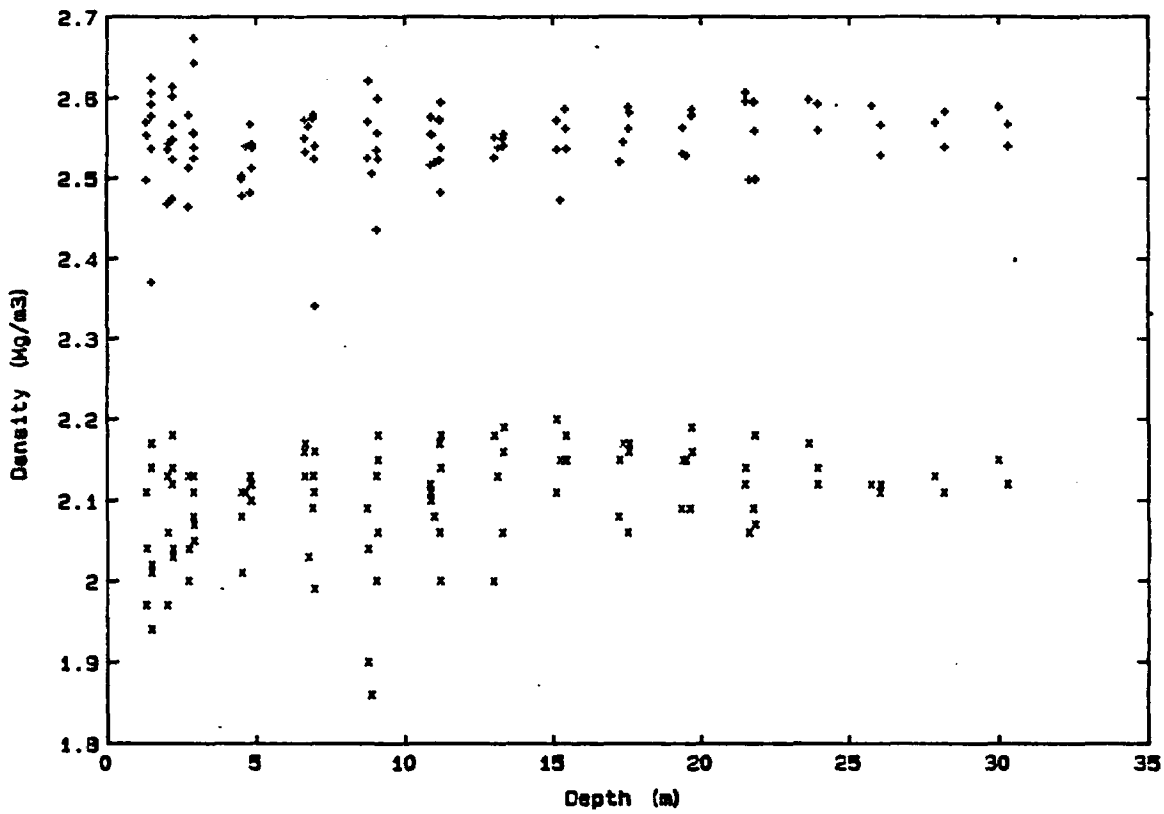


Figure 5: Bulk (x) and skeletal (+) density estimated from large Apache Leap tuff core segments.

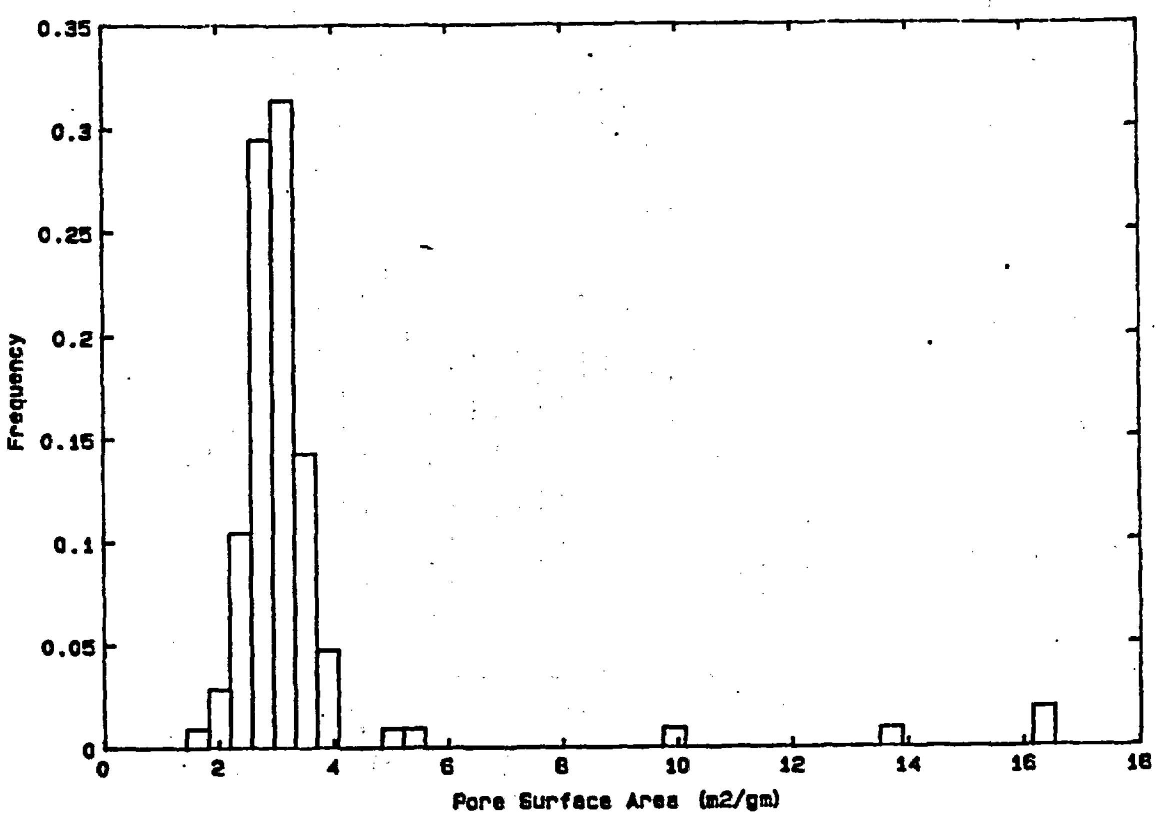


Figure 6: Pore surface area distribution of medium Apache Leap tuff core segments.

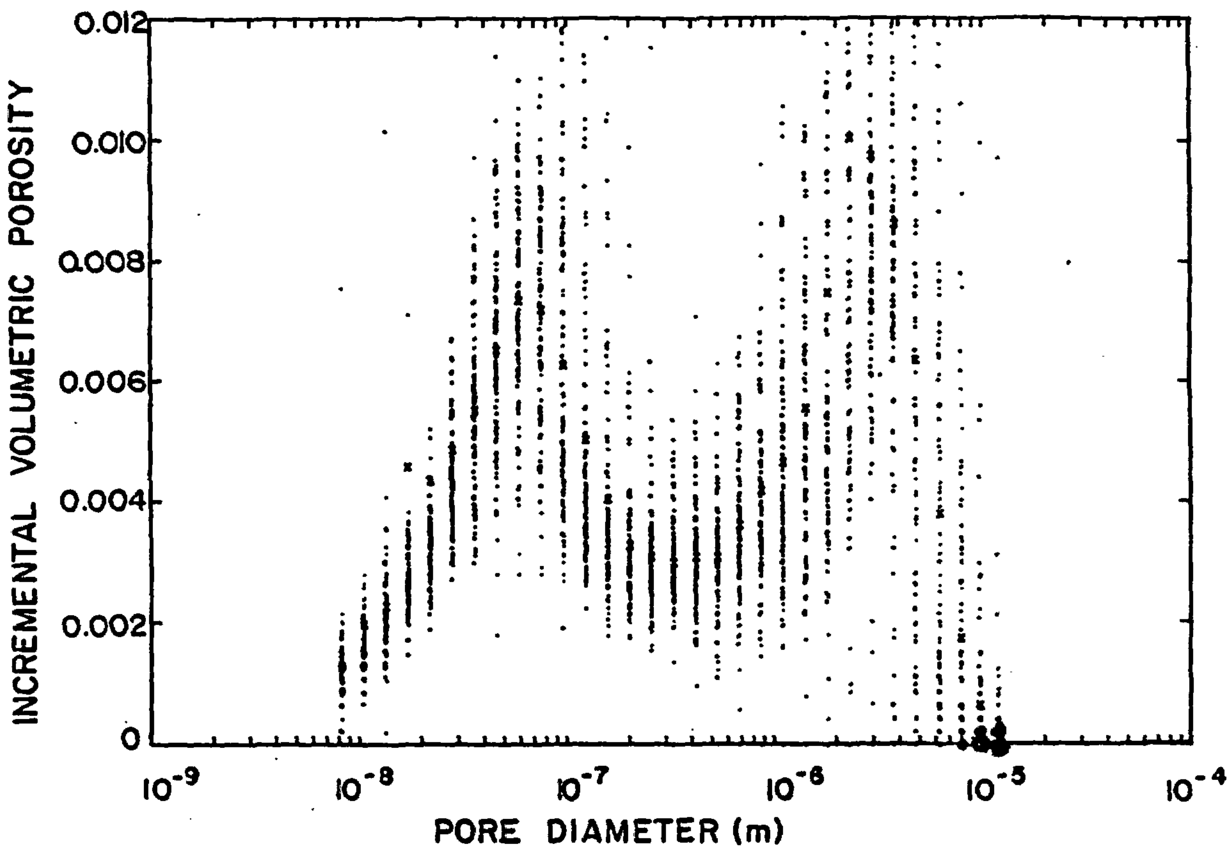


Figure 7: Incremental volumetric porosity (pore size distribution) of medium Apache Leap tuff core segments.

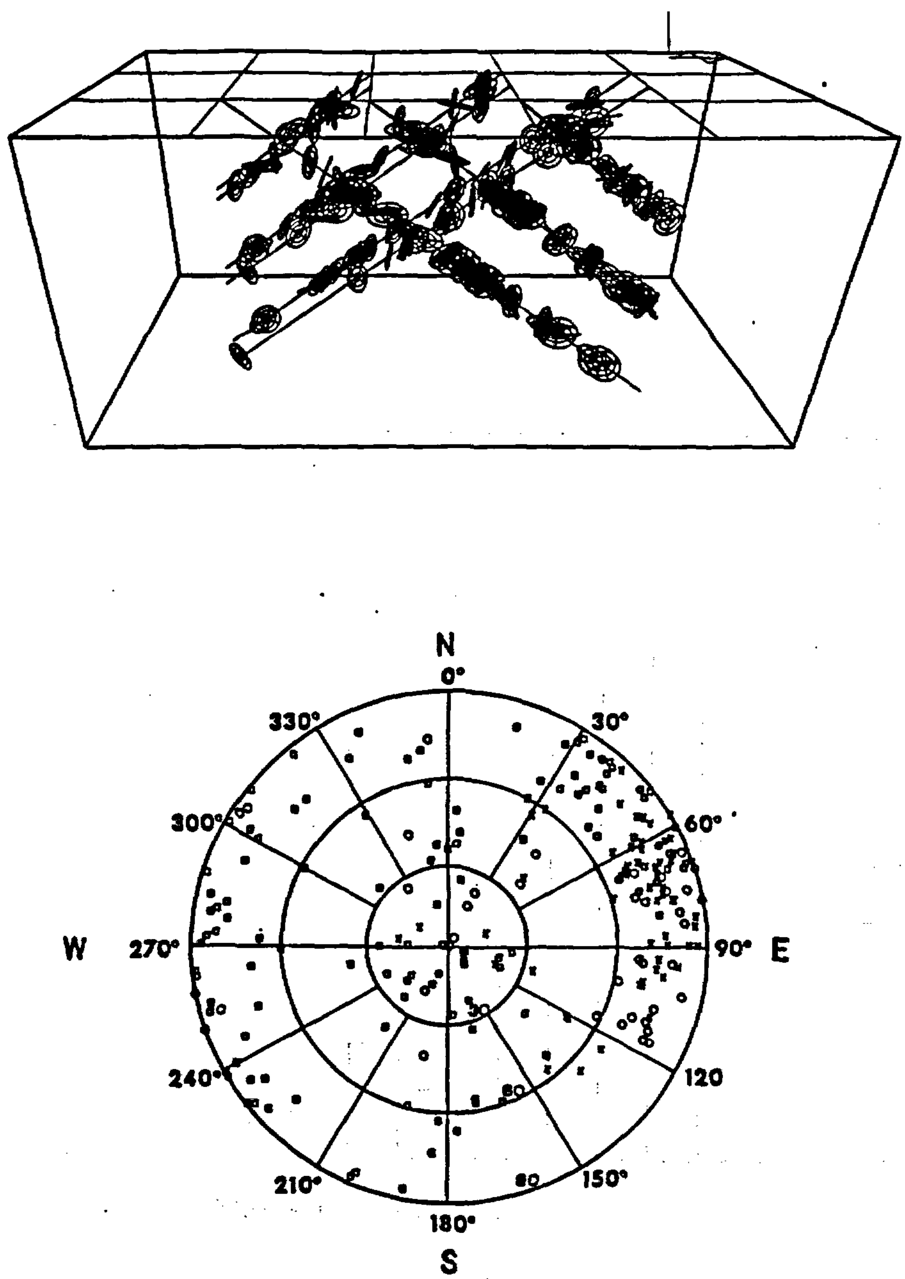


Figure 8: Fracture locations (above) and orientations (below) interpreted from Apache Leap tuff borehole cores.

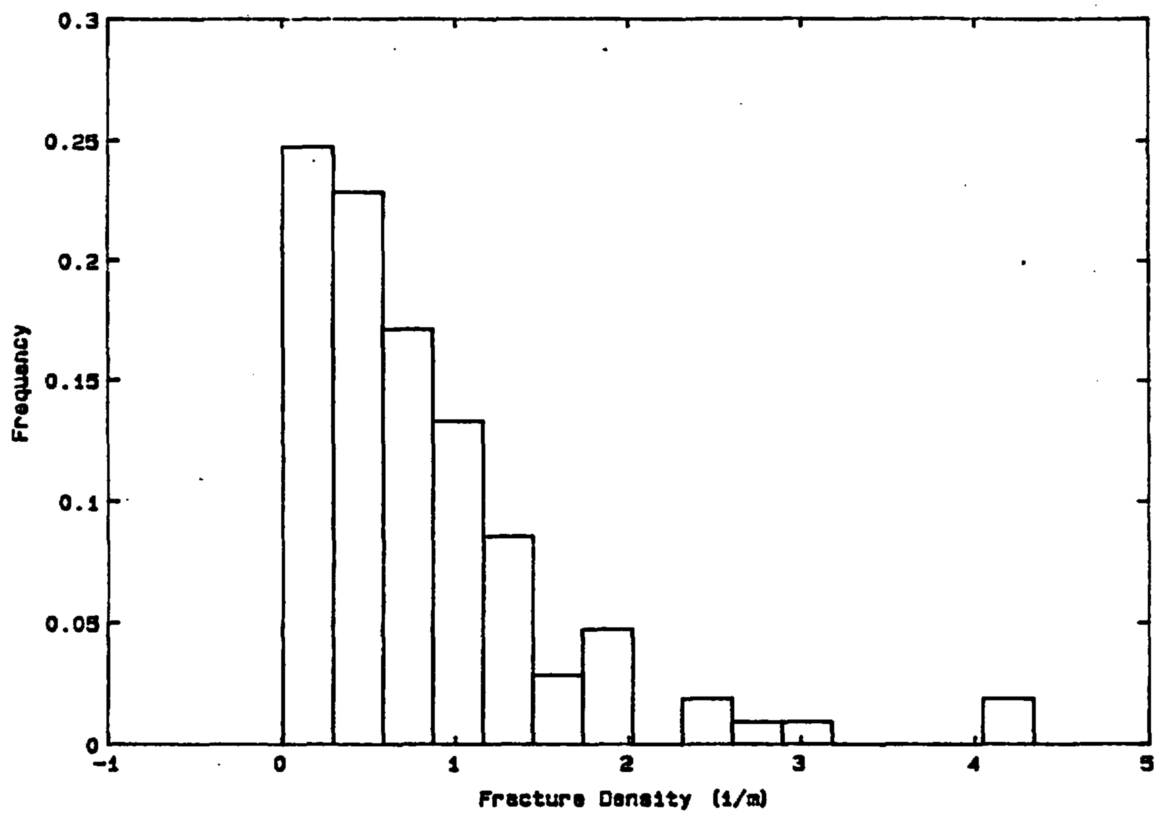


Figure 9: Fracture density distribution interpreted from Apache Leap tuff borehole cores.

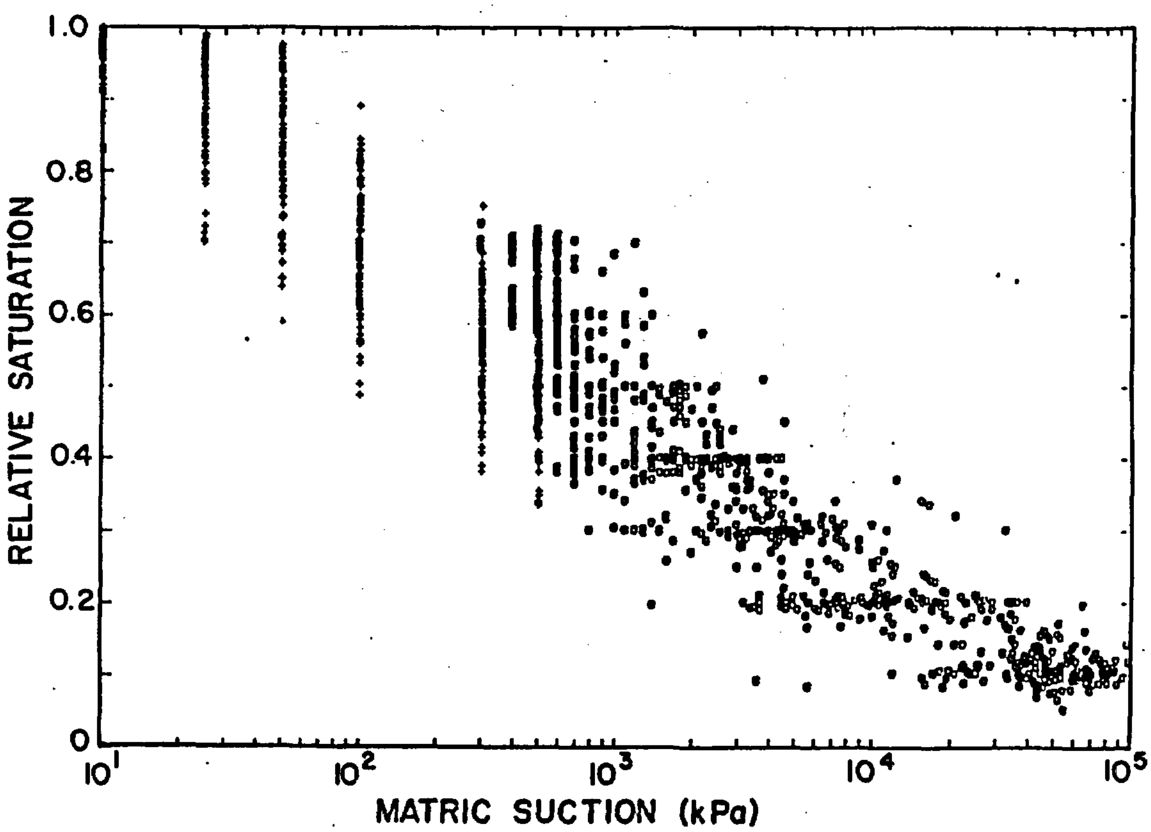


Figure 10: Characteristic curve values for 105 Apache Leap tuff core segments, (+) pressure extractor data using large segments, (o) psychrometer data using small segments.

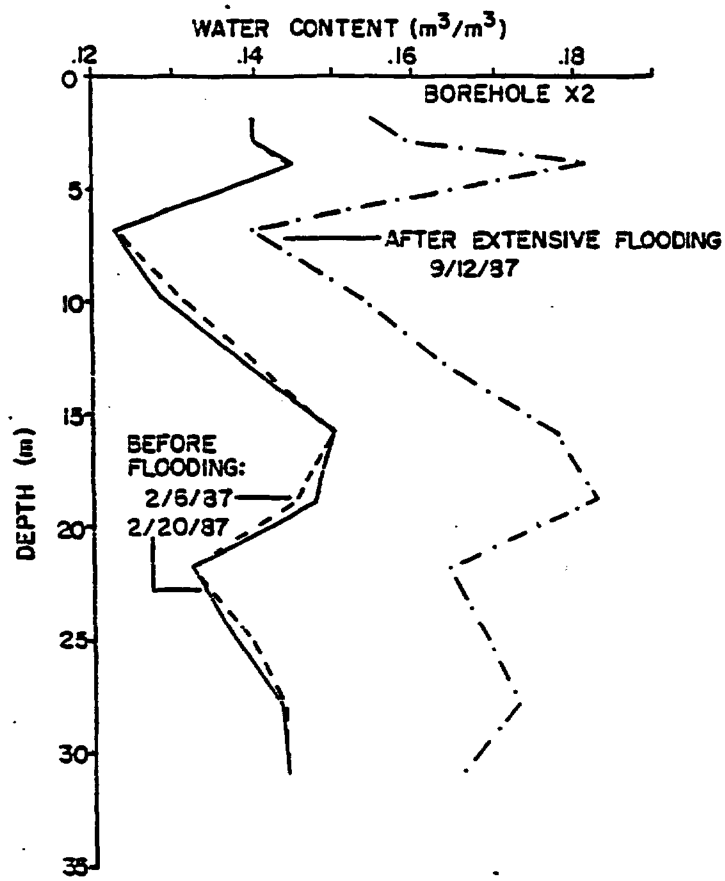


Figure 11: Water content profiles in Borehole X2 for different dates, before and after prolonged flooding of the borehole.

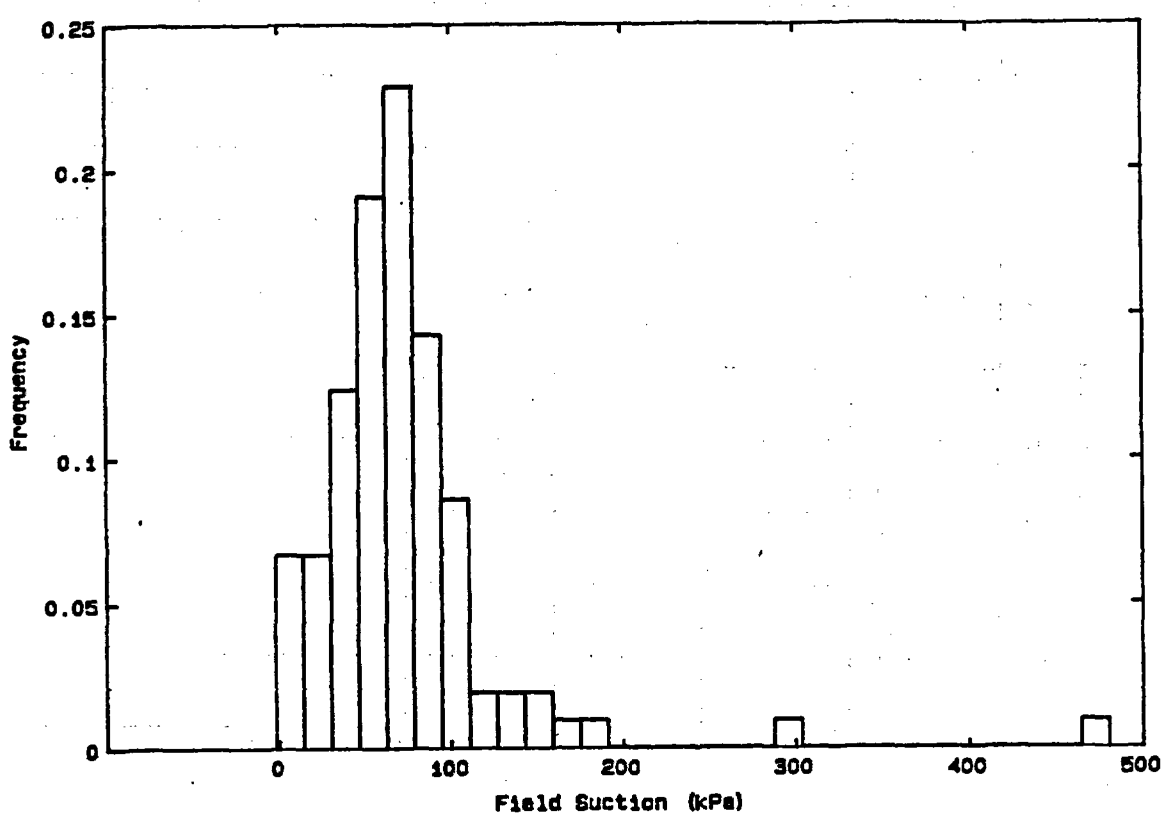


Figure 12: Field matric suction distribution inferred from laboratory characteristic curves and field neutron count data prior to flooding of boreholes.

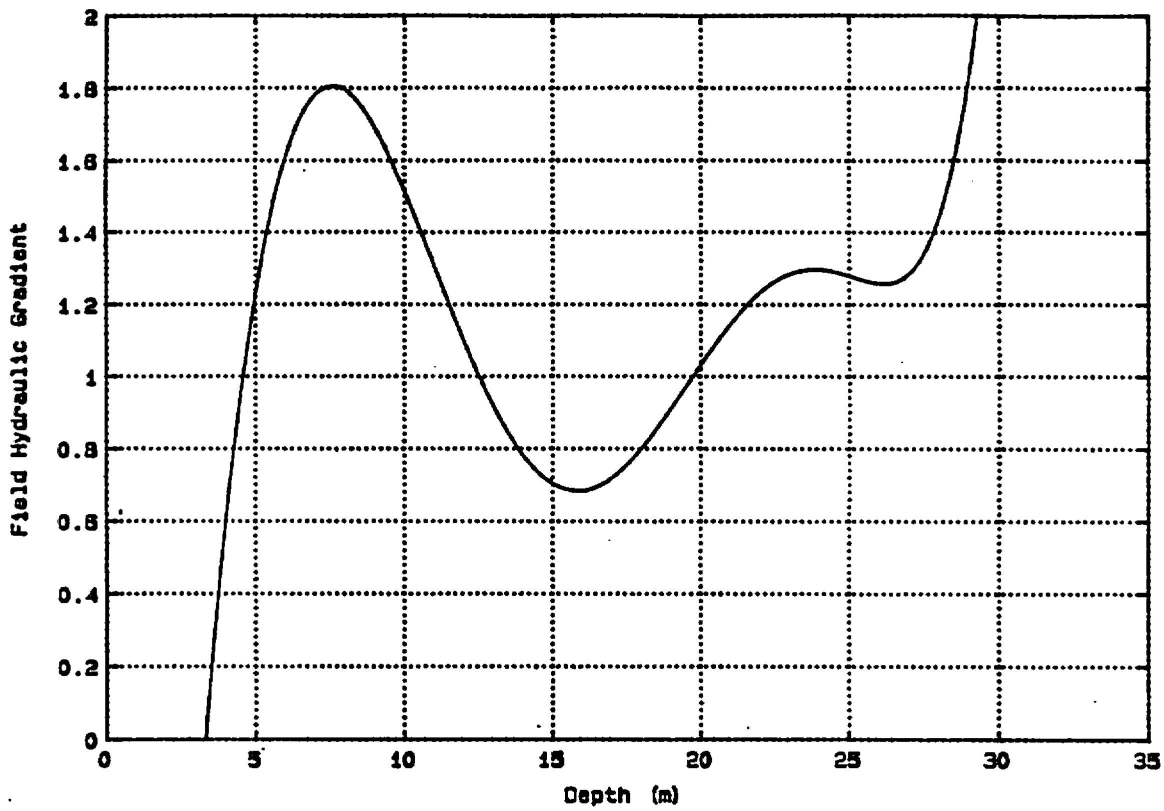


Figure 13: Vertical gradient inferred from least-squares polynomial fit of field matric suction distribution.

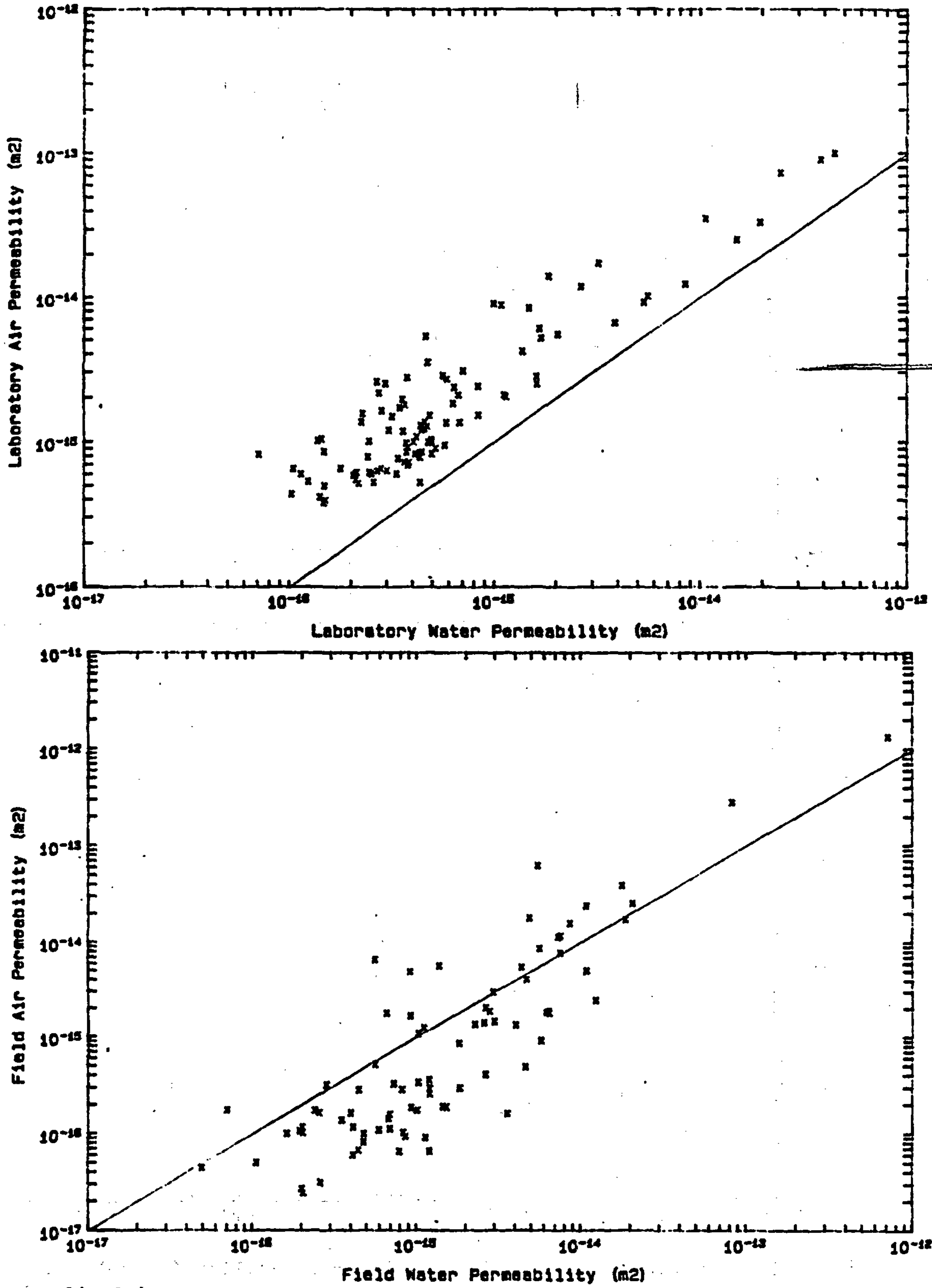
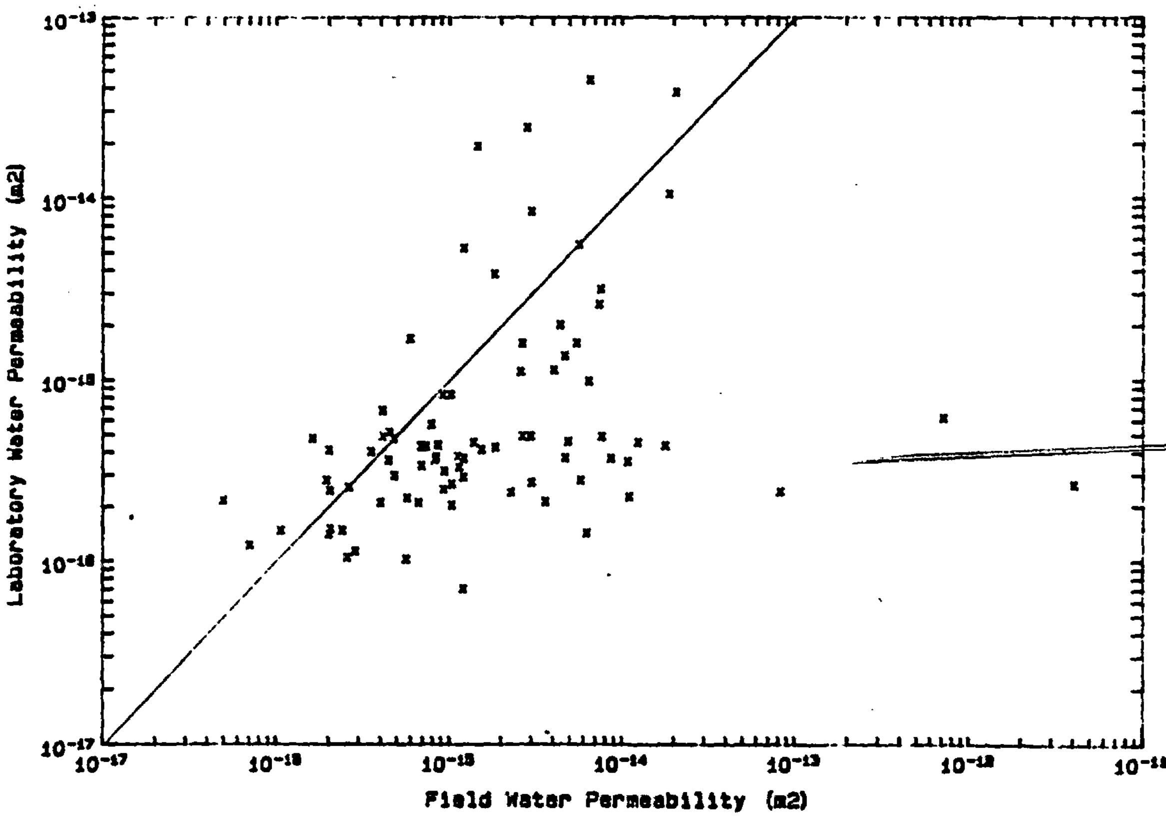


Figure 14: Laboratory hydraulic vs. pneumatic permeability (above) and field hydraulic vs. pneumatic permeability (below) for large Apache Leap tuff core segments.



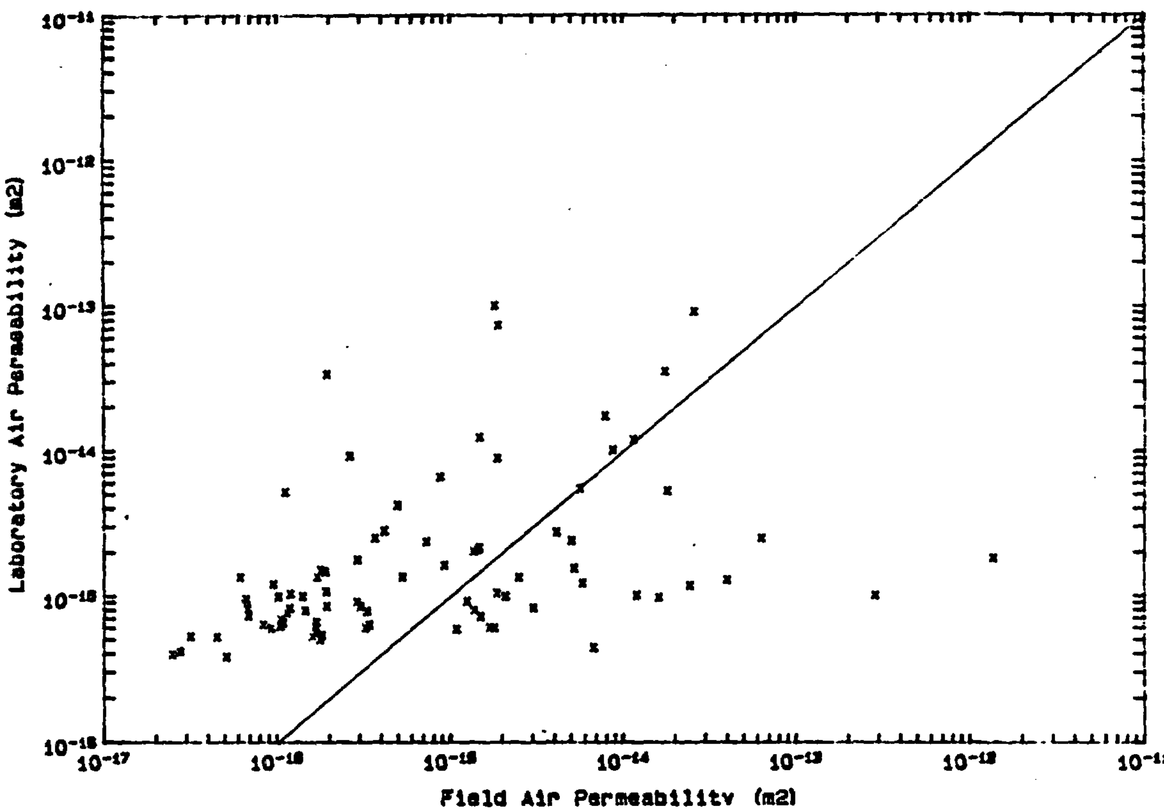


Figure 15: Laboratory vs. field hydraulic permeability (above) and laboratory vs. field pneumatic permeability (below) for large Apache Leap tuff core segments.

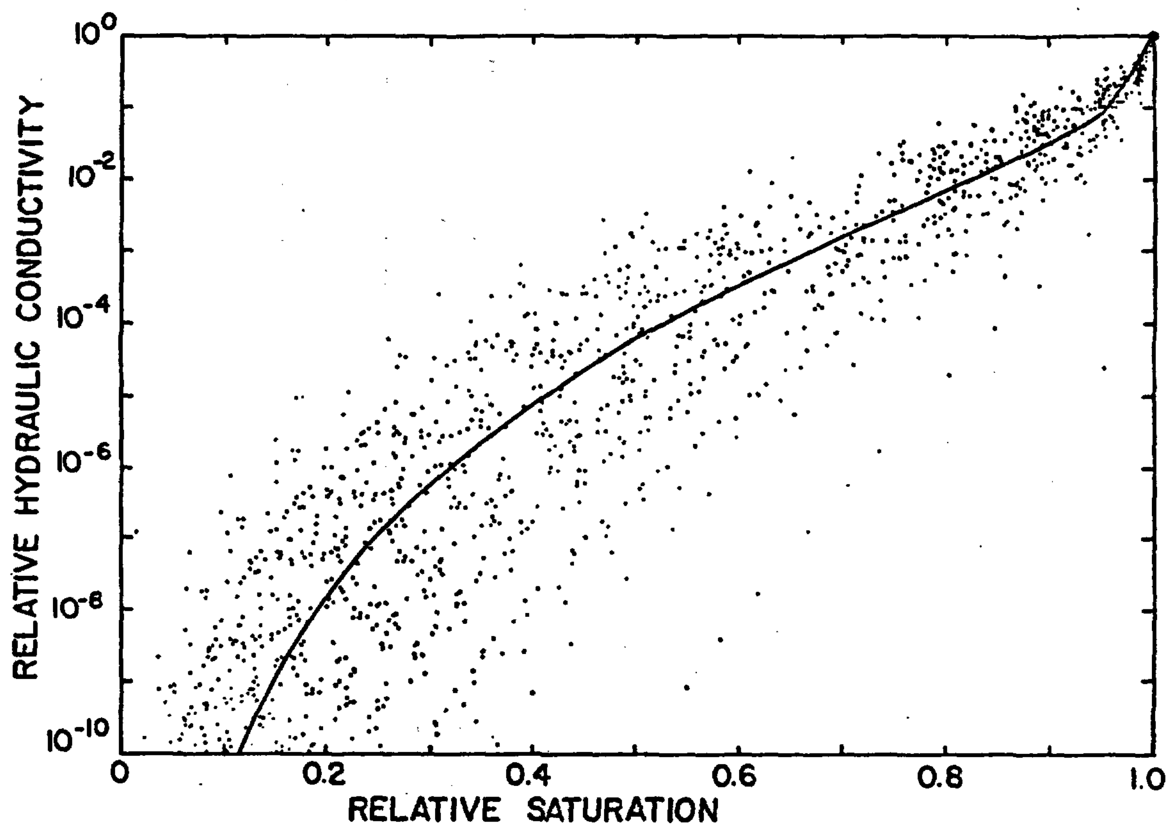


Figure 16: Relative hydraulic conductivity vs. relative saturation calculated from characteristic curves for large Apache Leap tuff core segments.

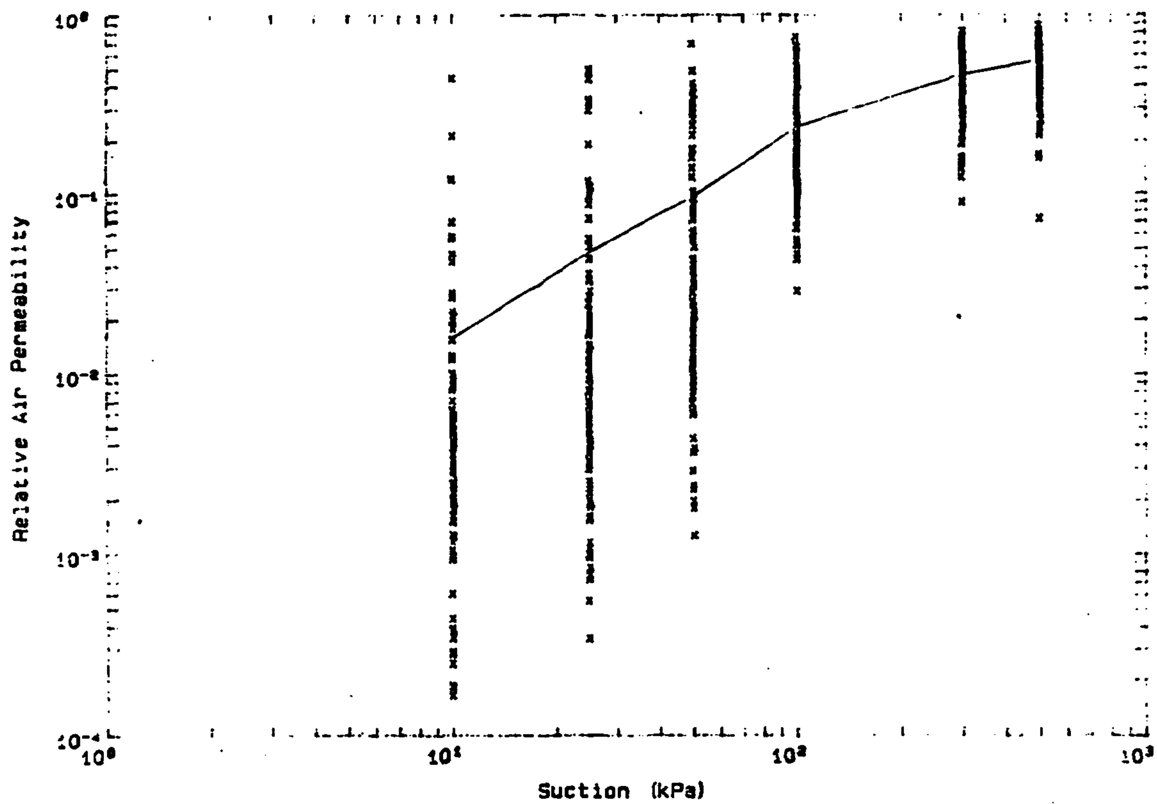


Figure 17: Observed relative pneumatic permeability vs. matric suction for large Apache Leap tuff core segments.

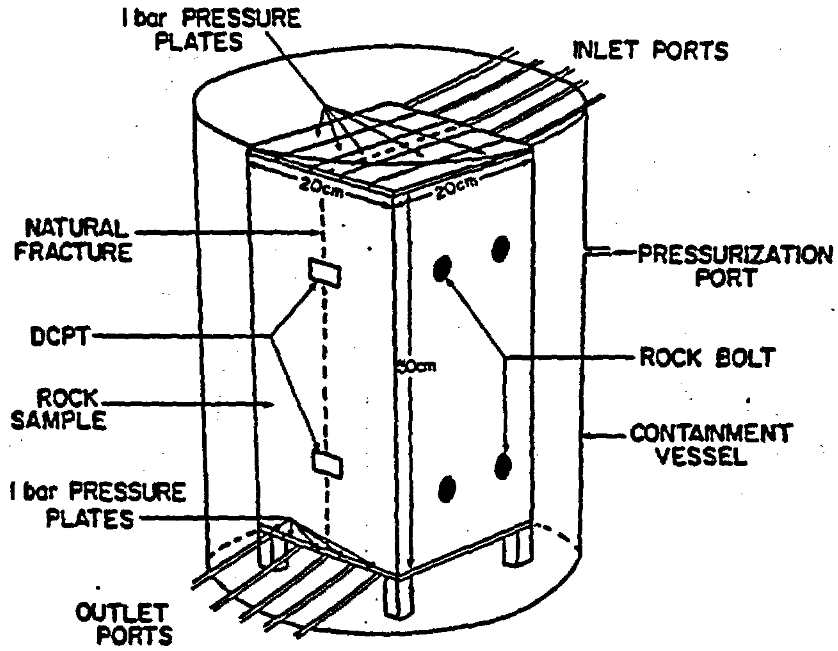


Figure 18: Laboratory arrangement for Apache Leap tuff block containing a single fracture.

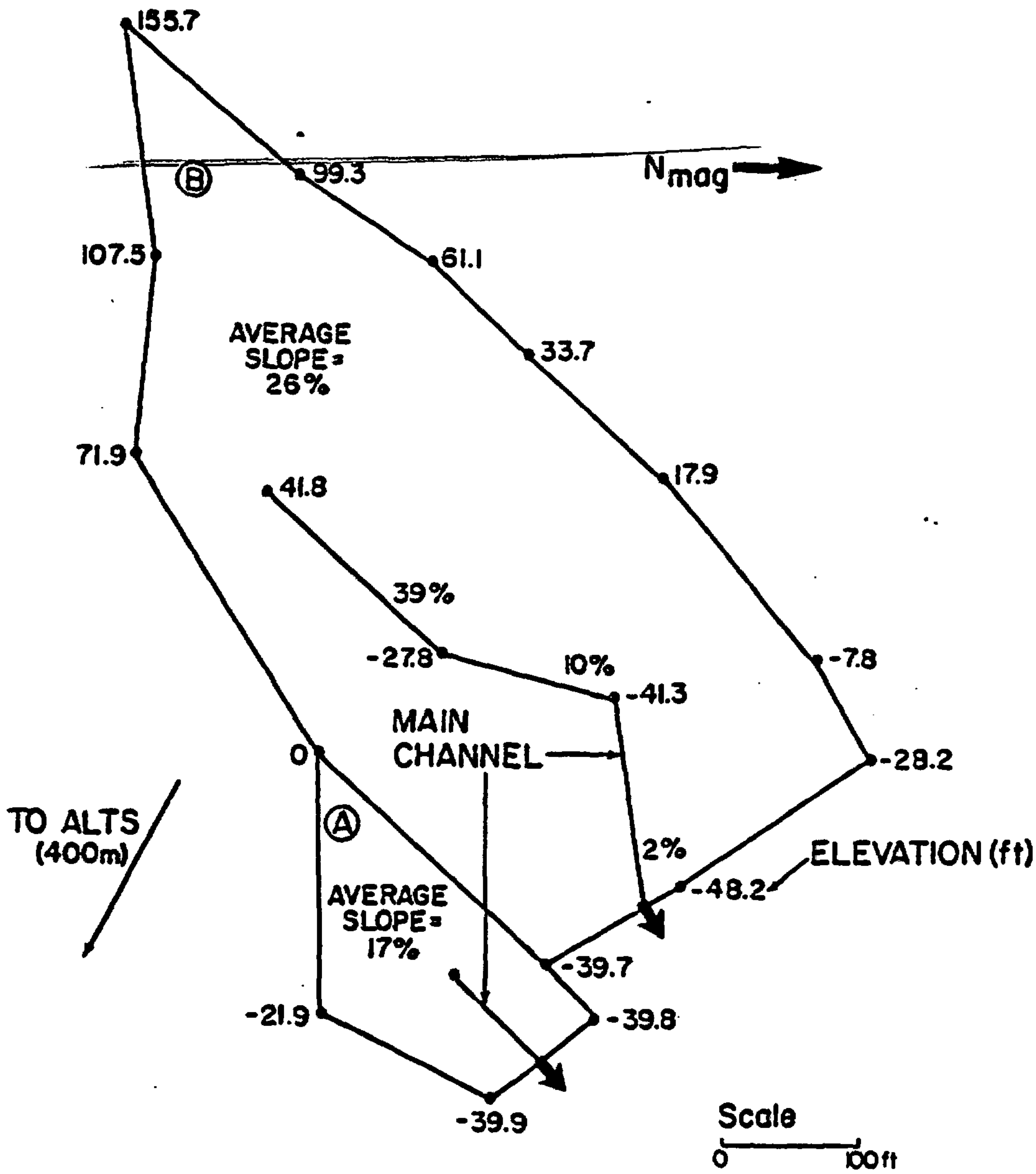


Figure 19: Plan view of two experimental watersheds showing location of runoff monitoring device and channel gradients.

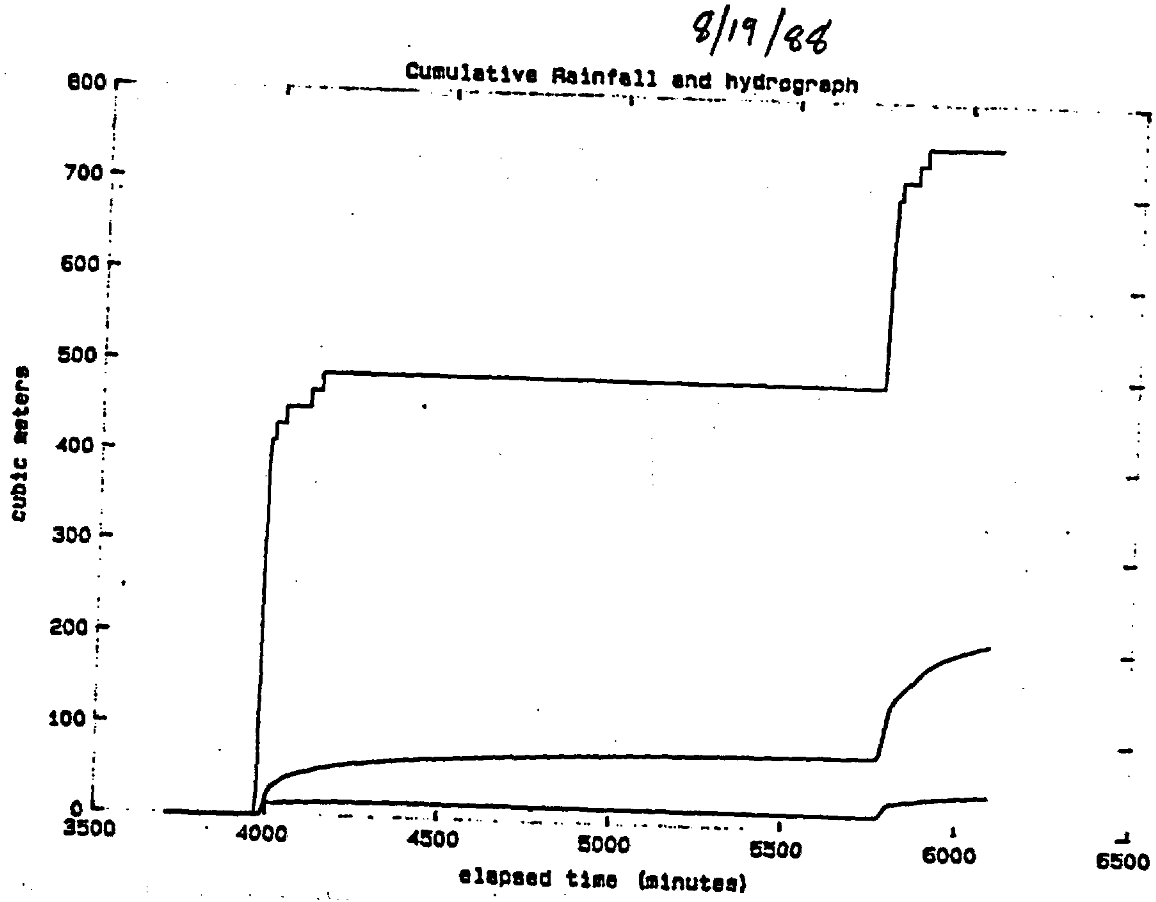


Figure 20: Runoff response of two watersheds (lower curves) to precipitation event (upper curve).

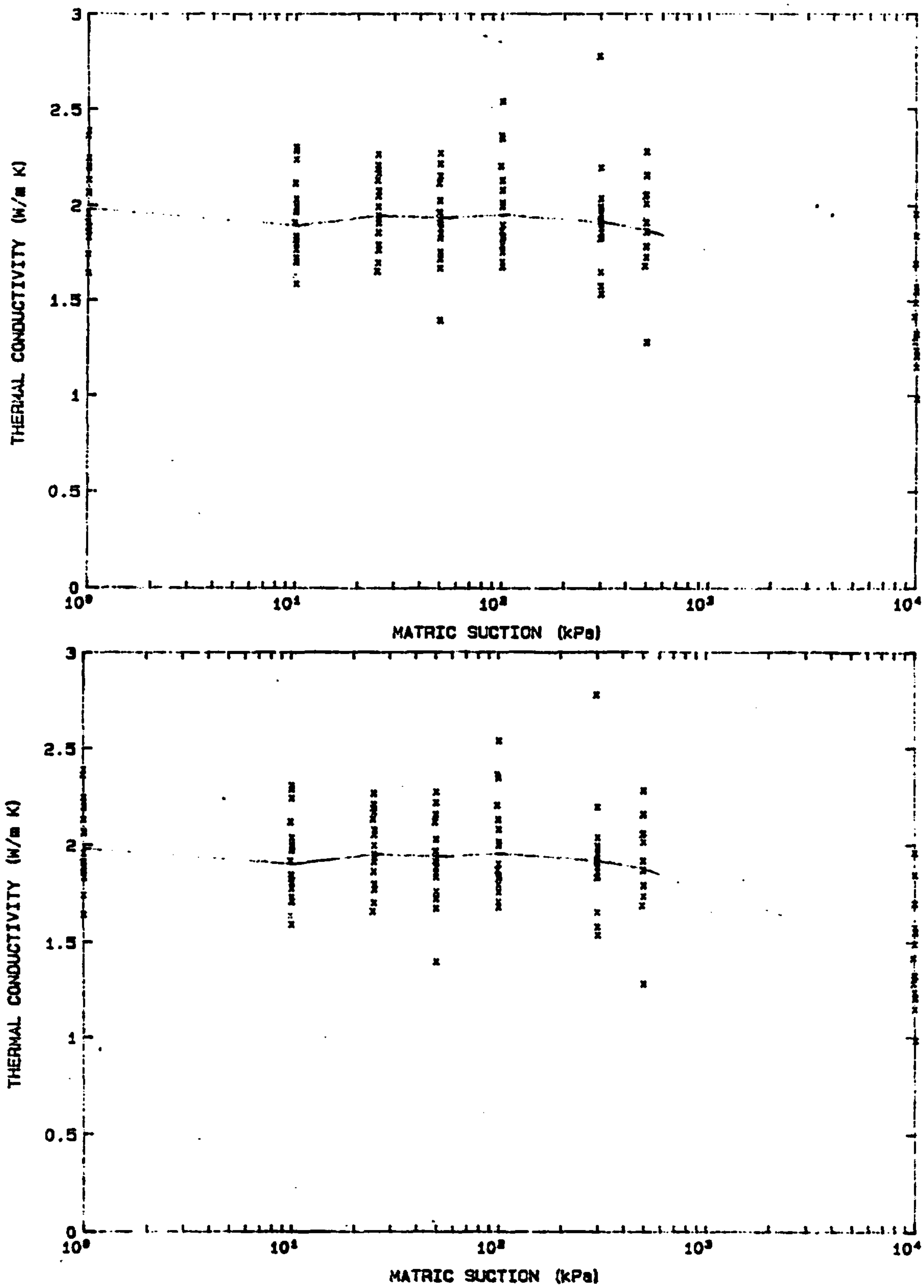


Figure 21: Thermal conductivity versus matric suction (above) and thermal diffusivity versus relative saturation (below) for large Apache Leap tuff core segments.

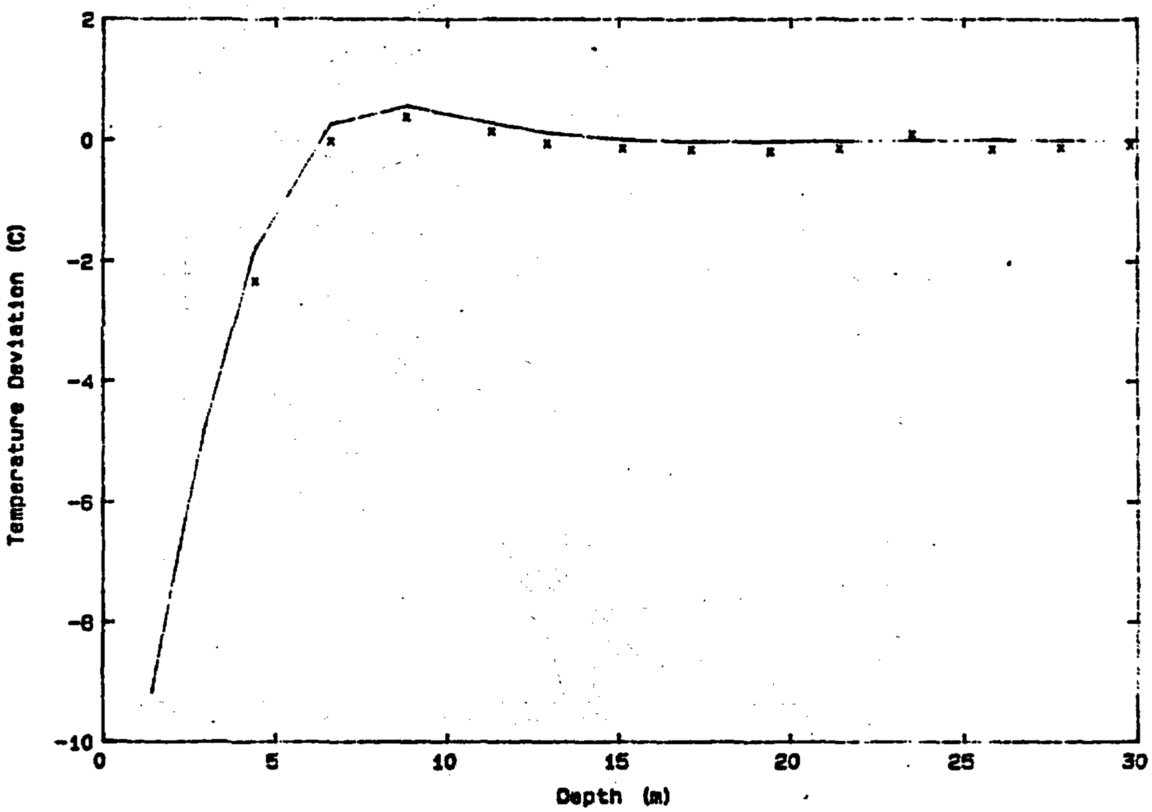


Figure 22: Observed and estimated thermal profile in a single borehole using laboratory estimate of thermal diffusivity.

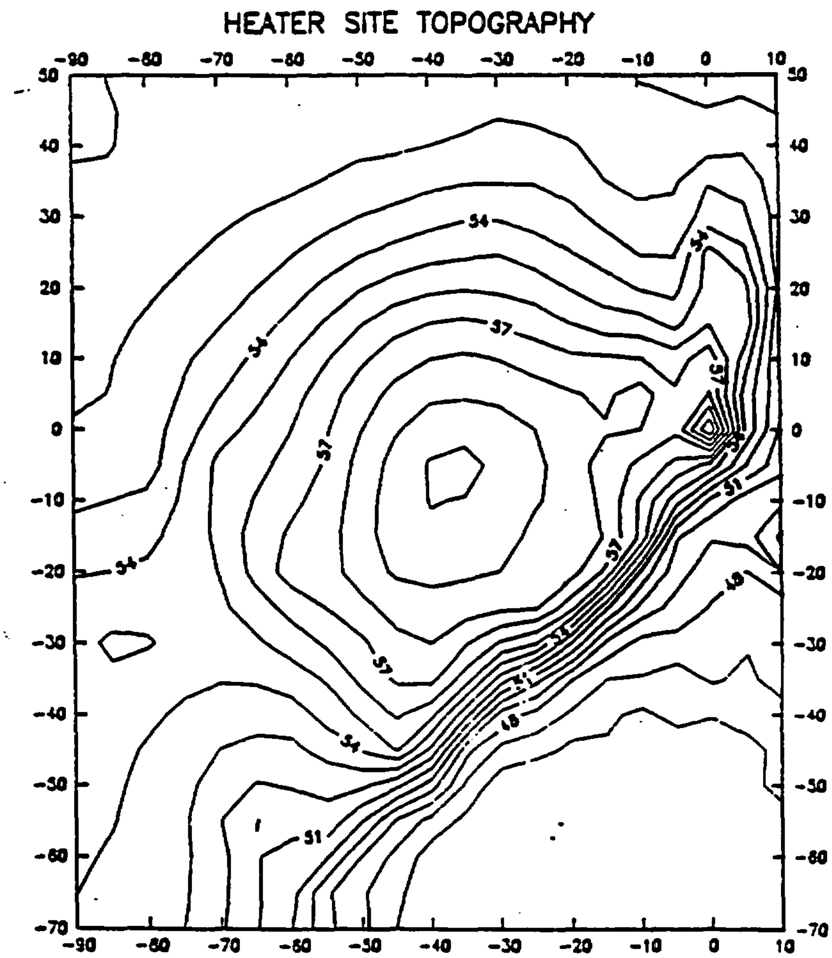


Figure 23: Topography of proposed field heater test site.

ABSTRACT

Numerical Simulation of Water Infiltration into an Unsaturated, Fractured Rock Mass

by E. M. Kwicklis and D. T. Hoxie
U. S. Geological Survey
Denver, Colorado

A preliminary investigation of the transient hydrologic interaction between variably saturated fractures and an adjacent rock matrix was conducted by numerically simulating the short-term infiltration of water ponded on the surface of an unsaturated, fractured rock mass. The model results indicated that water would readily infiltrate the fractures; would tend to be rapidly imbibed into the rock matrix adjacent to the fractures; and, subsequently, would be slowly redistributed within the rock mass. The geohydrologic setting considered consisted of a vertical, rectangular column of rock bounded laterally by vertically oriented fractures, each of which had an equivalent hydraulic aperture of 24 micrometers. The hydrologic properties of the rock matrix were assumed to be representative of a welded tuff, whereas those of the fractures were assumed to be analogous to a coarse sand. The initial saturation of the rock matrix was assumed to be 0.65, which corresponded to a pressure head of -11.0 meters in the matrix and an initial fracture saturation of 0.16.

In the first of three scenarios, a constant hydraulic head of +0.2 meter was imposed uniformly over the top of the fracture-bounded rock column

for 1 hour. Results indicated that although little water would infiltrate directly into the rock matrix across the upper boundary, the fractures would become saturated to a depth of about 0.5 meter. In the second scenario, the hydraulic head at the upper boundary was increased to +20.0 meters and was imposed for 1 hour. Again, results showed that little water would infiltrate directly into the rock matrix across the upper boundary; however, the depth of water penetration within the fractures would increase to 2.1 meters. After this second period of infiltration, recovery of the system was simulated. Results indicated that the fractures would desaturate, and that within 10 hours, the maximum fracture saturation would be near the value of residual saturation assumed for the fracture; after 24 hours, the maximum matrix saturation within a 0.1-millimeter distance from a fracture wall would decrease from 1.0 to 0.85 as a result of lateral movement of water further into the rock matrix. Complete re-equilibration of the entire rock-matrix block would require several weeks. Results from a third scenario showed that the depth of water penetration within the fractures was predicted to increase to 55 meters if the equivalent hydraulic aperture was assumed to be 250 micrometers and a hydraulic head of +0.2 meter was applied at the upper boundary for 30 minutes. Thus, the degree to which fractures become significant conduits for the transient movement of water within unsaturated rocks depends significantly on the effective fracture aperture.

NUMERICAL SIMULATION OF LIQUID-WATER INFILTRATION INTO AN UNSATURATED, FRACTURED ROCK MASS

E. M. Kwicklis

and

D.T. Hoxie

U. S. Geological Survey
Denver, Colorado

PURPOSE

1. To gain experience and insight into the methodology and pitfalls of simulating small-scale phenomena such as coupled flow of liquid water into and out of discrete fractures and enclosing matrix.

2. To test the applicability of different numerical simulators to solve such problems

- VS2D FD, Newton linearization
- VSFAST Galerkin FEM, Newton linearization
- UNSAT2 Galerkin FEM, Picard iteration
- TOUGH IFD, Newton linearization

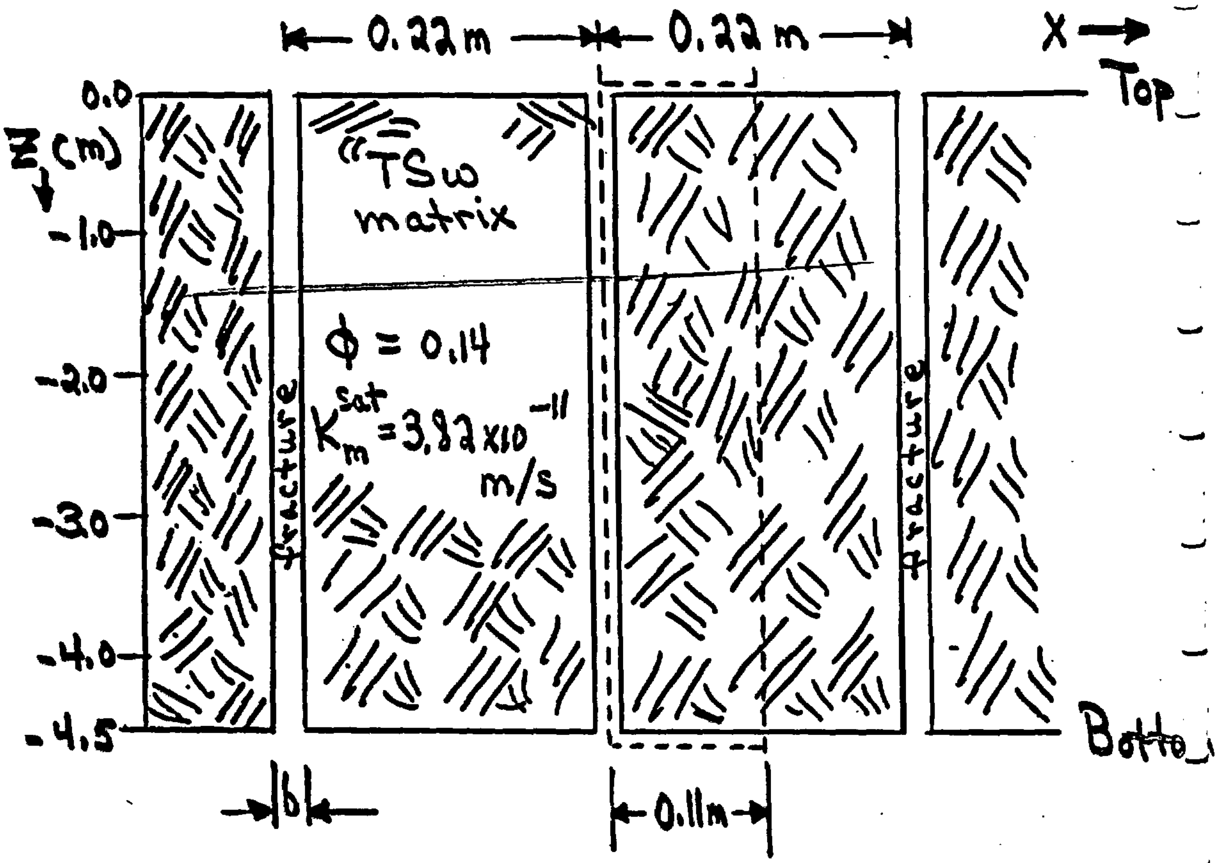
3

3. Specifically examine
   - stability
   - convergence
   - accuracy (truncation error)

4. Examine methods for calculating interface conductivities and mobilities
   - linear mean
   - harmonic mean
   - geometric mean
   - full upstream weighting

5. Assess overall computational efficiency: Does CPU time = accelerator time ?!

PHYSICAL MODEL



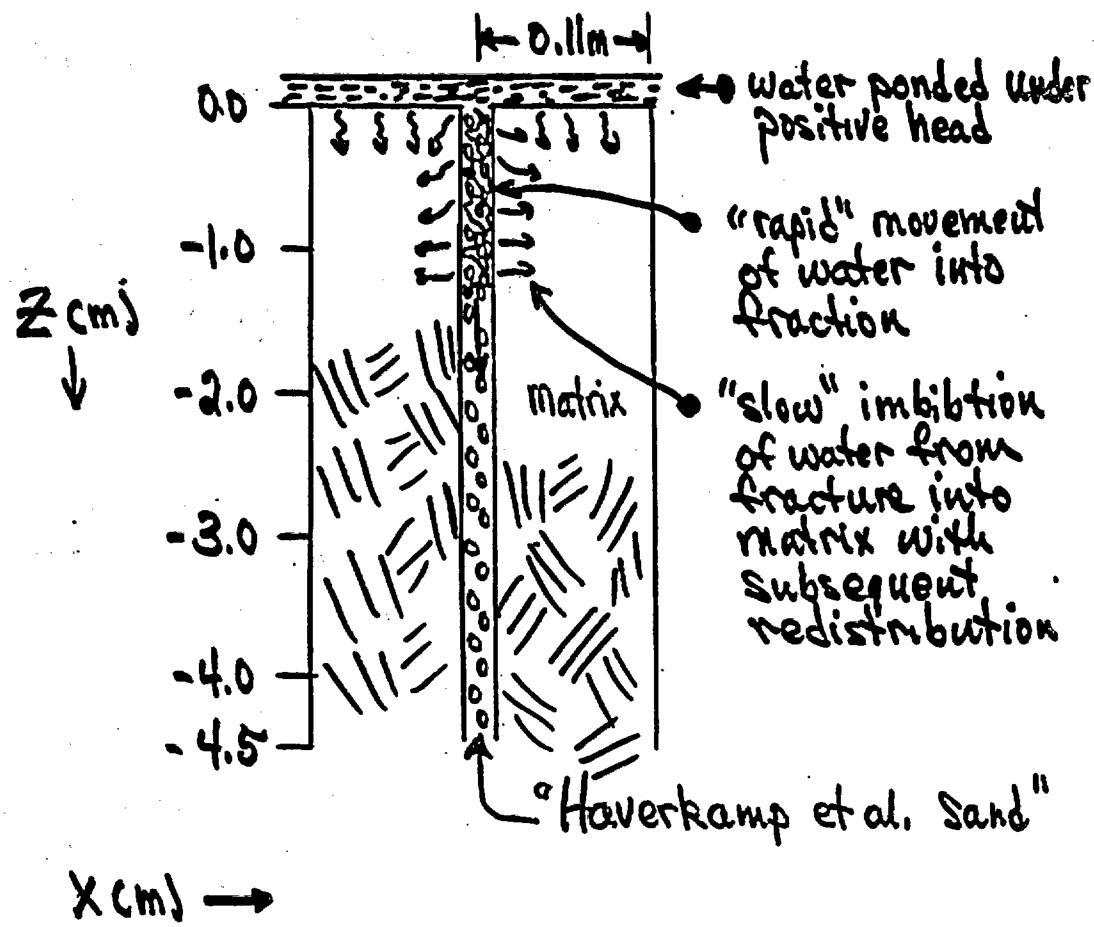
Fracture properties

- aperture $24\,\mu m \le b \le 250\,\mu m$
- $K_f^{sat} = \frac{b^2}{12} \frac{\rho_w g}{\mu_w}$
- $\phi_f = 1.0$

5

CONCEPTUAL MODEL

- Two Hydogeologic Units
  1. "Tuff" rock matrix
  2. Discrete fracture: $b = 24\mu m$
- Isothermal
- Passive gas phase



6

FLOW EQUATION

A. Derivation

1. Conservation of fluid mass within volume element V

2. Equation of motion: Darcy-Buckingham law

B. Result

$$V\left\{\rho_w\left[\frac{d\theta}{d\psi_w}+S_w S_s\right]\right\}\frac{\partial h}{\partial t}=\rho_w\sum_{k=1}^{m}A_k K^{sat}k_r(\psi_w)\frac{\partial h}{\partial n_k}$$

1. $h = \psi_w - z$ (L)
2. $\theta(\psi_w) = \phi S_w(\psi_w)$
3. $k_r = k_r(\psi_w)$
4. A_k = area of k^{th} face of ∂V
5. $\frac{\partial h}{\partial n_k}$ = outward normal gradient of h across face A_k of ∂V

7

PROBLEM DATA

A. Rectangular (finite-difference) grid with variable grid spacing in both z and x directions

1. "fine" spacing $\Delta z = 0.01\,m$
2. "course" spacing $\Delta z = 0.05\,m$

B. Material properties

1. $\phi_m = 0.14$ $\phi_f = 1.0$
2. Specific storage $S_s = \rho g (\phi \beta + \alpha)$
3. Moisture characteristic curves
   a. matrix: van Genuchten representation for TSw from Rulon et al. (1986)
   b. fracture: van Genuchten representation for Haverkamp et al. (1976) sand

8

C. Initial conditions: $t = 0$

1. $\psi_w^{matrix} = \psi_w^{frac} = -11.0$ m
2. $S_w^{matrix} = 0.65$

   $S_w^{frac} = S_r^{frac} = 0.159$

D. Boundary conditions: $z = 0$ m

Two cases:

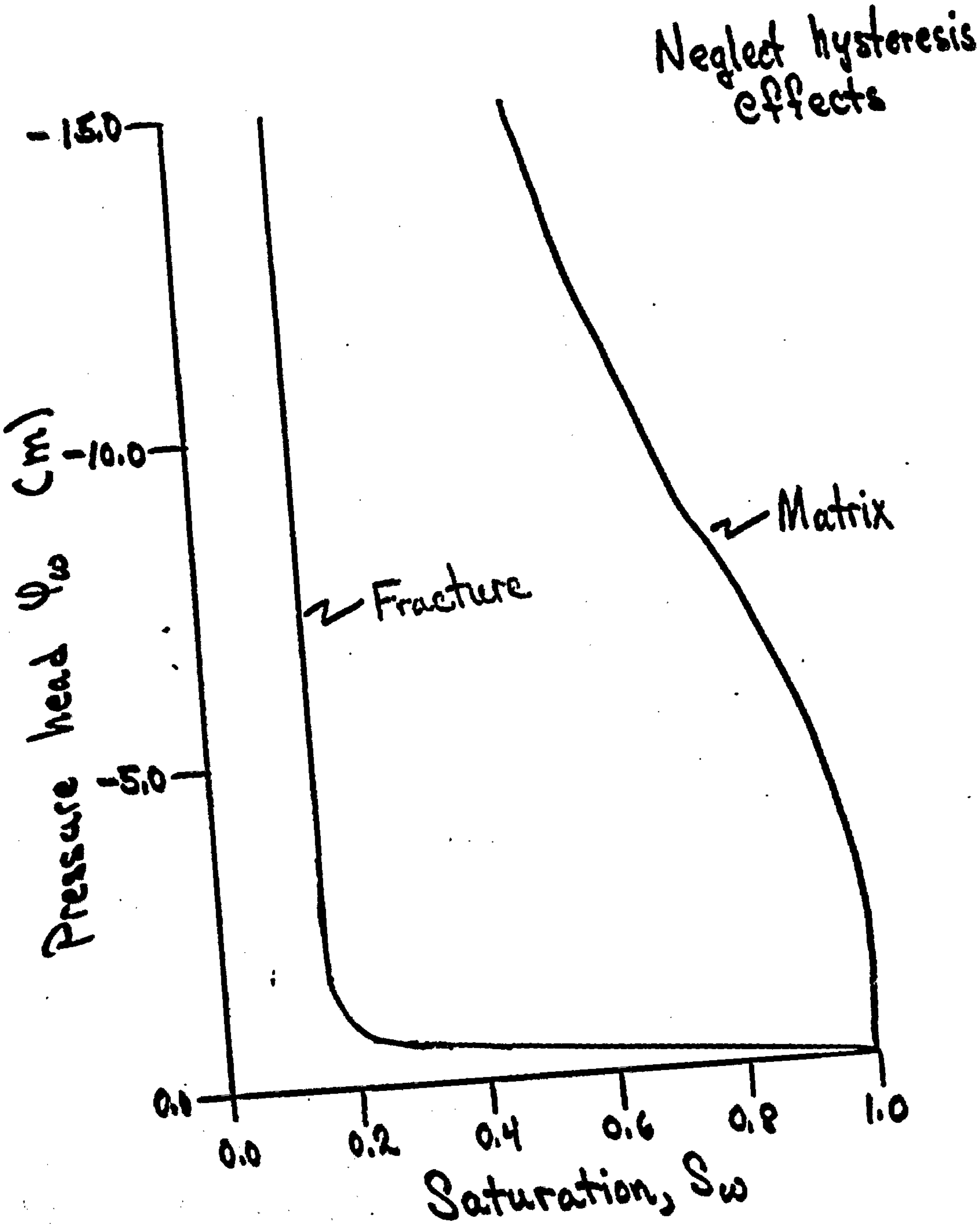
1. $\psi_w = +0.2$m $z = 0$ $0 < t \leq 60$ min
2. $\psi_w = +20.0$m $z = 0$ $0 < t \leq 60$ min

E. Fracture aperture

1. $b = 24\ \mu m$
2. $b = 250\ \mu m$

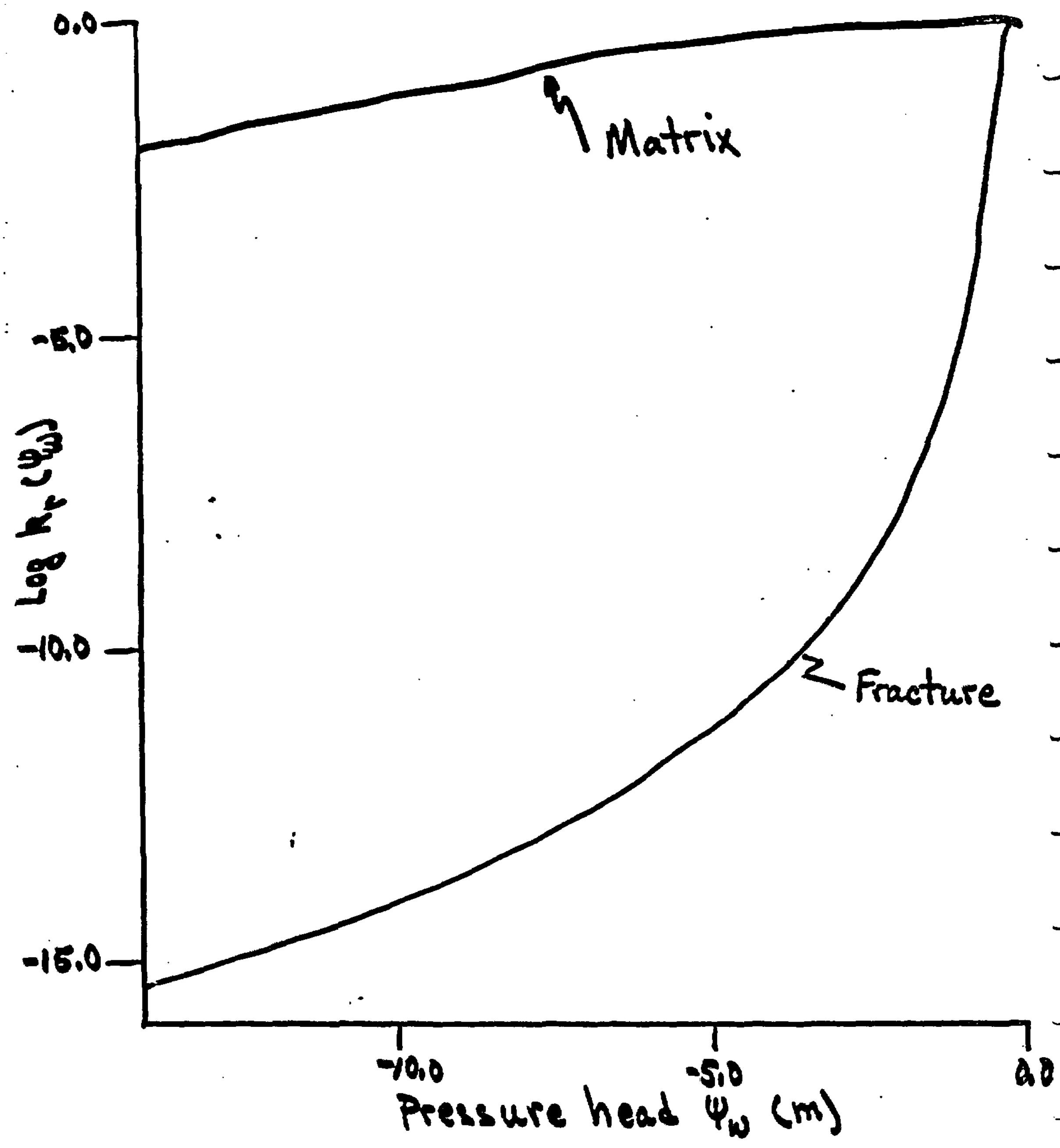
9

MOISTURE-RETENTION CURVES



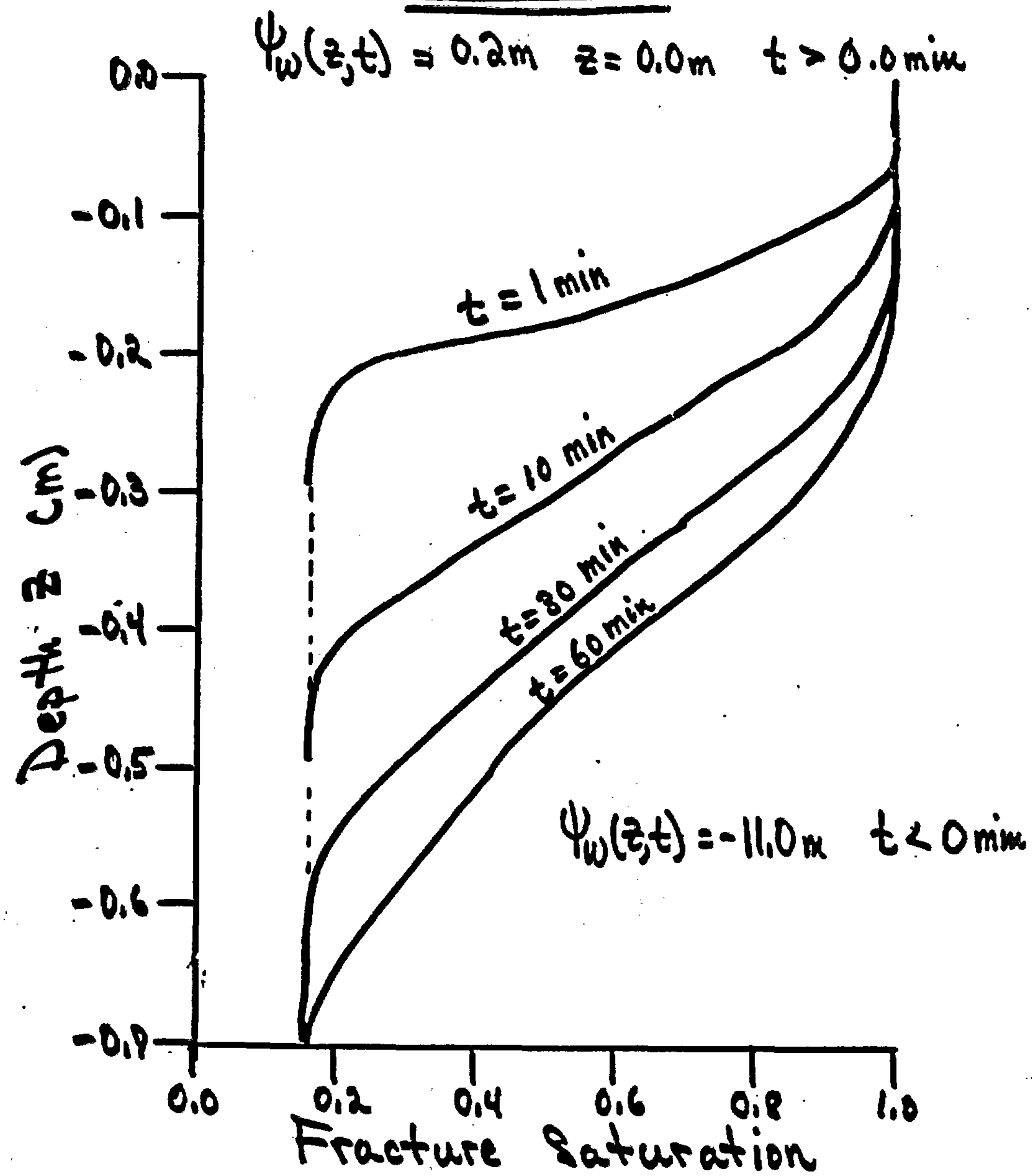
10

Log $k_r(\psi_w)$ vs ψ_w



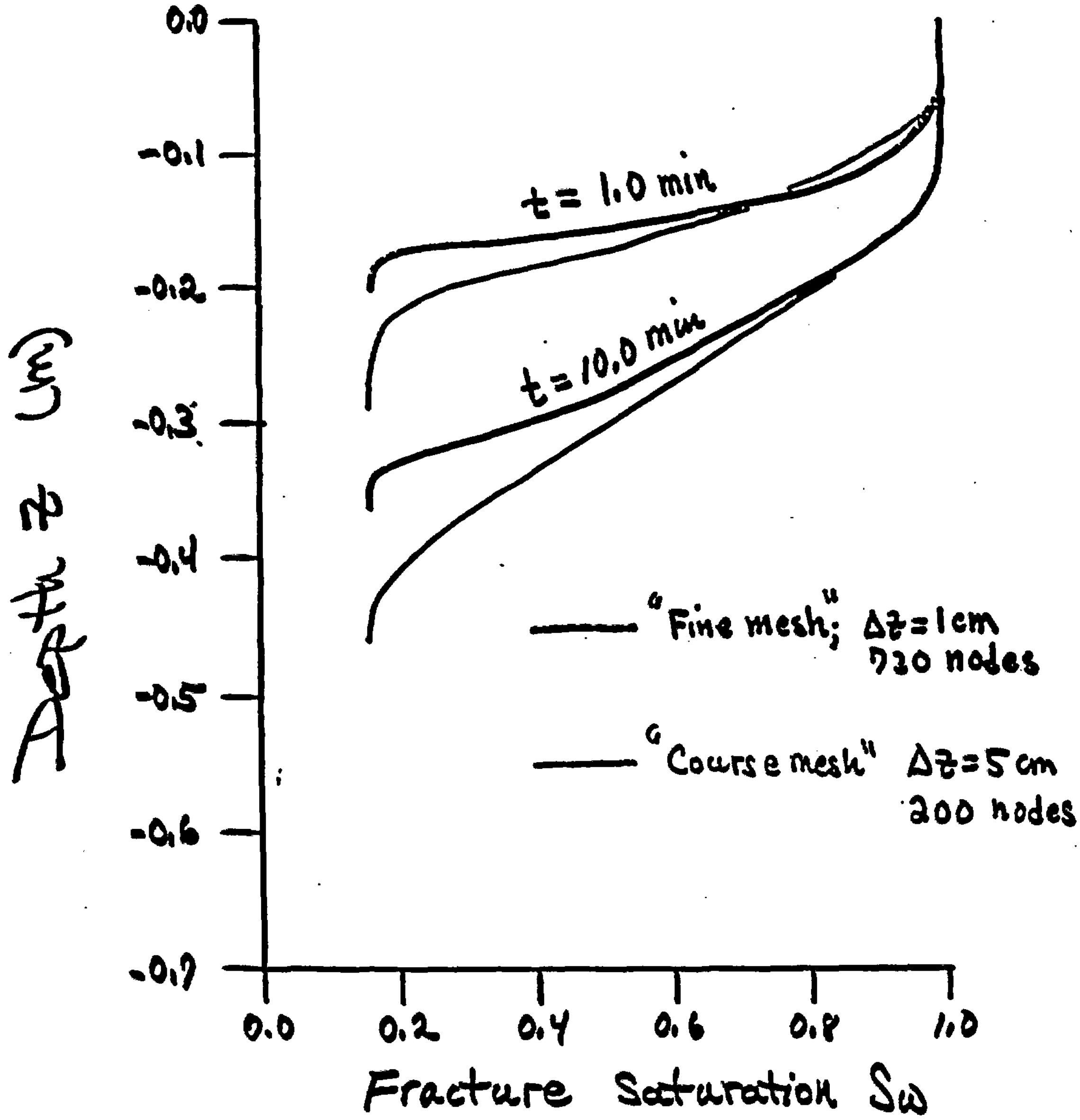
11 FRACTURE SATURATION PROFILES: VERTICAL INFILTRATION*

b = 24 μm



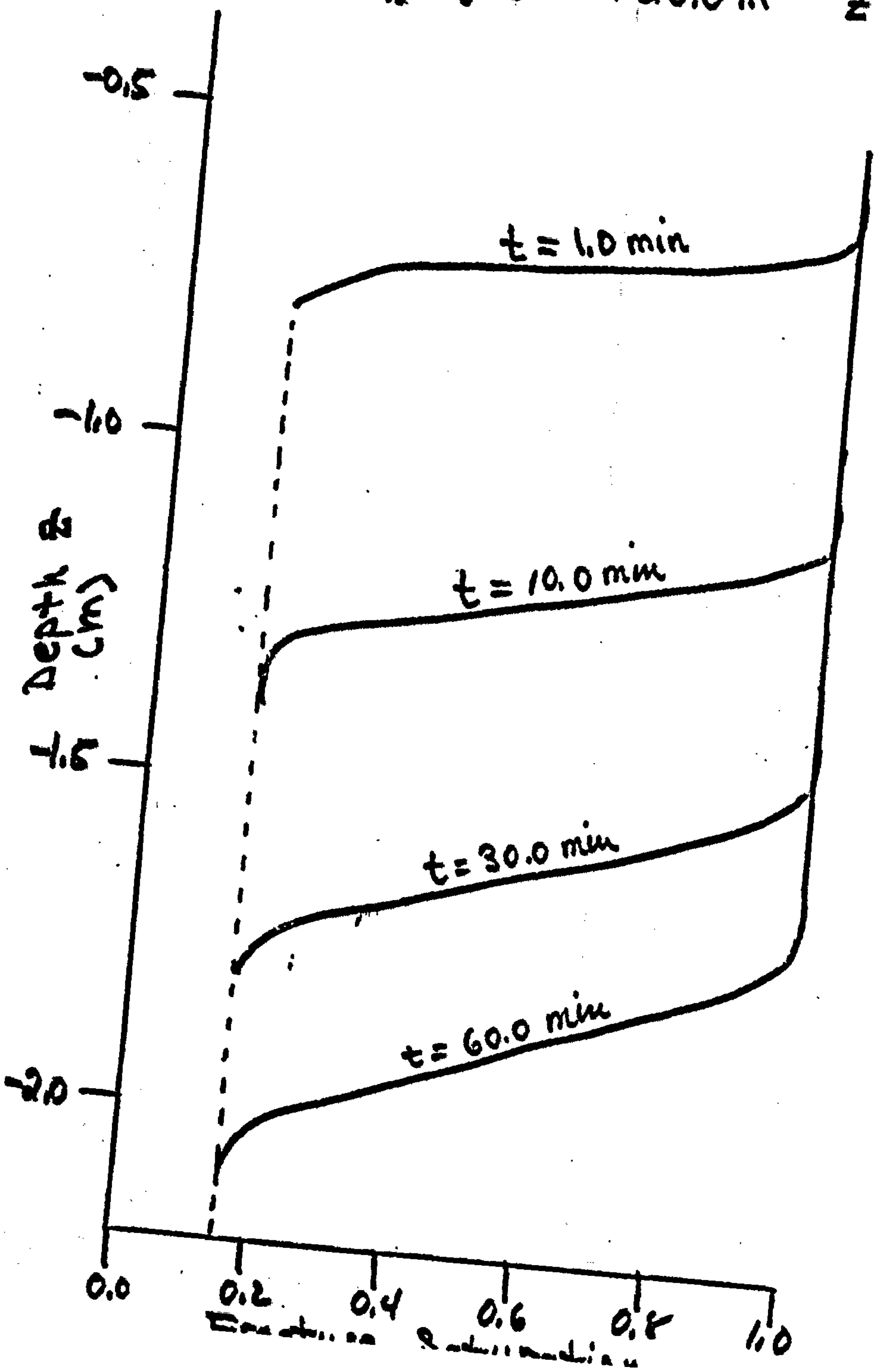
*All results shown were obtained with FD computer code VS2D.

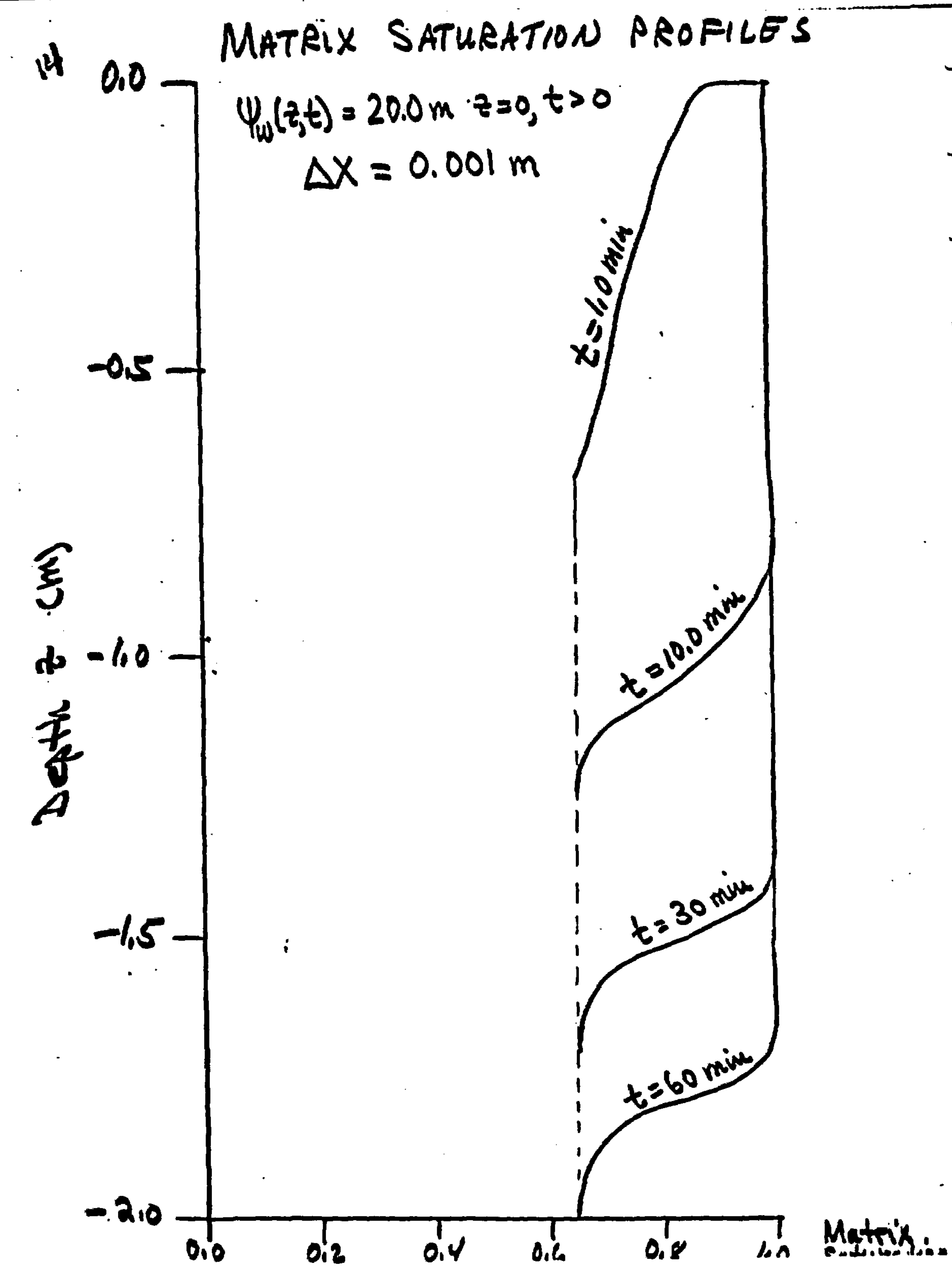
12 SOLUTION SENSITIVITY WITH RESPECT TO VERTICAL MESH SPACING Δz



13 FRACTURE SATURATION PROFILES

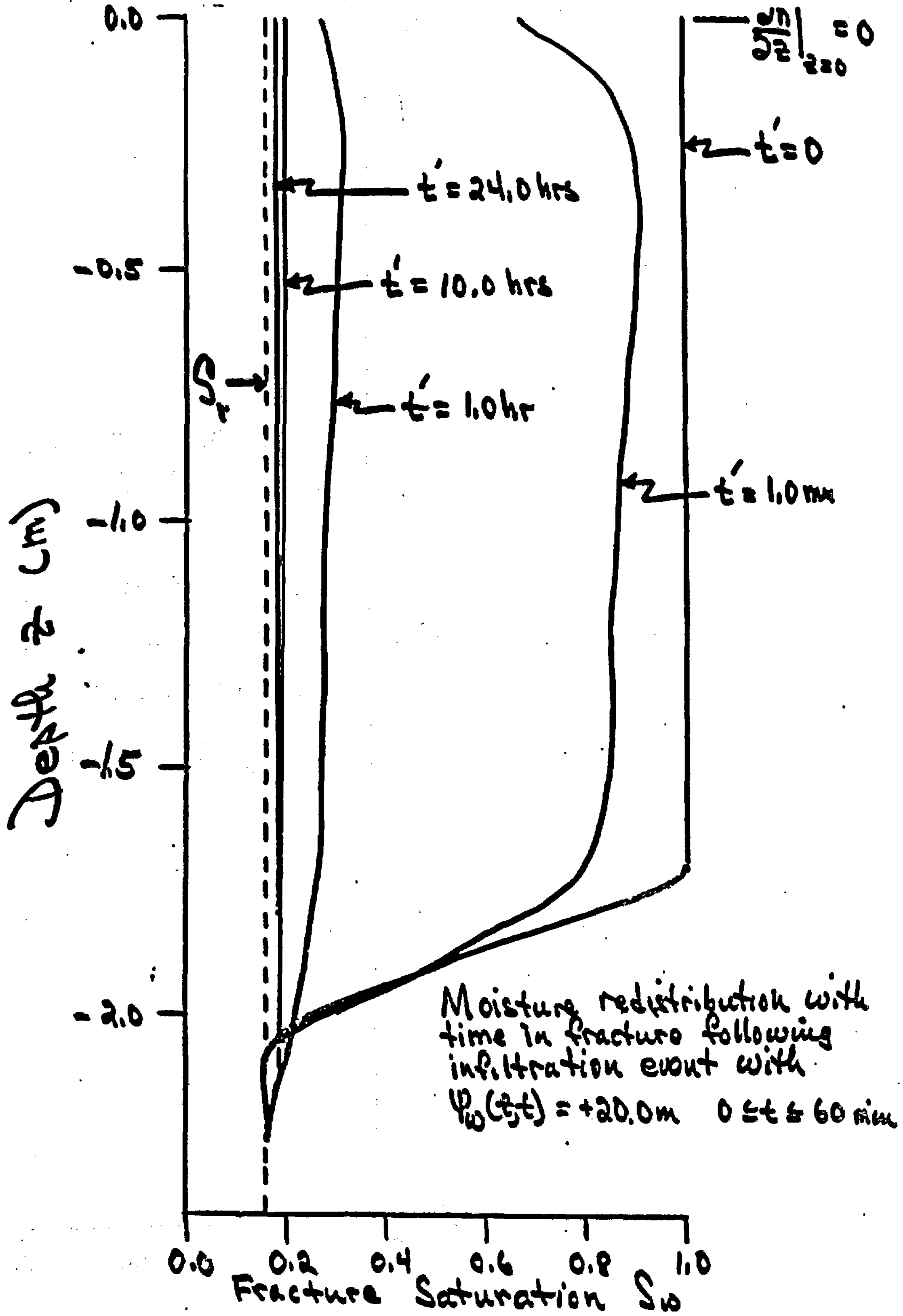
$\psi_w(z,t) = +20.0$ m $z=0,\ t>0$





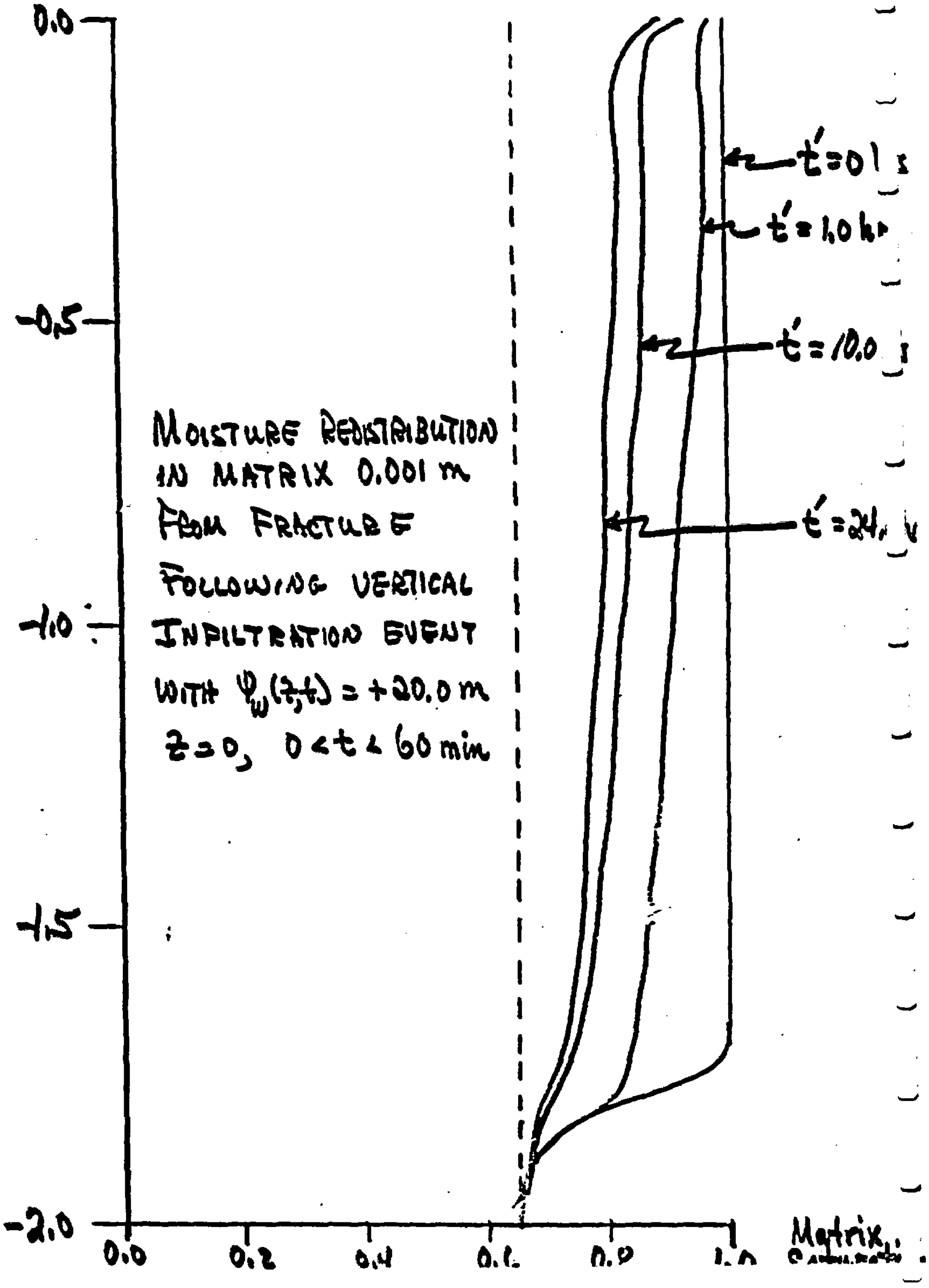
MATRIX SATURATION PROFILES
14
$\Psi_w(z,t) = 20.0$ m $z=0, t>0$
$\Delta X = 0.001$ m
$t=1.0$ min
$t=10.0$ min
$t=30$ min
$t=60$ min
0.0
-0.5
-1.0
-1.5
-2.0
Depth (m)
0.0
0.2
0.4
0.6
0.8
1.0
Matrix

15



0.0
-0.5
-1.0
-1.5
-2.0
Depth (m)
$\left.\frac{\partial n}{\partial z}\right|_{z=0} = 0$
t' = 0
t' = 24.0 hrs
t' = 10.0 hrs
S_r
t' = 1.0 hr
t' = 1.0 min
Moisture redistribution with time in fracture following infiltration event with
$\psi_w(z,t) = +20.0$ m $0 \le t \le 60$ min
0.0
0.2
0.4
0.6
0.8
1.0
Fracture Saturation S_w

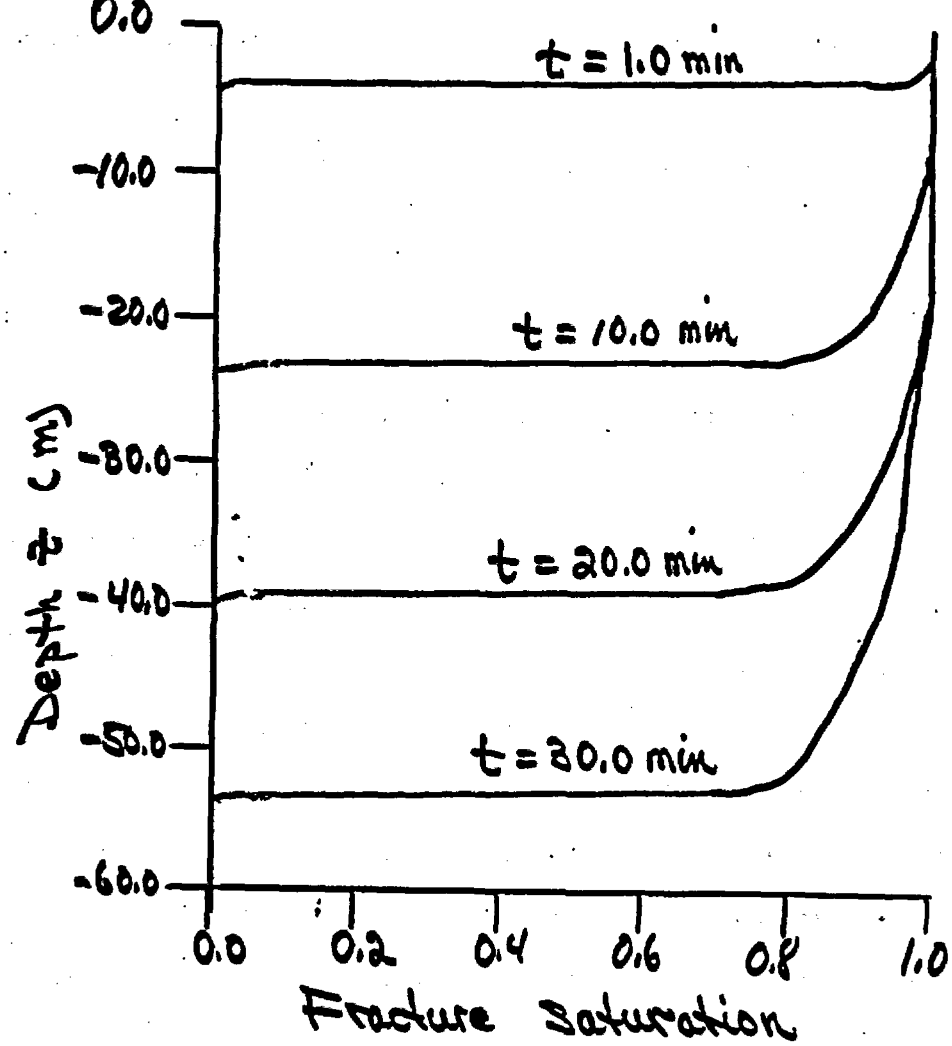
16



0.0
-0.5
-1.0
-1.5
-2.0
0.0
0.2
0.4
0.6
0.8
1.0
Matrix
t′=0.1
t′=1.0 hr
t′=10.0
t′=24.
MOISTURE REDISTRIBUTION IN MATRIX 0.001 m FROM FRACTURE FOLLOWING VERTICAL INFILTRATION EVENT WITH $\Psi_w(z,t) = +20.0$ m
$z=0$, $0<t<60$ min

17

SATURATION PROFILES IN A FRACTURE
WITH $b = 250\,\mu m$
$\psi_w(z,t) = 0.2\,m \quad z = 0 \quad t > 0$



Numerical Simulations to Aid in the Design and Interpretation of Percolation Tests in the Proposed Exploratory Shaft Facility, Yucca Mountain, Nevada

by Edward M. Kwicklis, Hydrologist, U. S. Geological Survey, Denver, Colorado

ABSTRACT

In order to help assess the potential of the proposed host rock at Yucca Mountain, Nevada, to isolate high-level nuclear waste, the U. S. Geological Survey plans to conduct various hydraulic and pneumatic tests. One of these tests presently planned for the Exploratory Shaft Facility is the Percolation Test.

The Percolation Test will provide information concerning: (1) The conditions under which flow in fractures predominates, rather than flow in the matrix; (2) the degree of hydraulic connection between the fracture and matrix-pore domains; and (3) the relation between effective bulk-rock properties (such as conductivity, moisture content or dispersivity) and bulk-rock matric potential.

Several objectives of the proposed test require that steady flow of water be established within a volume of fractured, welded tuff for a range of bulk-rock matric potentials and moisture contents. However, due to the extremely low hydraulic conductivity of the welded-tuff matrix, steady-state flow conditions may be difficult to achieve within a reasonable time, especially when flow is predominantly through the matrix. Numerical simulations indicate that it is more feasible to first establish steady flow for wet or near-saturated conditions, under which flow in fractures predominates, and then to

re-establish steady flow at incrementally increasing matric suctions, until the fracture system is effectively drained.

Several of these simulations depicted the pattern of wetting in a 1 cubic-meter volume of welded tuff that contained four vertical, parallel fractures, each with an equivalent hydraulic aperture of 250 micrometers, that are spaced 25 centimeters apart. Infiltration of water into the block was assumed to take place either by ponding water above a clay layer placed on the block surface, by maintaining a constant tension in ceramic plates that were hydraulically connected to the rock surface, or by sprinkling water onto a sand bed placed above the block surface. For each infiltration mechanism, the initial applied boundary condition was chosen such that substantial flow in fractures resulted, and the adjacent matrix blocks were wetted with water imbibed from the fractures.

Simulations that used ceramic porous plates at the upper and lower boundaries of the block indicated that, at small applied matric suctions, significant pressure-head loss would occur across the thickness of the plate near large-aperture fractures. Hence, the matric potential within the rock mass may be different from the applied potential. The numerical results, thus, emphasized the need to monitor in situ tension. The inclusion of a permeable sand layer between the plates and the block would reduce head loss across the plates and, thus, minimize lateral variations in pressure head across the upper and lower block surfaces. The addition of the sand layers between the block and the plates also would result in narrower zones in which "end effects", or fracture-matrix matric potential disequilibrium, could be discerned.

Simulations of tracer transport through a block of fractured rock placed between two porous plates indicated that the shape of the breakthrough curve, as well as the percentage of tracer that would be irrecoverable for a test of 2-month duration, is a function of the effective matrix diffusivity. The effect of matrix diffusion on the breakthrough of the tracer would become more pronounced as the flux through the fracture network decreased, even when the overall flux through the rock remained fracture dominated. The percentage of the tracer that would be irrecoverable during the test period became larger as the flux through the fracture decreased.

The sprinkler-imposed, steady-flux method was determined to be an effective way to introduce water into a fractured, porous medium. Water can be removed from the rock mass by applying a suction to a ceramic porous plate that is hydraulically connected to the rock by the permeable sand layer. Simulation of water movement through a block containing two parallel fractures with hydraulic apertures of 25.0 and 250.0 micrometers demonstrated that, at certain fluxes and for certain, fixed, lower-boundary conditions, the spatial distribution of pressure heads would be quite complex, even in a homogeneous matrix.

Additional simulations were performed that treated a fractured rock mass as a composite porosity medium. Such an approach ignores the heterogeneity introduced by the presence of the fractures and considers the rock as a homogeneous material characterized by effective parameters. Using this approach, it was determined that unless the rock volume to be tested was isolated from the surrounding rock, lateral flow components could markedly delay the attainment of vertical steady-state flow conditions beneath the infiltration surface. However, even under these conditions, the test can be satisfactorily designed and interpreted.

Numerical Simulations to Aid in the Design and Interpretation of Percolation Tests in the Proposed Exploratory Shaft Facility, Yucca Mountain, Nevada

Edward M. Kwicklis

U. S. Geological Survey, Denver, CO

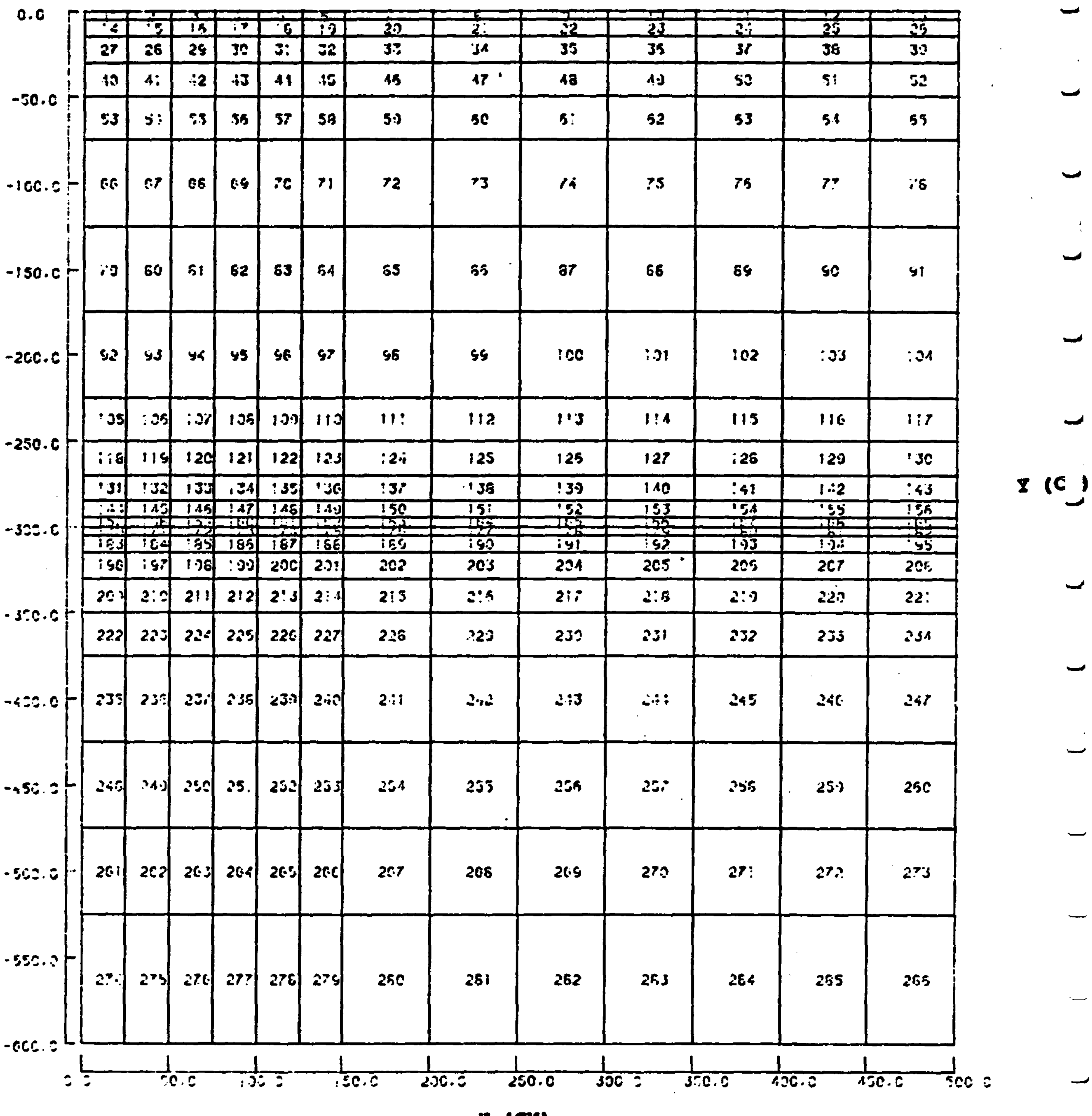
OBJECTIVES OF PERCOLATION TEST:

- Examine Conditions under which Flow in Fractures Predominates
- Investigate the degree of Hydraulic Connection Between the Fracture and Matrix–Pore Domains
- Explore the Relation Between Effective Bulk–Rock Properties and Bulk–Rock Matric Potential
- Model Validation

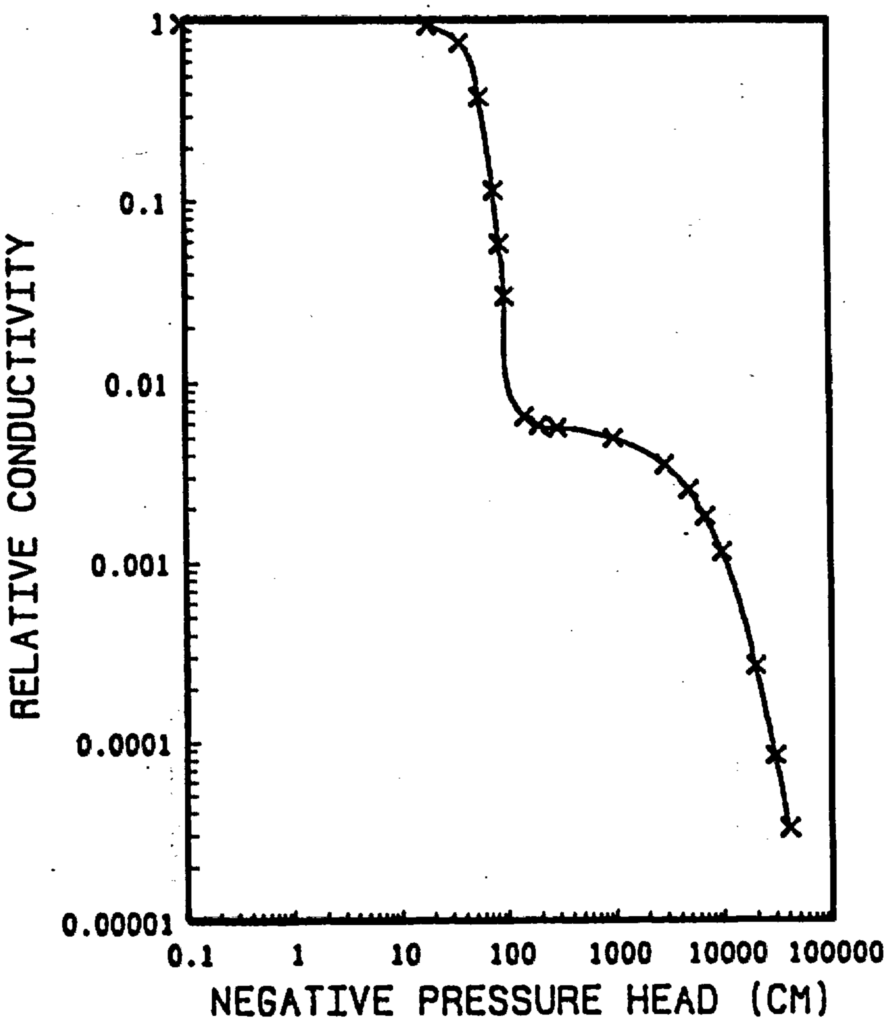
NUMERICAL SIMULATIONS EXAMINED

- Feasibility of Attaining Steady–State Flow
- Duration of Various Phases of the Percolation Test
- Various Infiltration Mechanisms
  - a) Crust–Imposed, Steady–Flux Method
  - b) Steady–State, Head Control Method
  - c) Sprinkler–Imposed, Steady–Flux Method
- Non–Vertical Flow Components
- Spatial Variation of Pressure Head Due to Presence of Fractures of Different Aperture

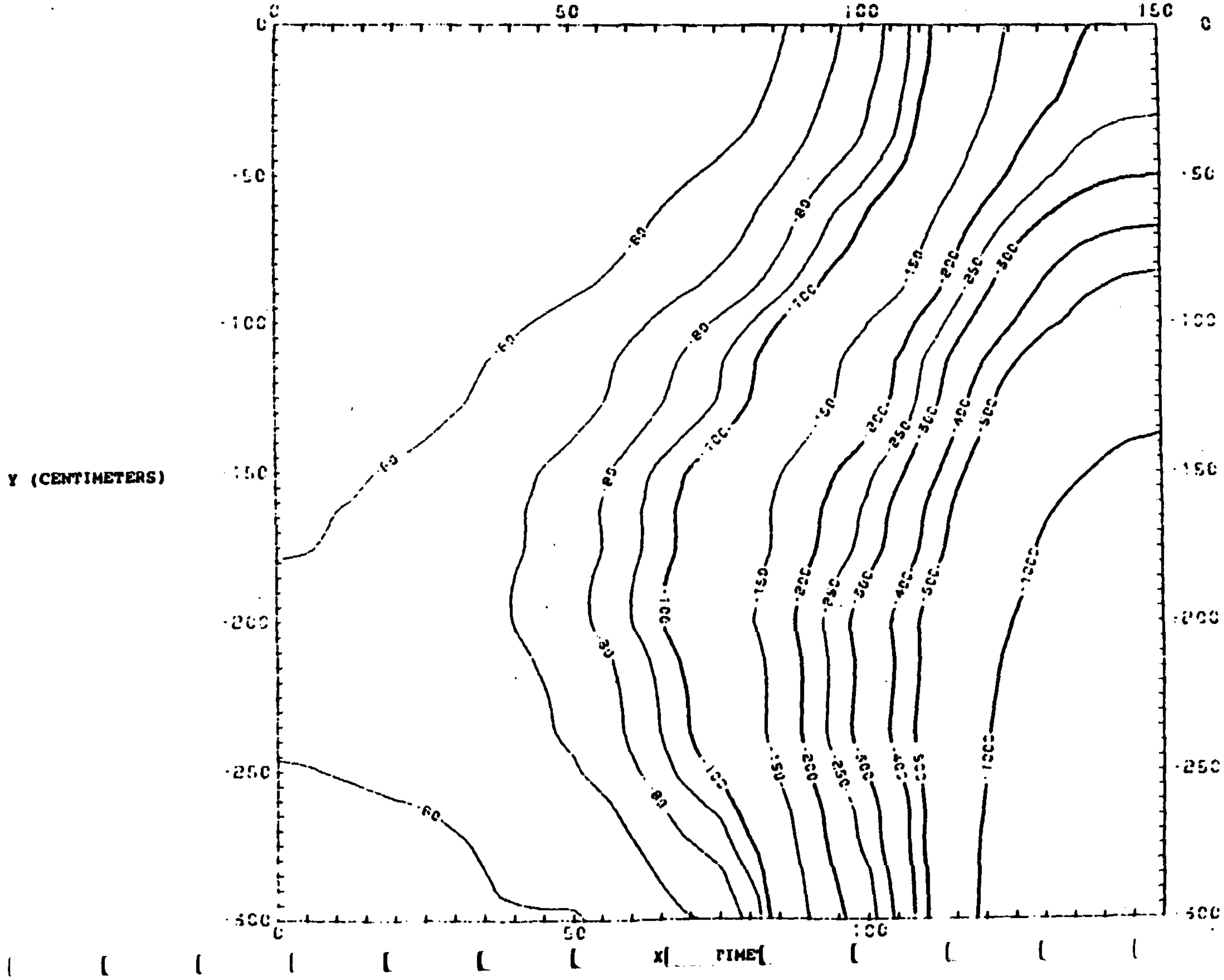
COMBINED M-F PERM CURVES. 3.0 M TEST SECTION. ASSESS NON-VERTICAL FLOW



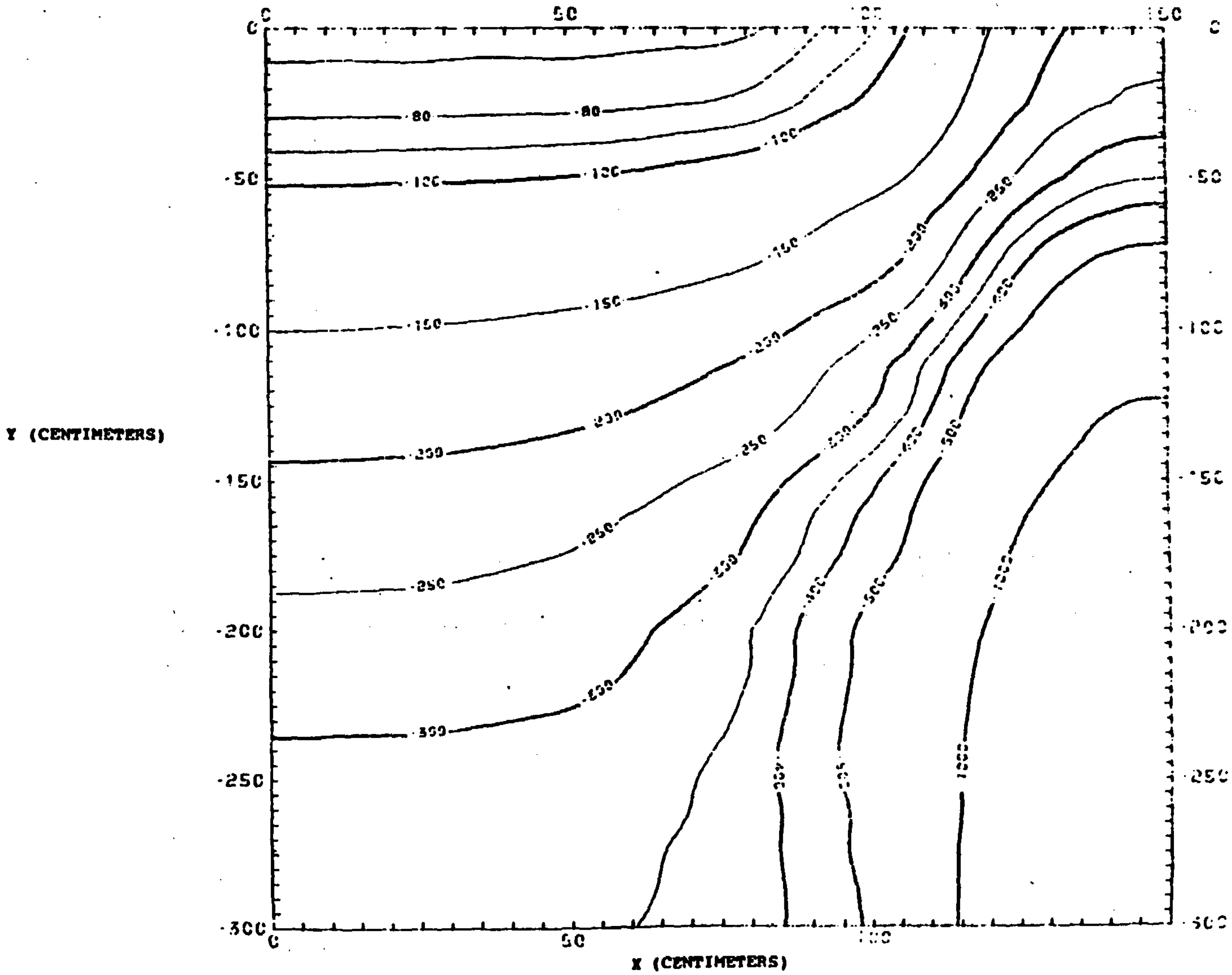
RELATIVE CONDUCTIVITY VERSUS PRESSURE HEAD
USED IN SIMULATIONS TO EXAMINE LATERAL FLOW



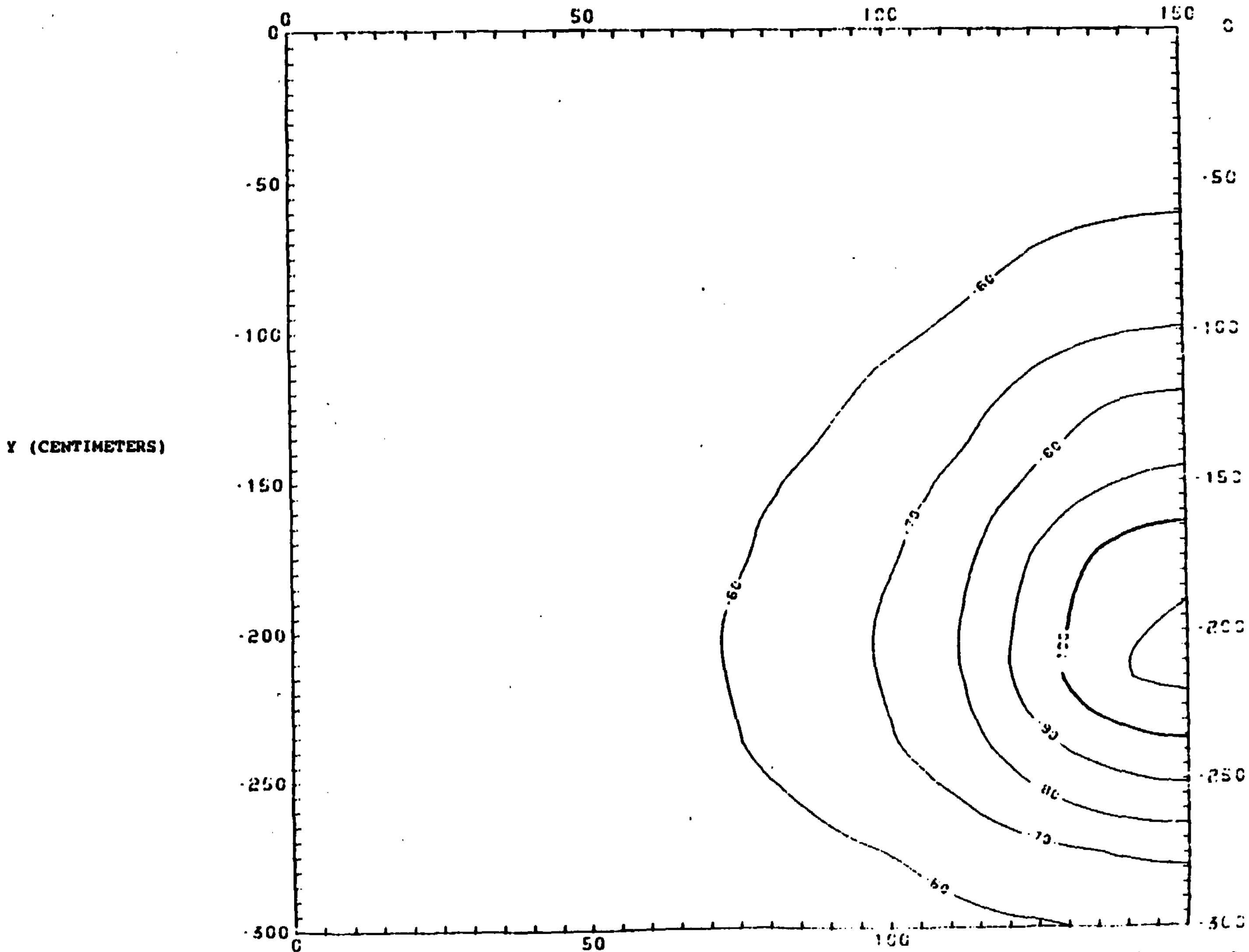
Pressure-head contours at the end of 3 years for the anisotropic case involving the 2-meter by 2-meter infiltration surface.



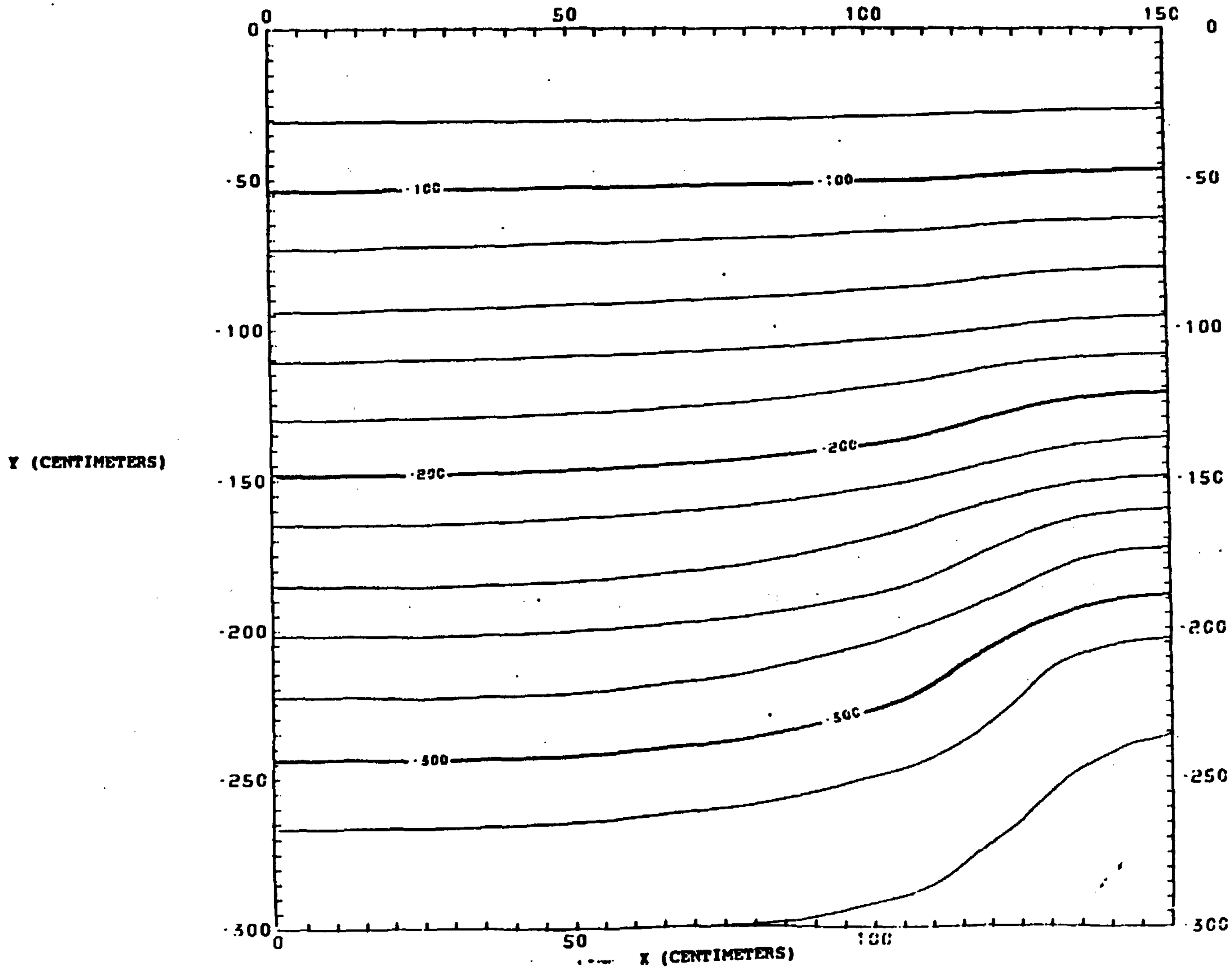
Total-head contours at the end of 3 years for the anisotropic case involving the 2 meter by 2 meter infiltration surface.



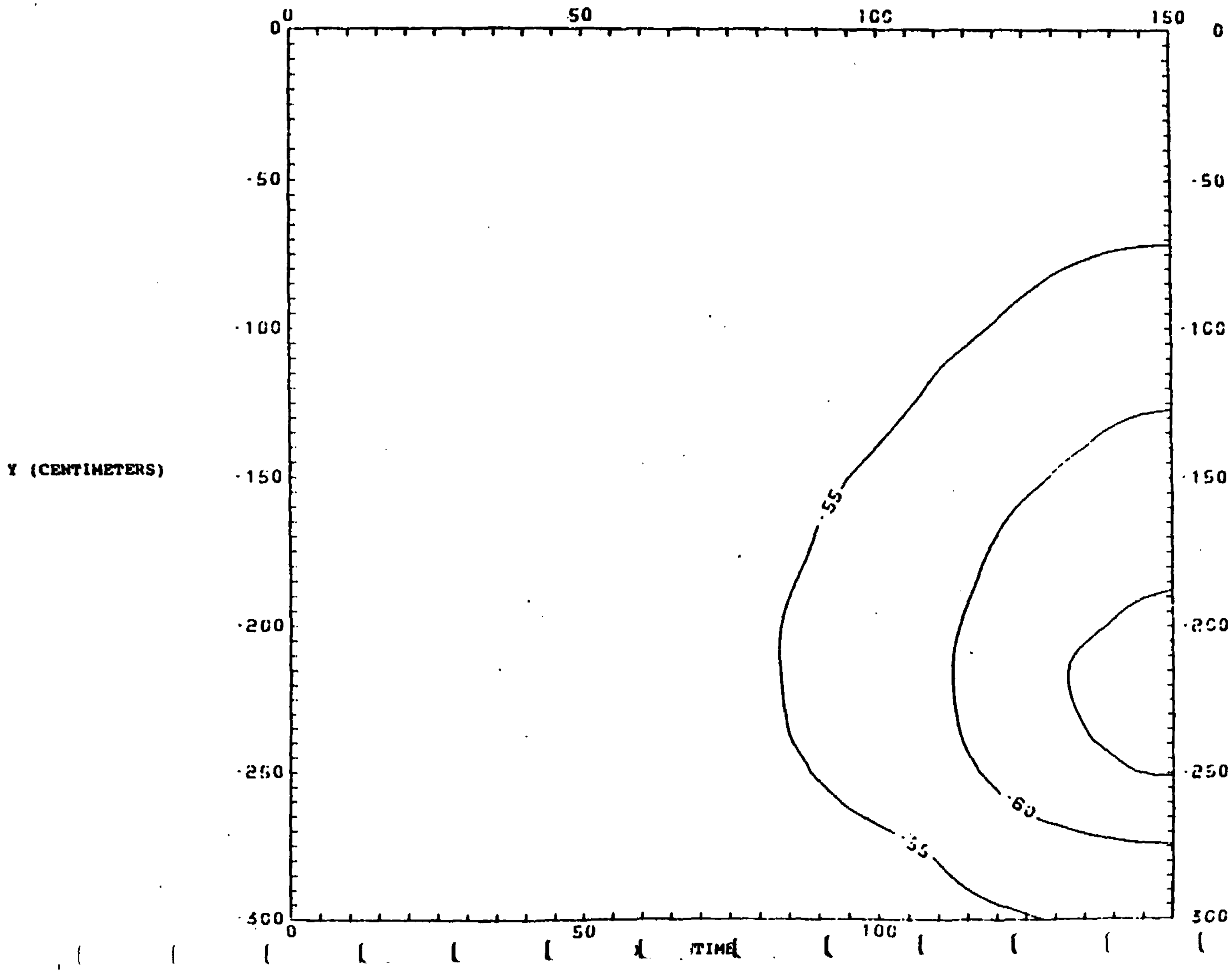
Pressure-head contours at the end of 1 year for the anisotropic case involving the 4-meter by 4 meter infiltration surface.



Total-head contours at the end of 1 year for the case involving the 4-meter by 4-meter infiltration surface.



Pressure-head contours at the end of 2 years for the anisotropic case involving the 4-meter by 4-meter infiltration surface.



Total-head contours at the end of 2 years for the anisotropic case involving the 4-meter by 4-meter infiltration surface.

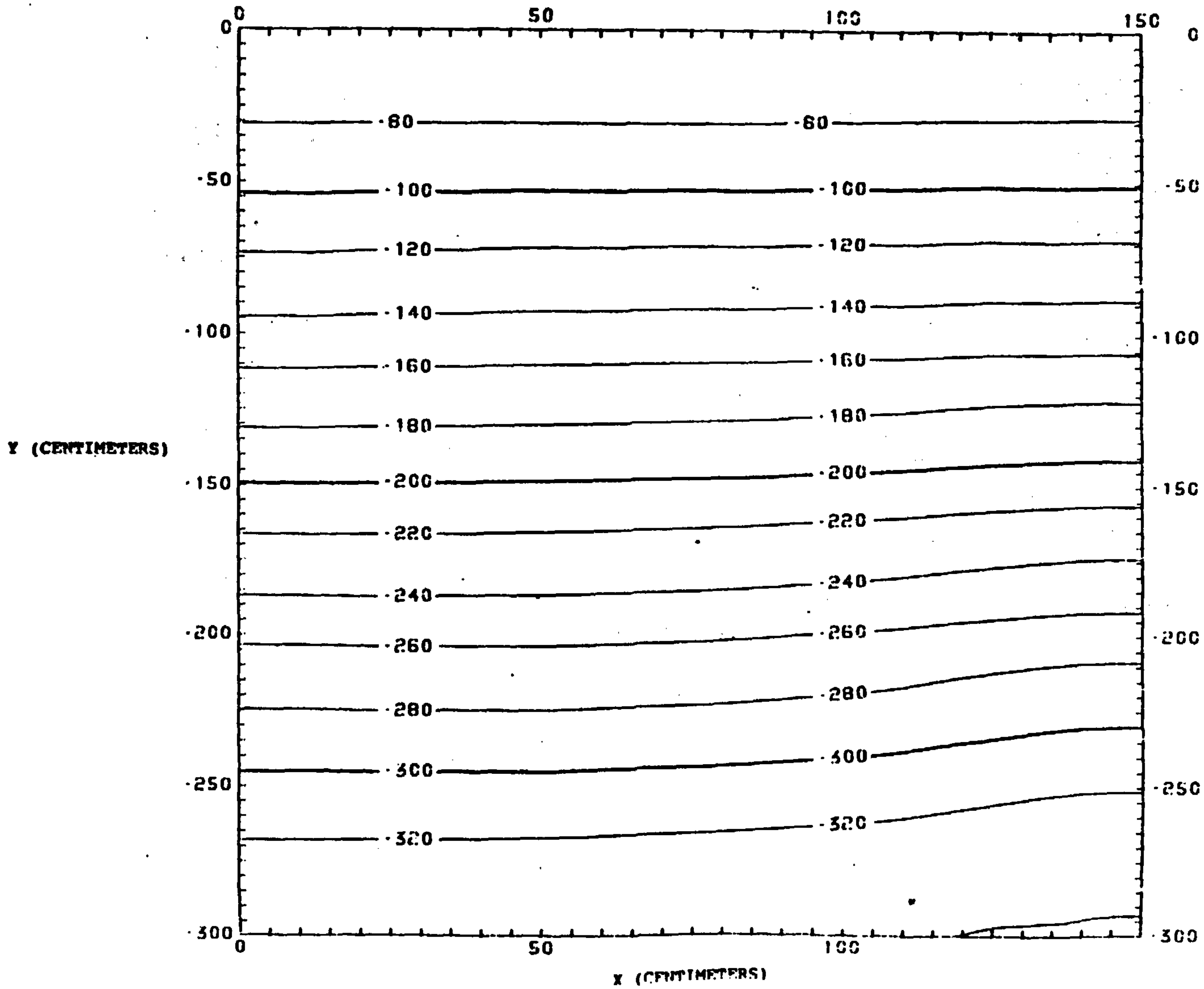
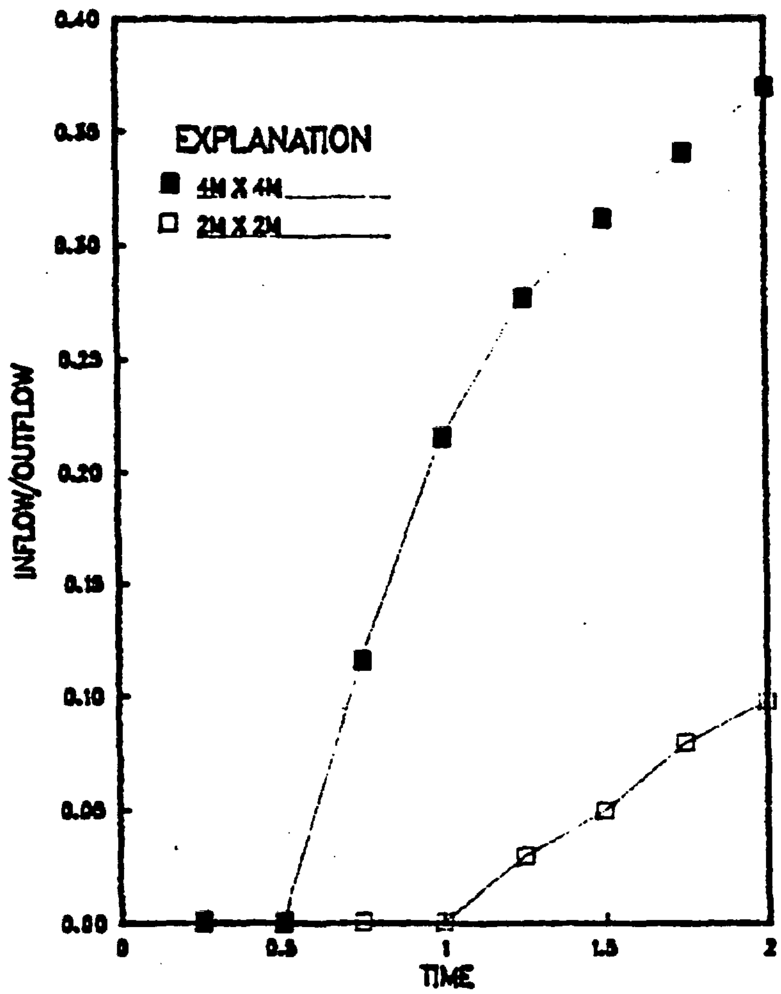
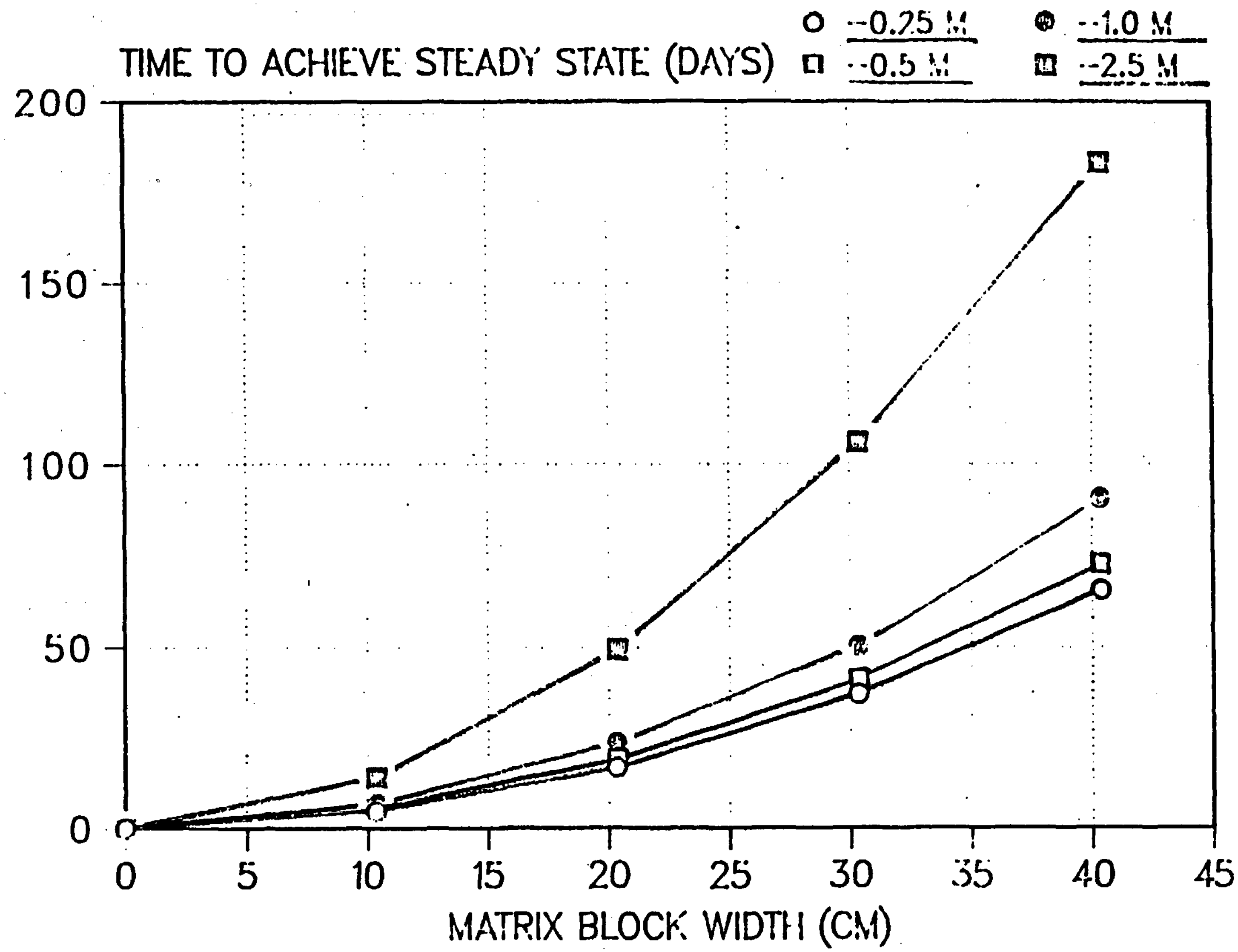
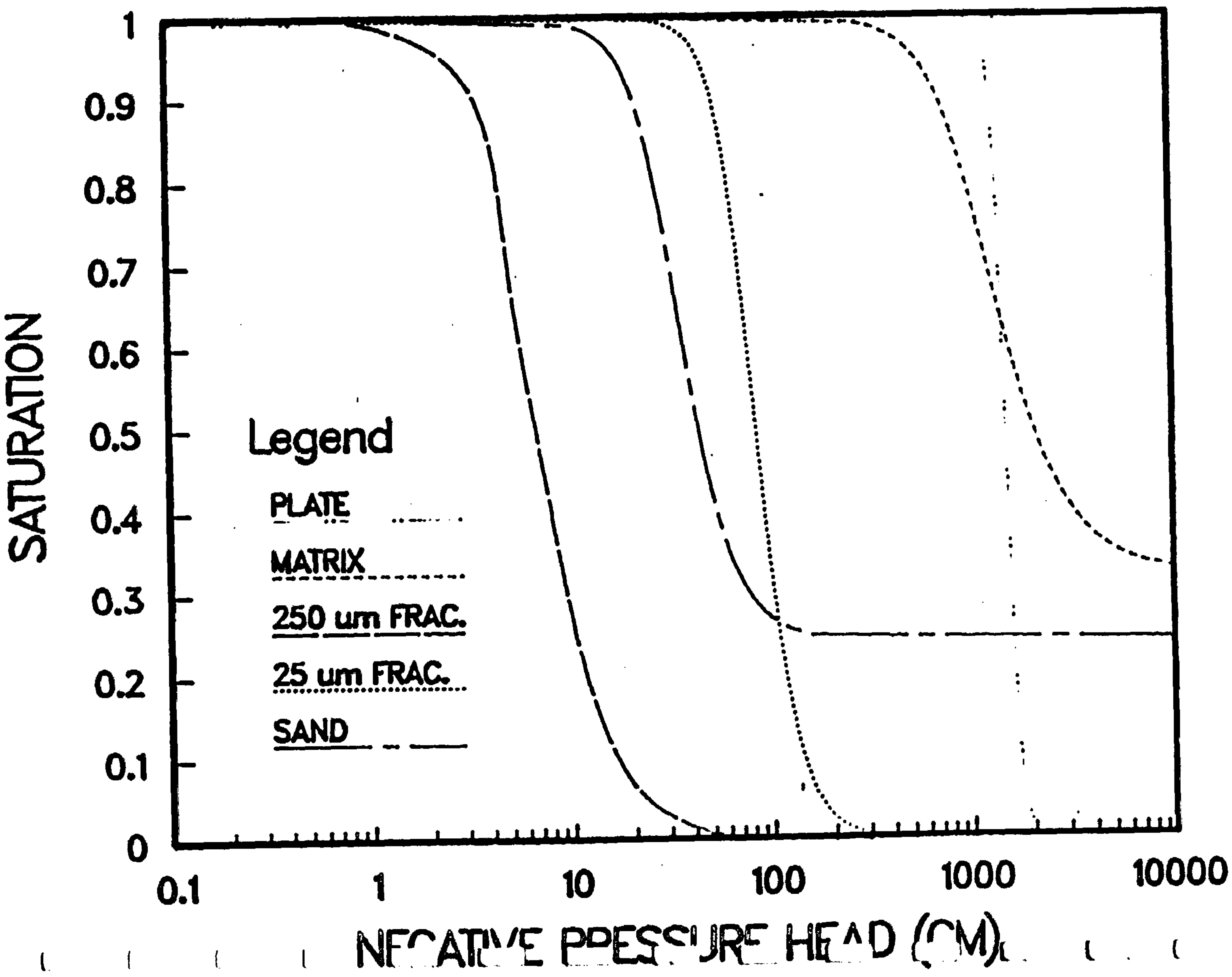


TABLE COMPARING THE RATIO OF OUTFLOW TO INFLOW FOR THE 2 METER BY 2 METER INFILTRATION SURFACE WITH THE 4 METER BY 4 METER SURFACE

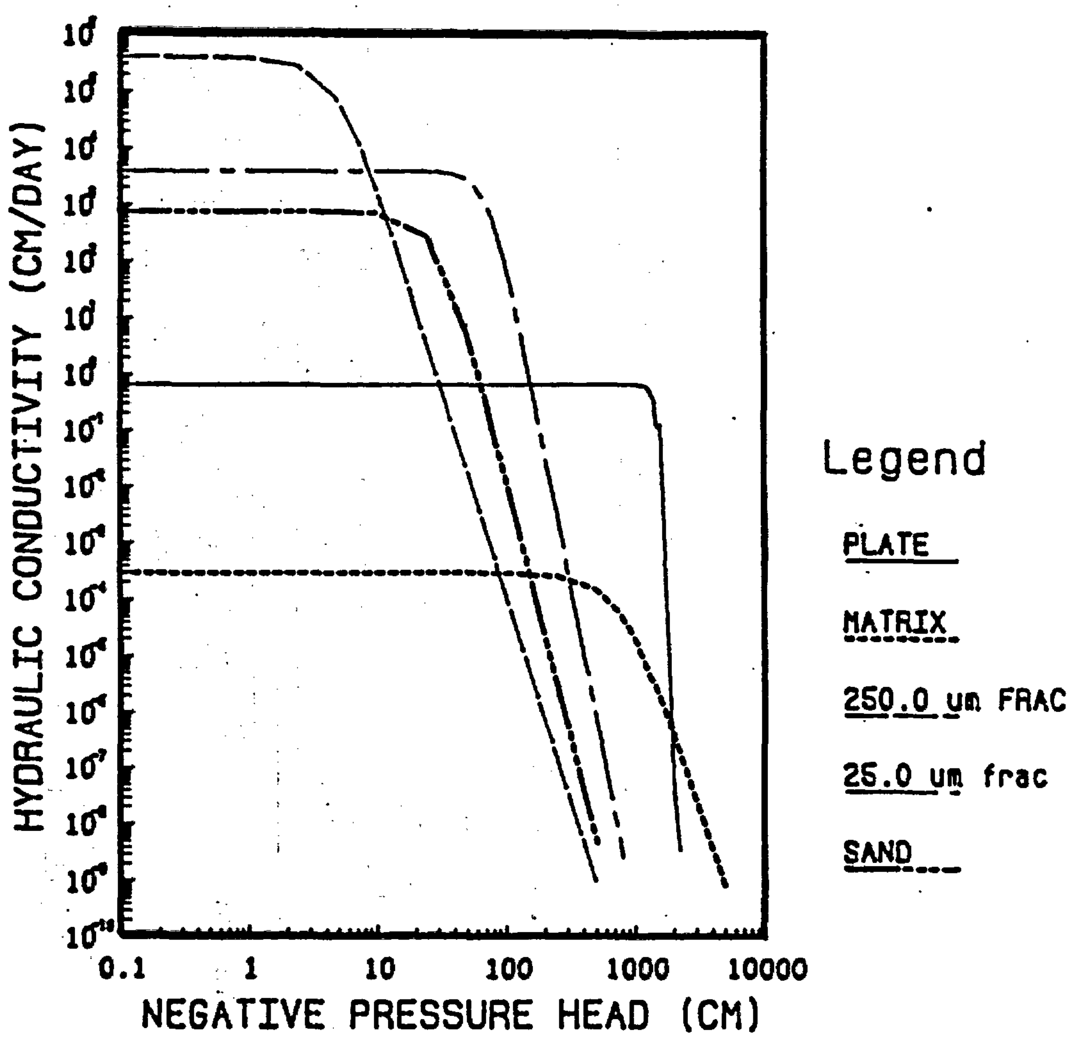


STEADY STATE TIME VS. MATRIX BLOCK WIDTH

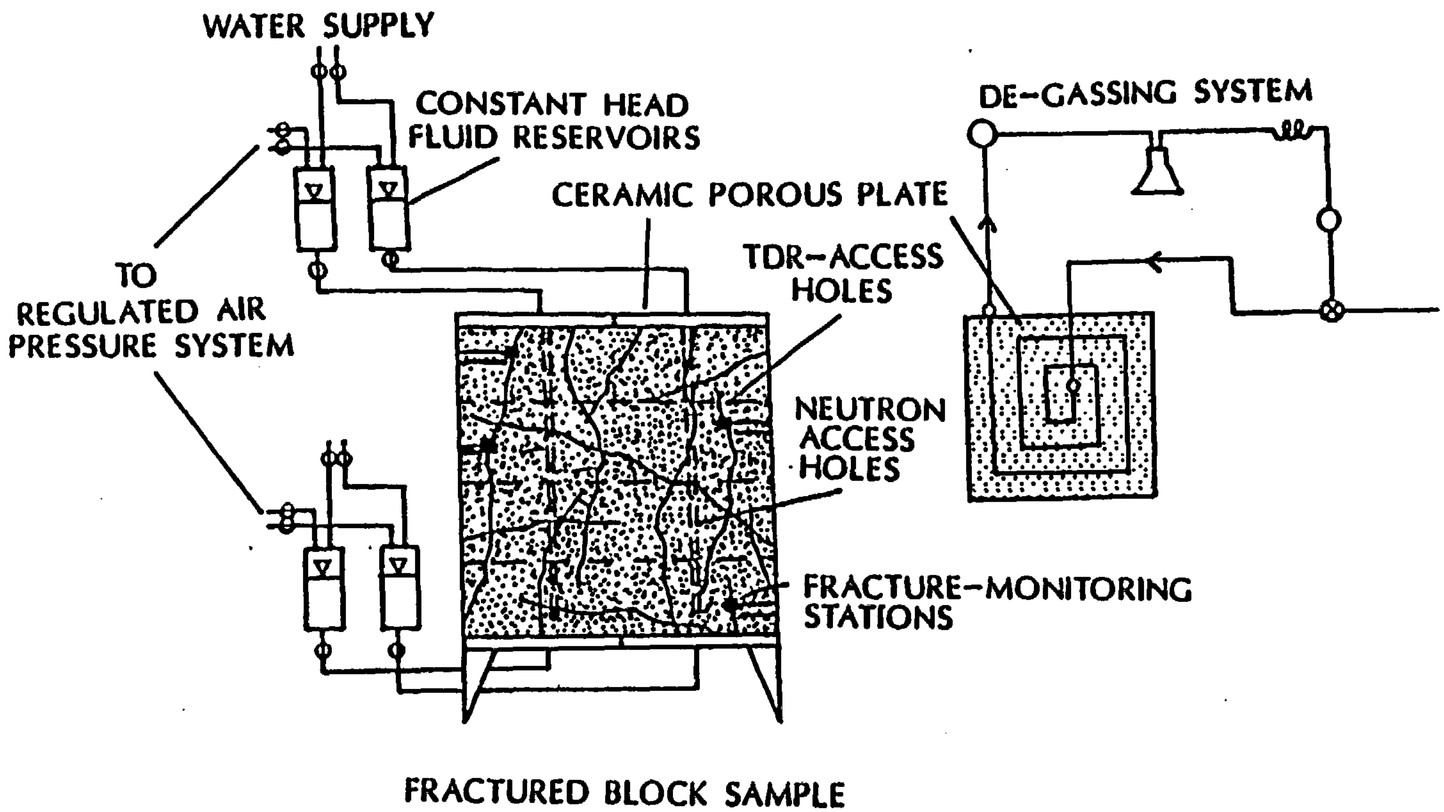



SATURATION
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.1
1
10
100
1000
10000
NEGATIVE PRESSURE HEAD (CM)
Legend
PLATE
MATRIX
250 um FRAC.
25 um FRAC.
SAND

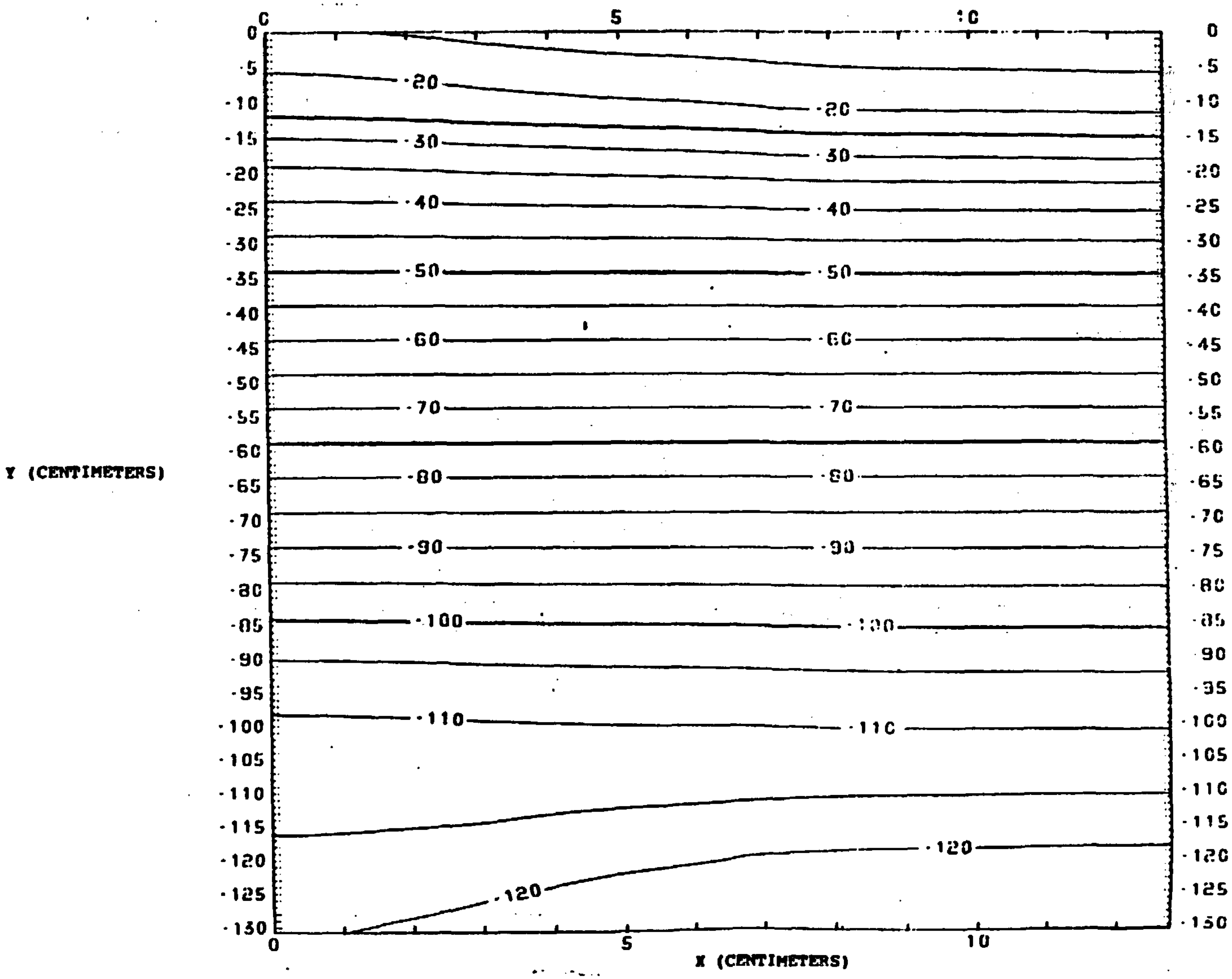
EFFECTIVE CONDUCTIVITY VERSUS PRESSURE HEAD



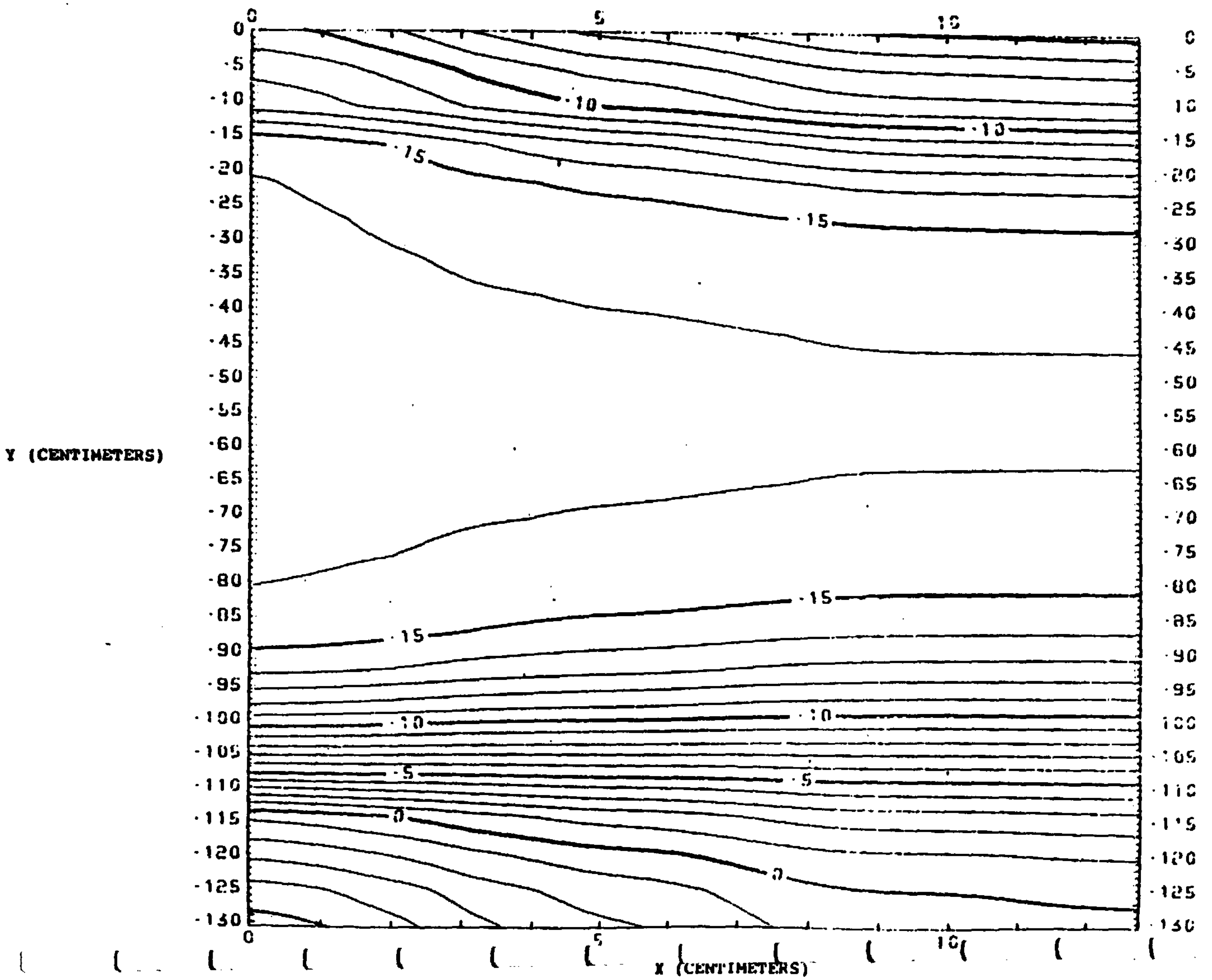
CONCEPTUAL DESIGN OF PERCOLATION TEST



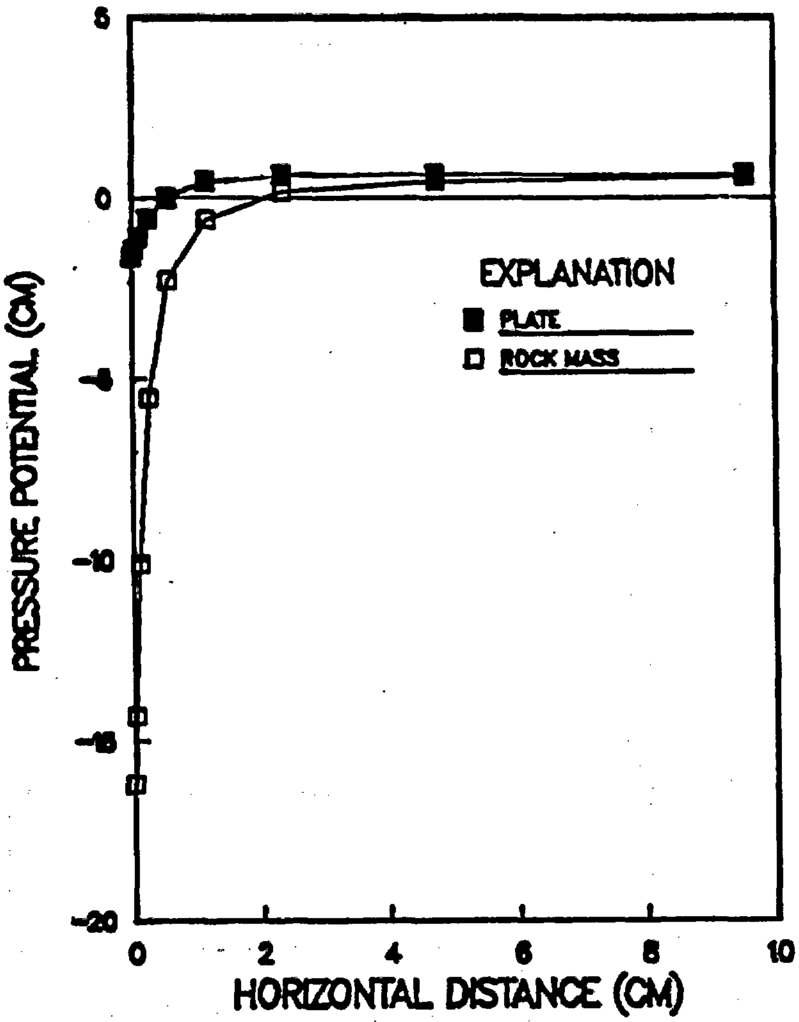
Steady-state total-head contours obtained using the head-control method for the case in which the bubbler heights are exactly level with the outer surfaces of the porous plates.



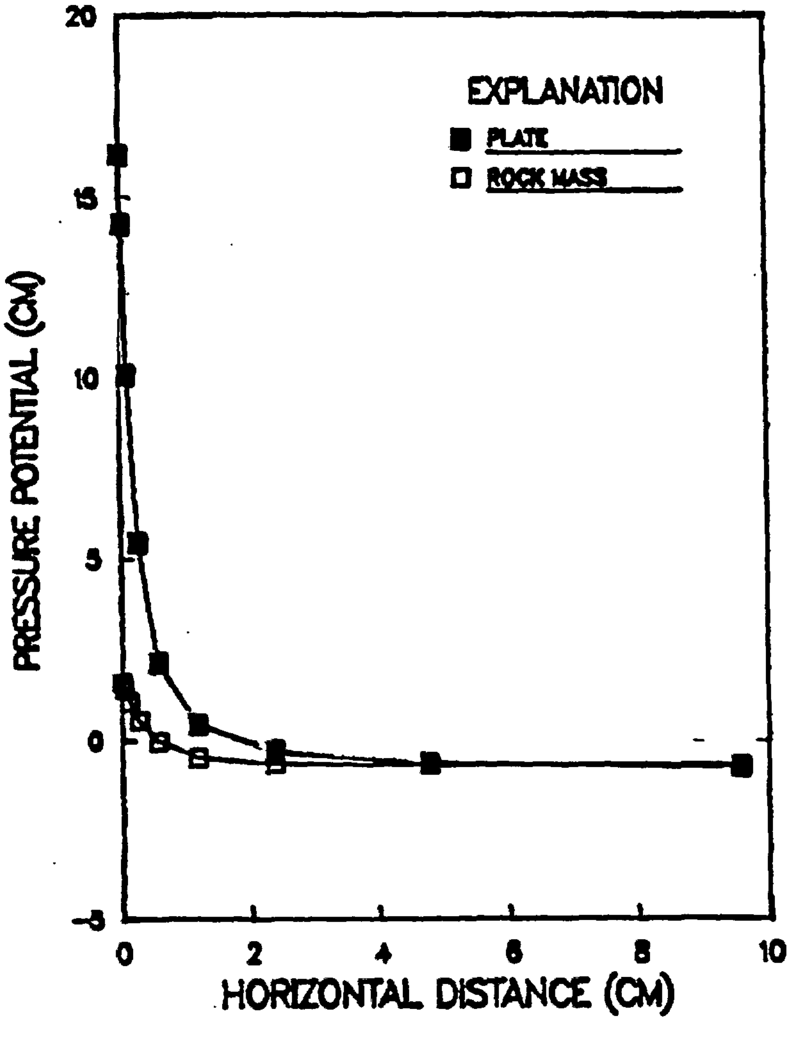
Steady-state pressure potential contours obtained using the head-control method for the case in which the bubbler heights are exactly level with the outer surfaces of the porous plates



PRESSURE POTENTIAL GRADIENTS AT THE BASE OF THE UPPER POROUS PLATE AND AT THE UPPERMOST NODES IN THE ROCK MASS



PRESSURE POTENTIAL GRADIENTS AT THE TOP OF THE LOWER POROUS PLATE AND AT THE LOWERMOST NODES IN THE ROCK MASS



MATRIC POTENTIAL GRADIENTS AT A DEPTH OF APPROXIMATELY 6 CM BENEATH IMPEDING LAYER

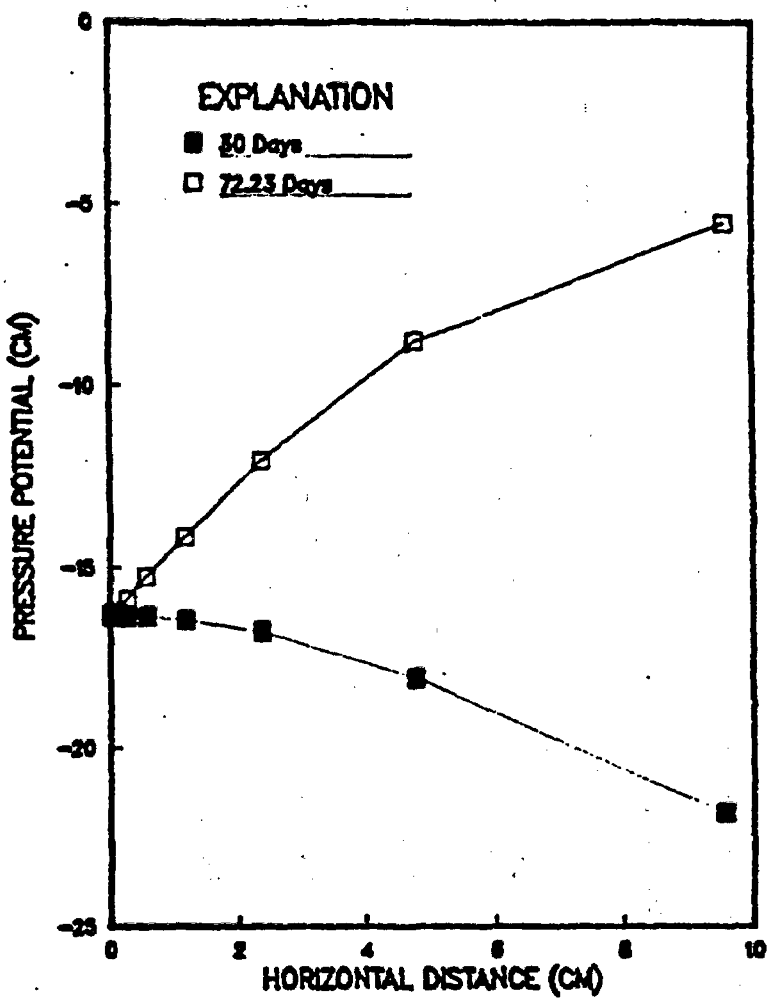
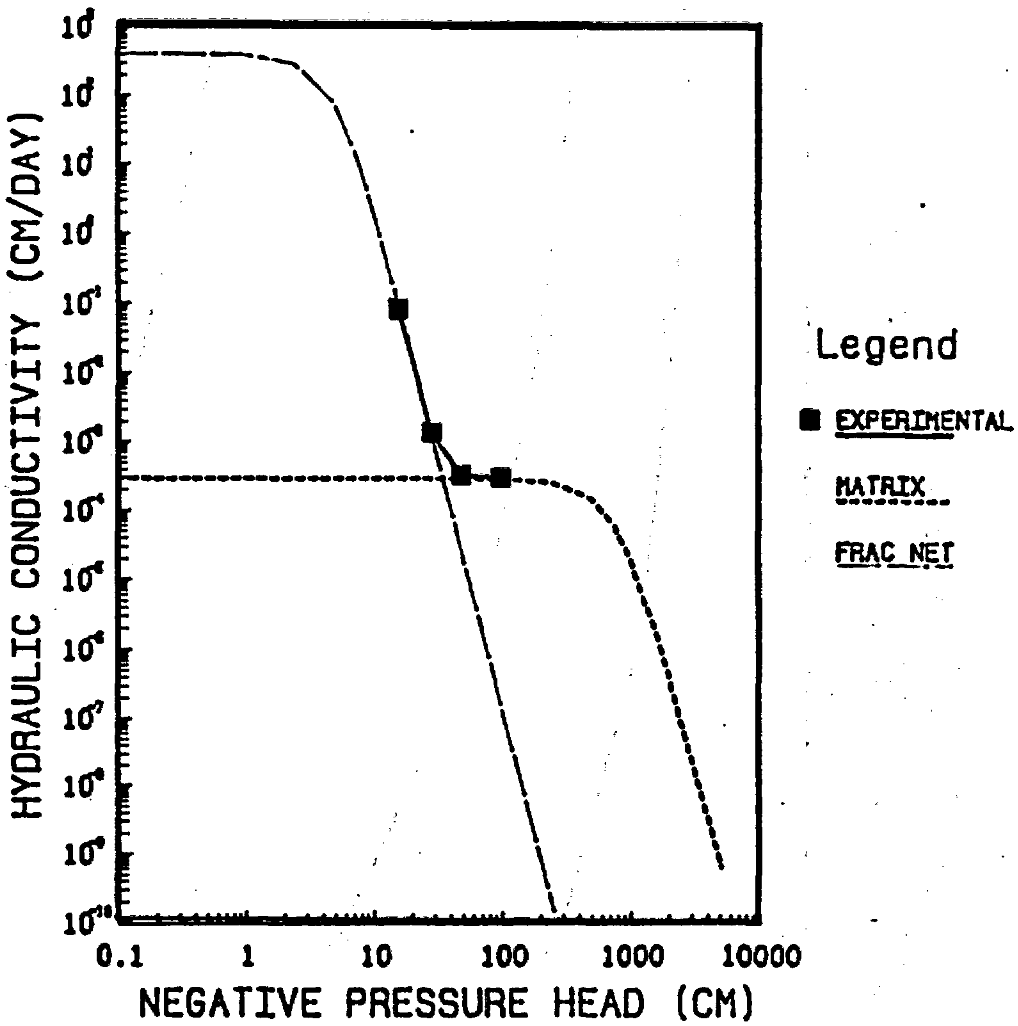


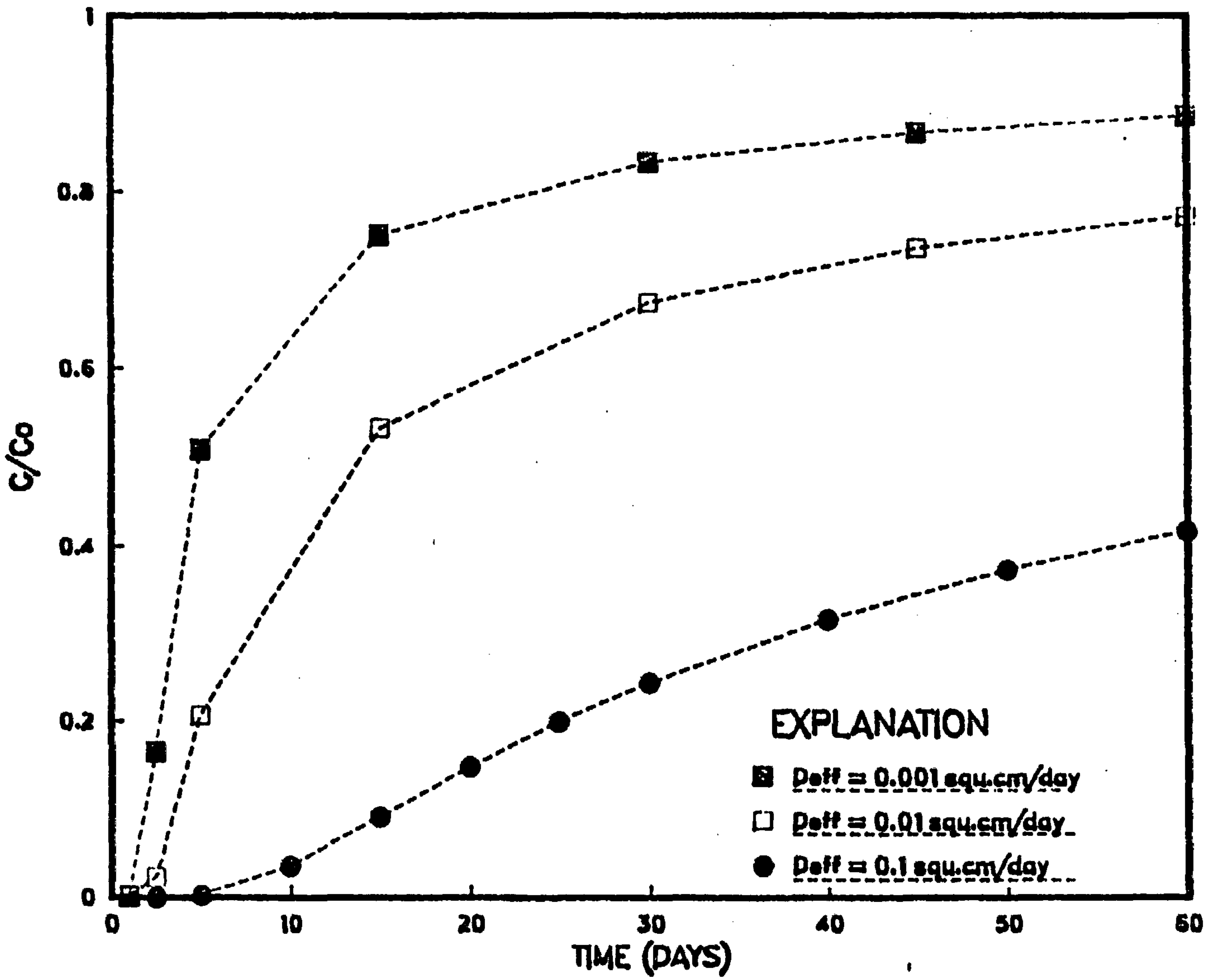
TABLE I

Applied Suction (cm)	Equilibrium Suction (cm)	Inflow (cm^3/day)	Outflow (cm^3/day)	K_{equiv} (cm/day)
0.0	-16.2	905.30	904.30	9.053×10^{-2}
-30.0	-29.3	15.11	15.13	1.511×10^{-3}
-50.0	-49.3	3.59	3.69	3.590×10^{-4}
-100.0	-99.5	3.26	3.40	3.250×10^{-4}

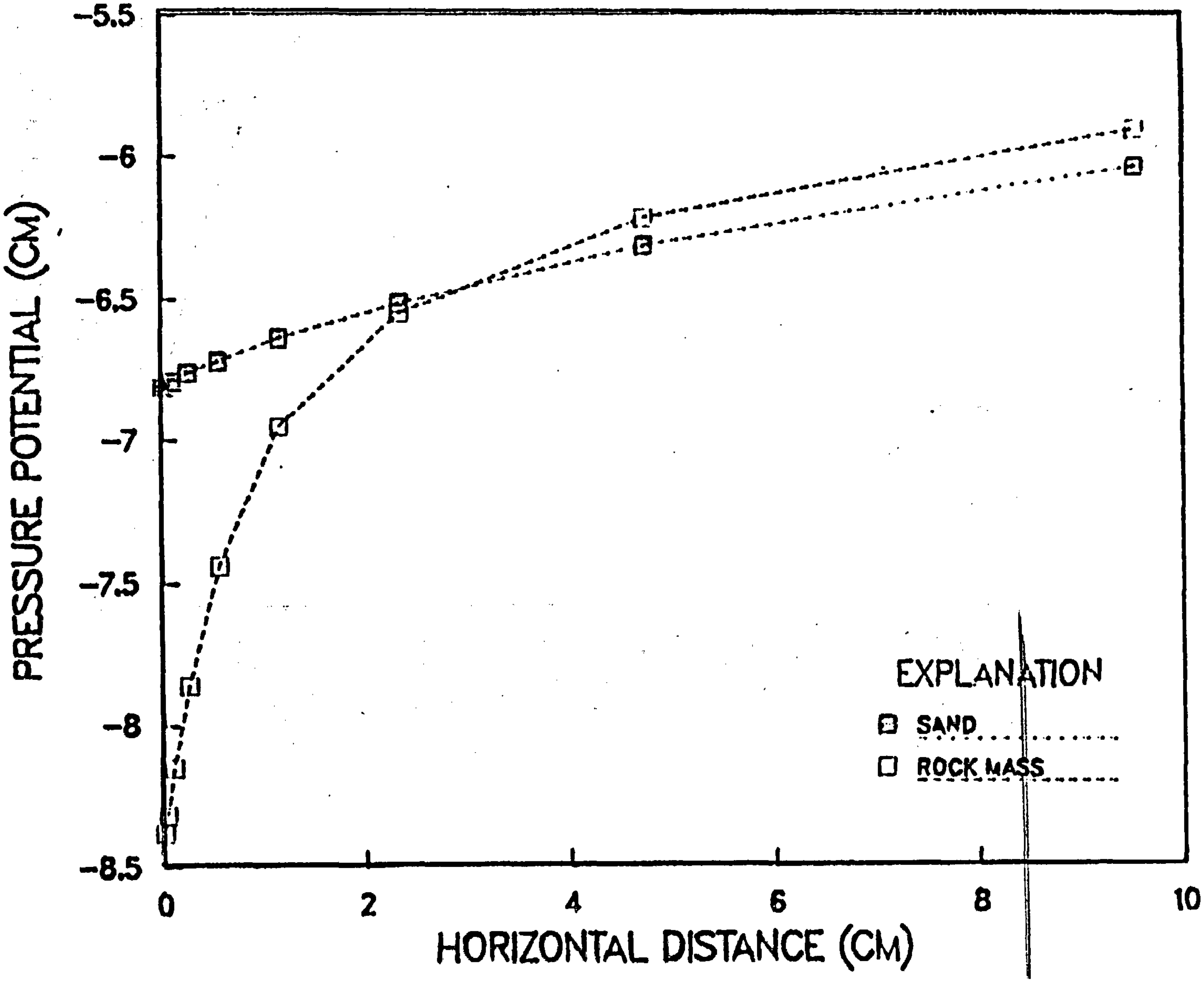
SIMULATED EXPERIMENTAL RESULTS



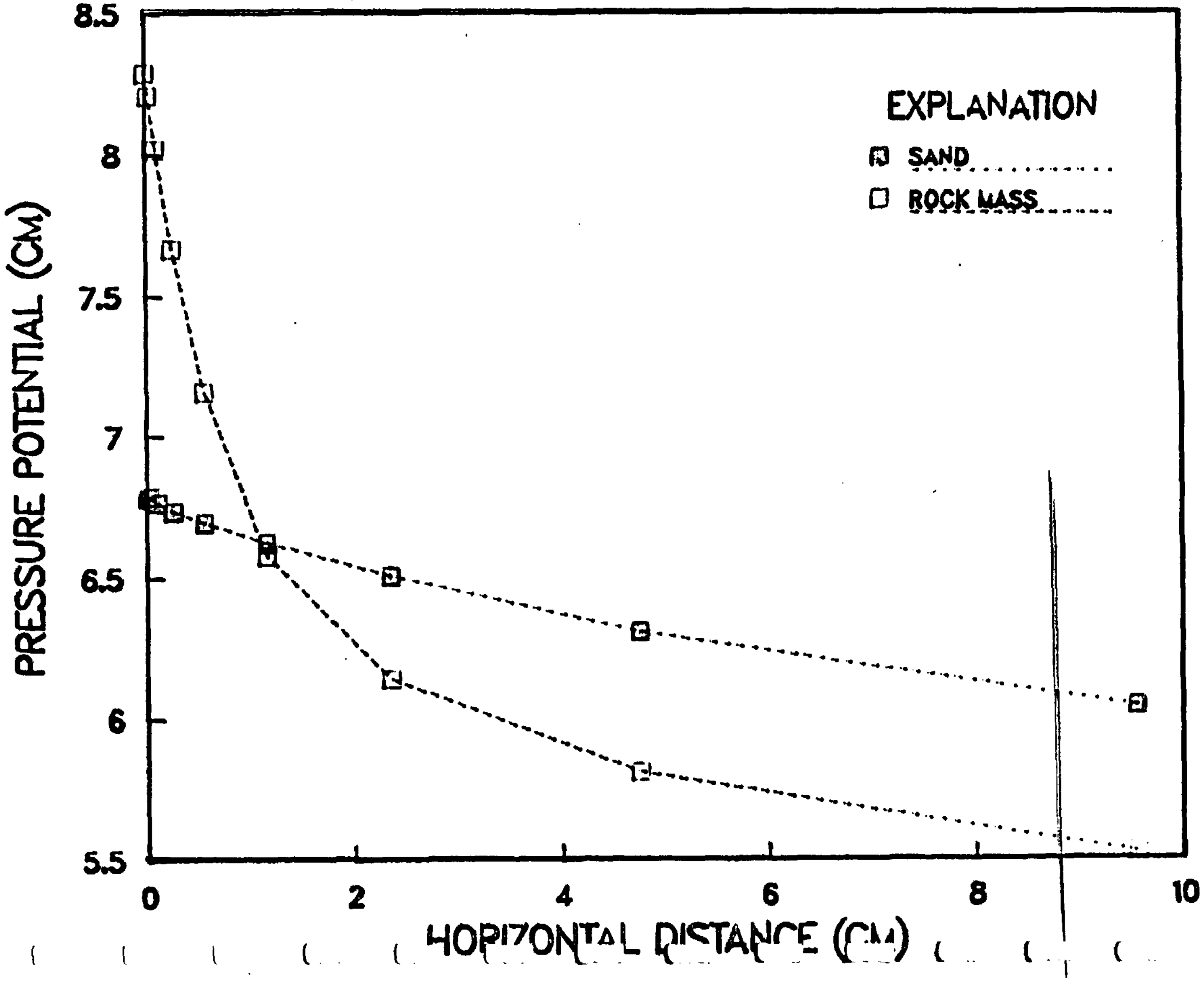
TRACER BREAKTHROUGH CURVES
FOR VARIOUS VALUES OF MATRIX DIFFUSIVITY

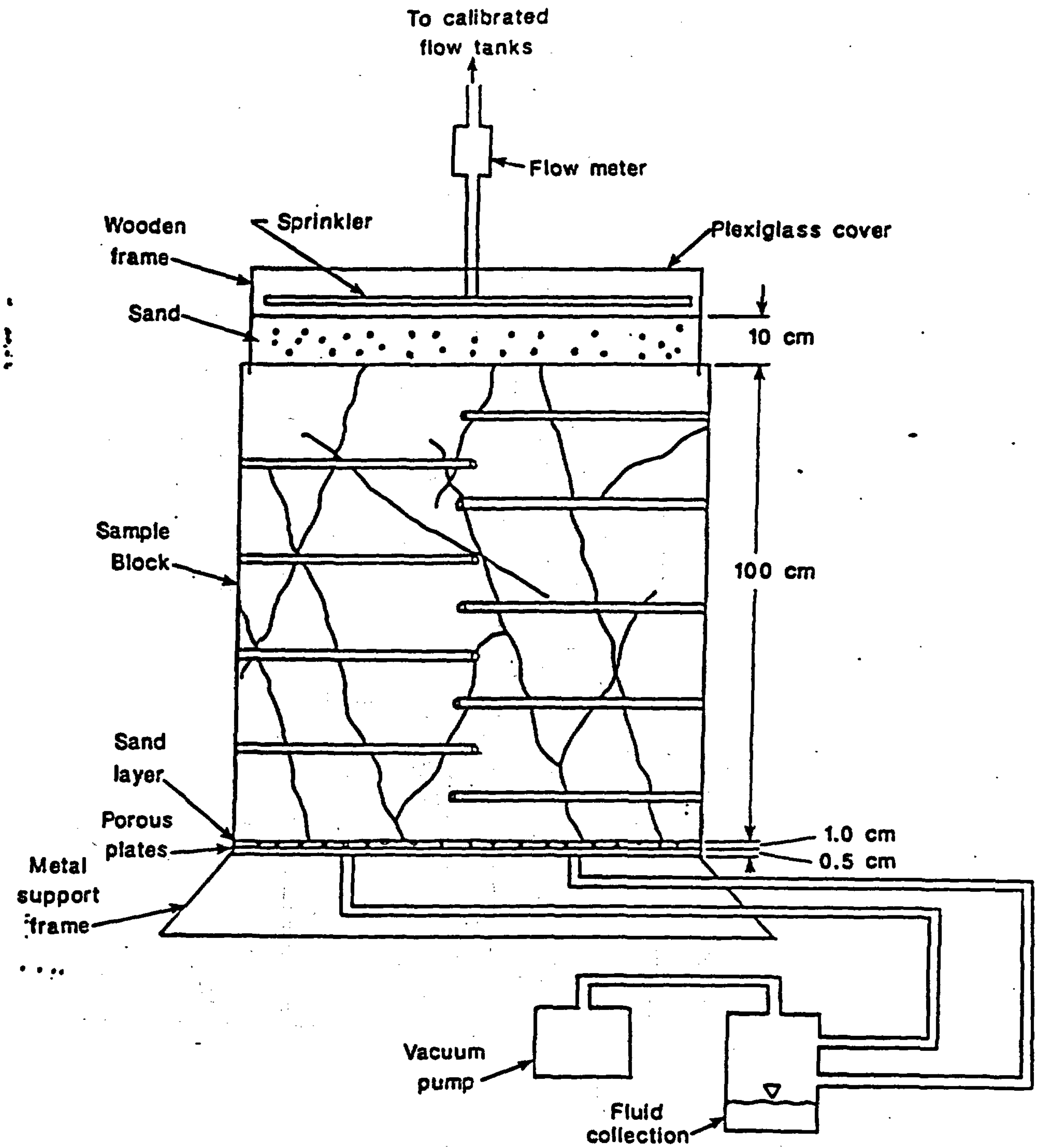


STEADY-STATE PRESSURE POTENTIAL GRADIENTS
AT THE BASE OF THE UPPER SAND LAYER AND
AT THTE UPPERMOST NODES IN THE ROCK MASS

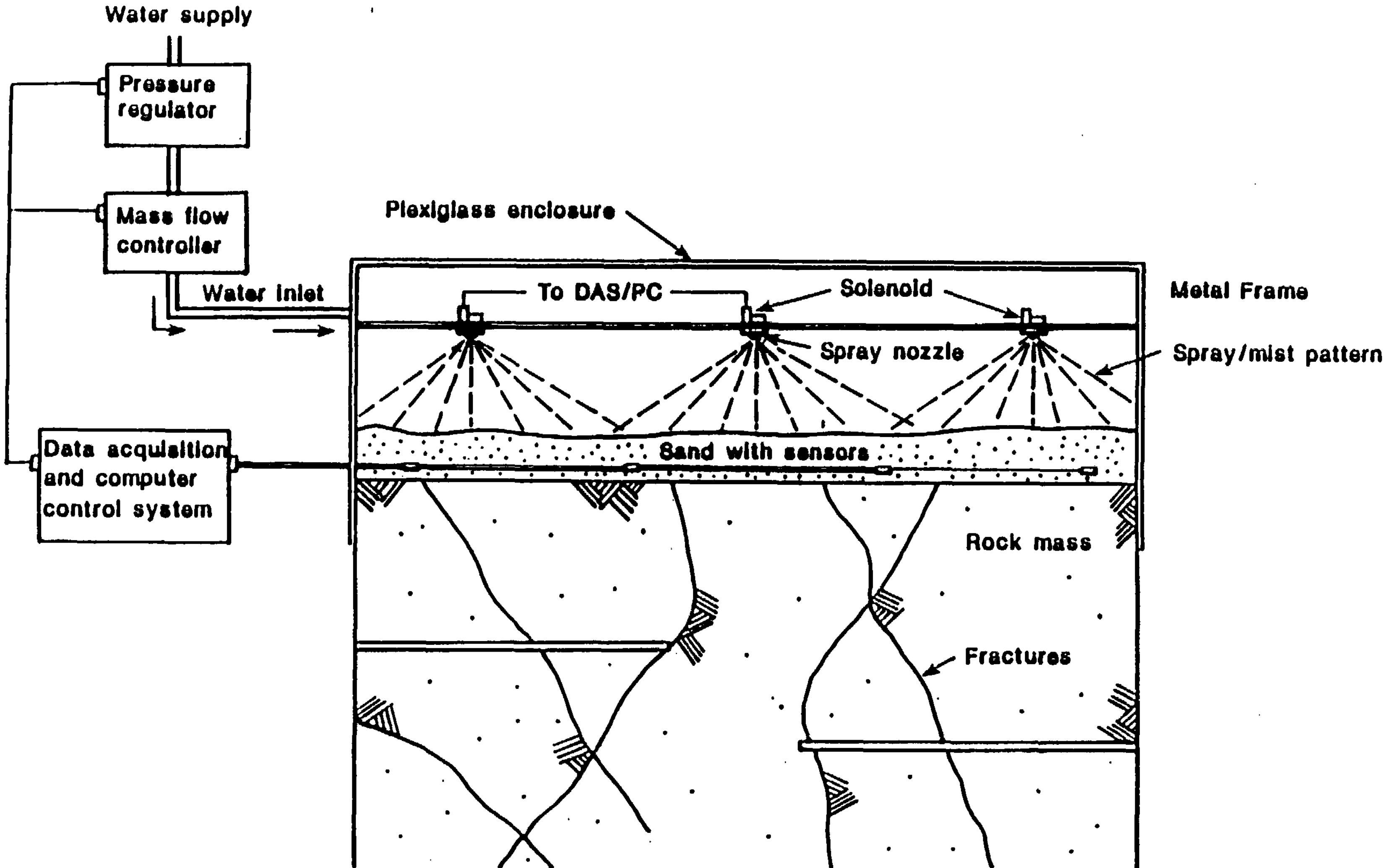


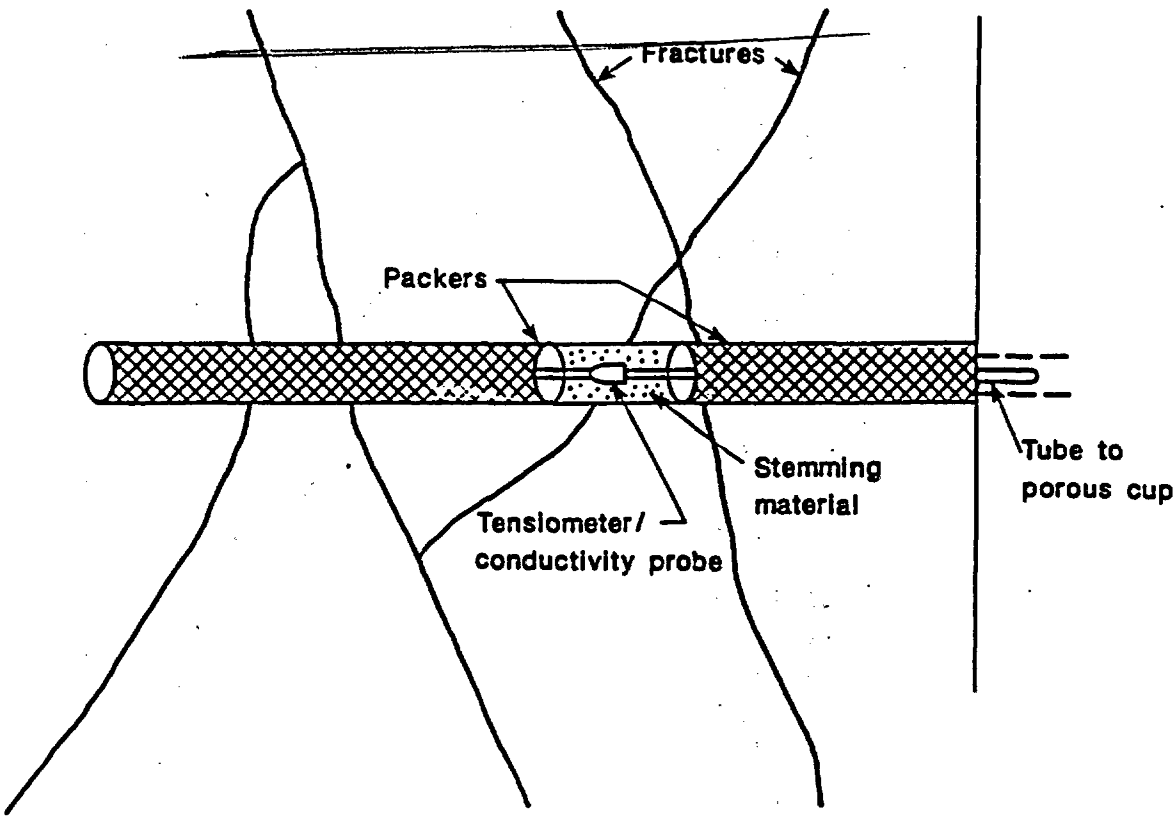
STEADY-STATE PRESSURE POTENTIAL GRADIENTS ACROSS THE LOWERMOST NODES IN THE ROCK MASS AND ACROSS THE TOP OF THE LOWER SAND LAYER



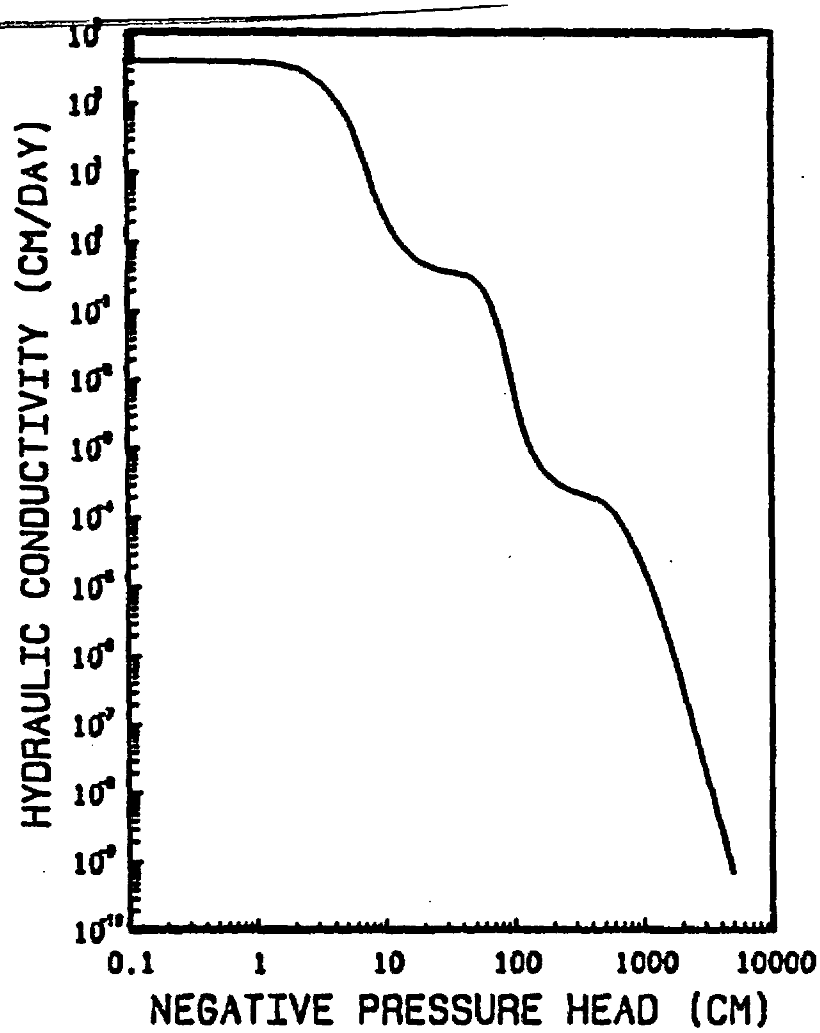


CONCEPTUAL DESIGN OF PERCOLATION TEST

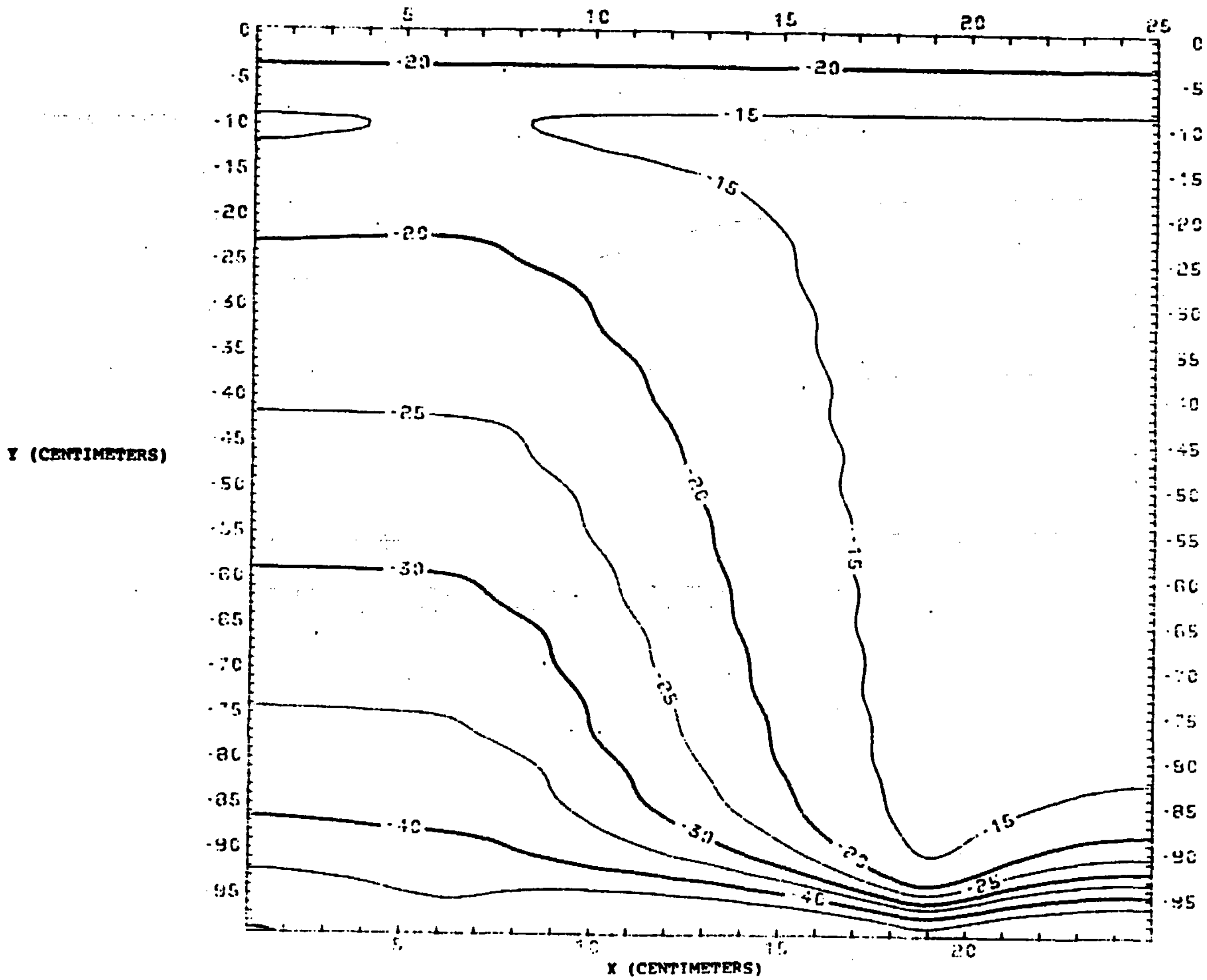

Water supply
Pressure regulator
Mass flow controller
Water inlet
Plexiglass enclosure
To DAS/PC
Solenoid
Metal Frame
Spray nozzle
Spray/mist pattern
Data acquisition and computer control system
Sand with sensors
Rock mass
Fractures


Fractures
Packers
Stemming
material
Tube to
porous cup
Tensiometer/
conductivity probe

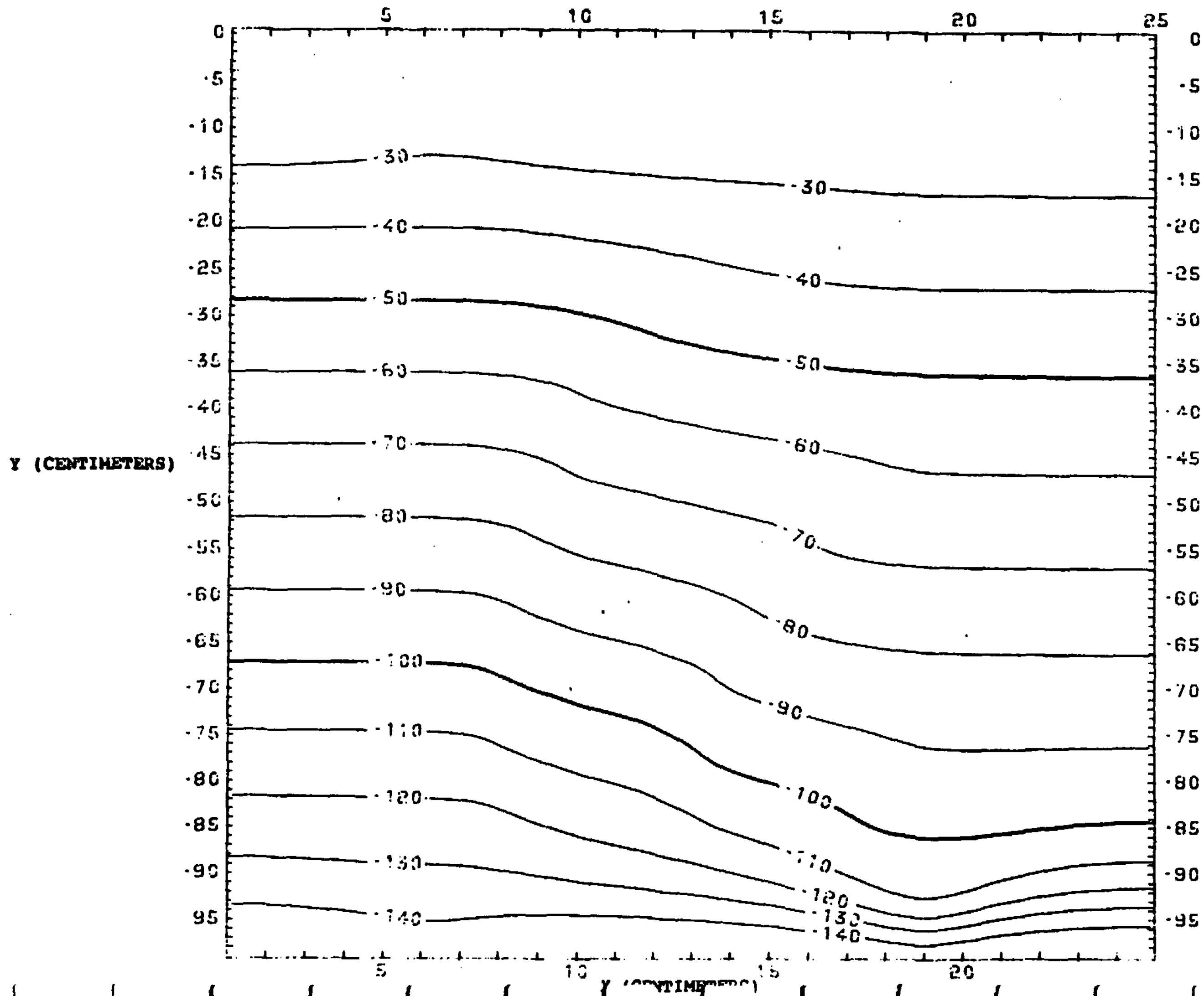
EFFECTIVE CONDUCTIVITY VERSUS PRESSURE HEAD
FOR A BLOCK CONTAINING FOUR 250 MICRON AND FOUR 25.0
MICRON FRACTURES



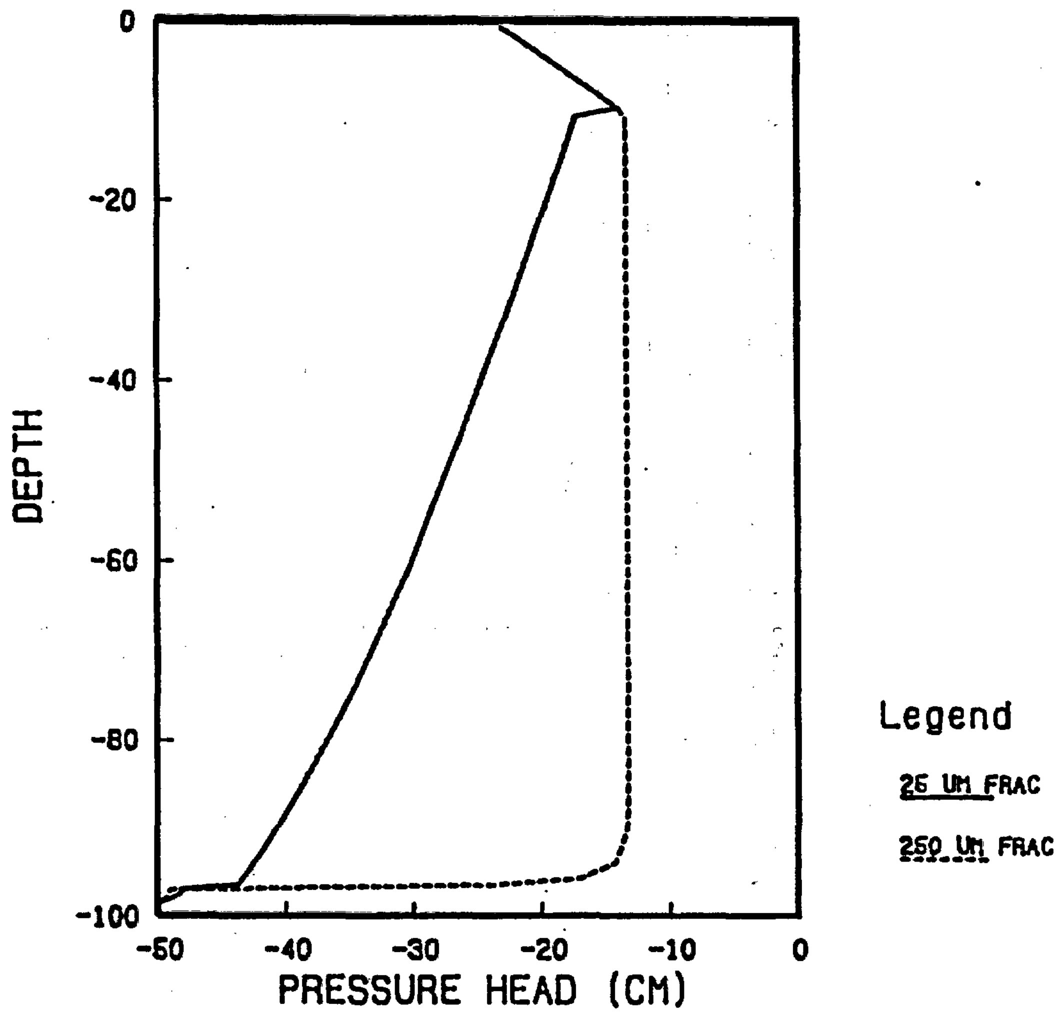
Steady-state pressure-head contours for the sprinkler-imposed steady-flux method. The flux is 0.905 cm/day and the lower boundary has a fixed pressure-head of -50.0 cm.



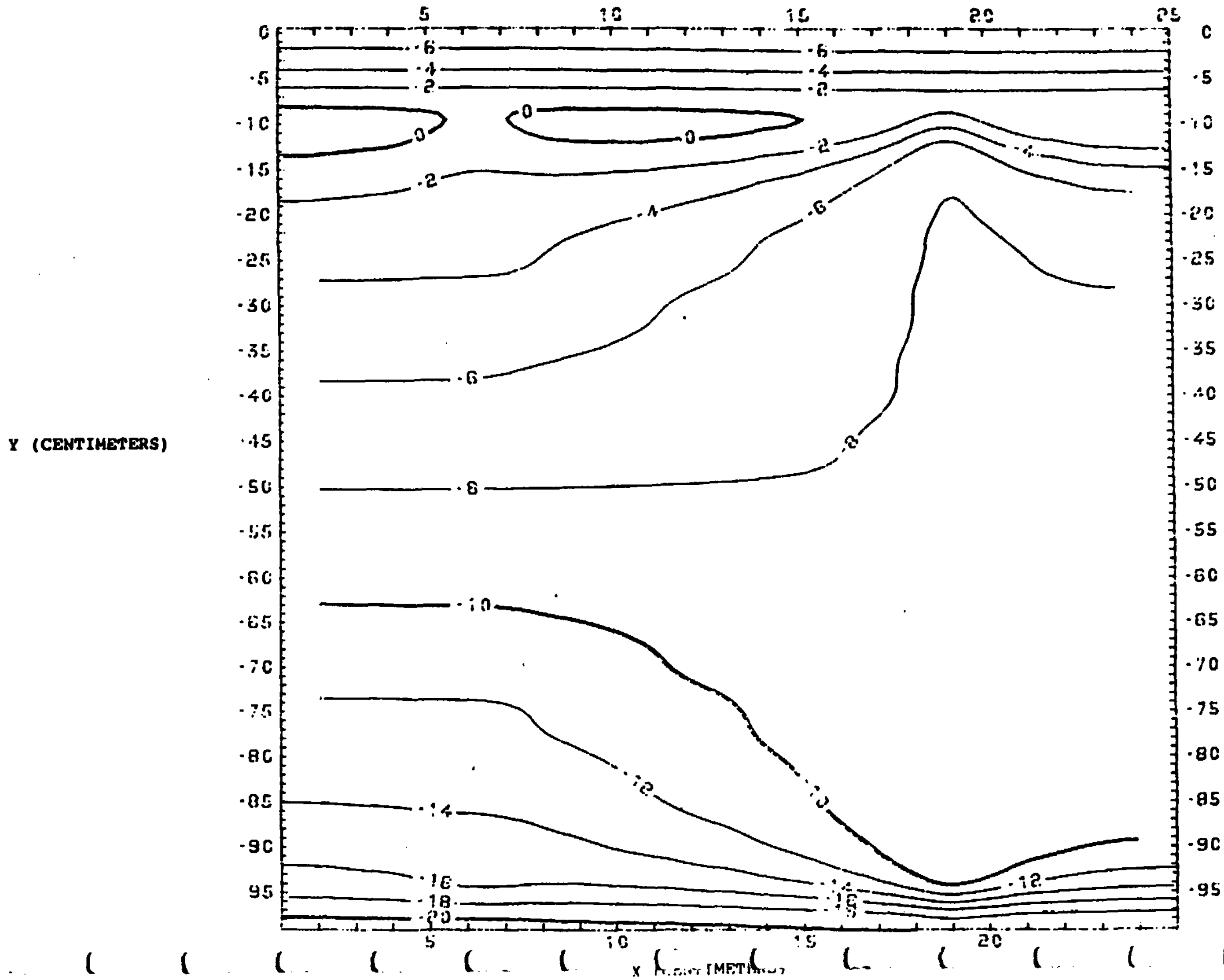
Steady-state total-head contours for the sprinkler imposed steady-flux method. The flux is 0.905 cm/day and the lower boundary has a fixed pressure-head of -50.0 cm.



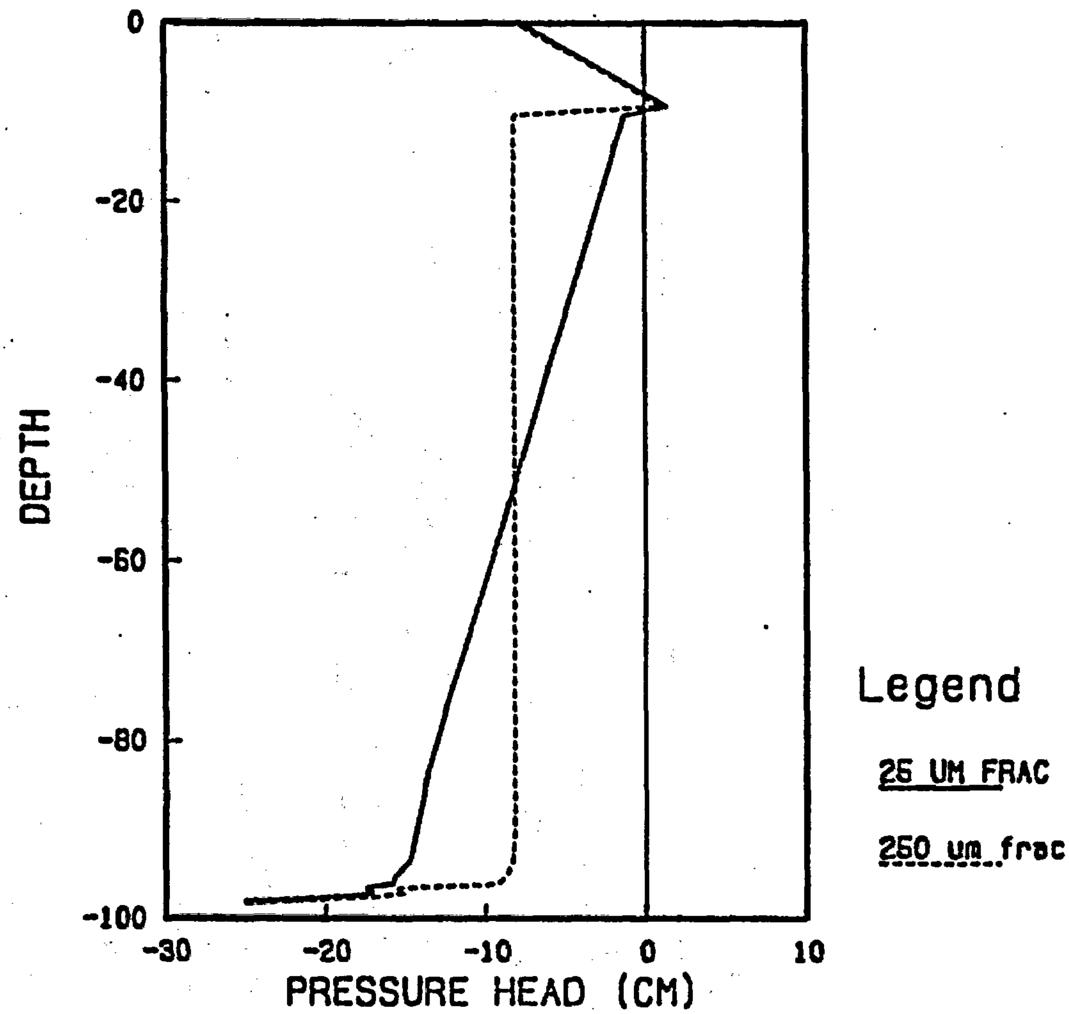
PRESSURE HEAD VERSUS DEPTH FOR THE COLUMNS
OF NODES CONTAINING THE FRACTURES



Steady-state pressure-head contours for the sprinkler-imposed steady-flux method. The flux is 9.05 cm/day, and the lower boundary has a fixed pressure-head of -25.0 cm.



PRESSURE HEAD VERSUS DEPTH FOR THE COLUMNS
OF NODES CONTAINING THE FRACTURES



CONCLUSIONS:

- Steady–flow conditions are attainable over a broad range of fluid fluxes, provided conditions are initially wet.
- It is necessary to monitor matric potentials in situ, regardless of the infiltration mechanism.
- Significant lateral flow may occur during a truly in situ test. In this case, the test may be interpreted using concepts developed for the double–ring infiltrometer.
- Spatial variability in matric potential will exist even in a homogeneous matrix, due to the presence of the fractures.

Models of Unsaturated Flow in a Fractured Porous Medium

N.M. Okusu, R.W. Zimmerman, G.S. Bodvarsson,
K. Karasaki, and J.C.S. Long

Earth Sciences Division
Lawrence Berkeley Laboratory

As part of the LBL-USGS cooperative project, different models for evaluating flow in unsaturated, fractured rocks are being developed. These models include 2- and 3-dimensional fracture/matrix mesh generators and a semi-analytic approach for evaluating fracture/matrix interaction. The purpose of the models is to assist with the design and analysis of prototype and exploratory shaft tests being carried out by the USGS at the Yucca Mountain site.

The mesh generating programs discretize both the fracture network and the surrounding rock matrix so that the mass, heat, and chemical transport through the system may be evaluated using integral finite-difference codes. The fracture network used by the programs may be either specified by the user or automatically generated with random fracture locations and statistically distributed fracture parameters. The rock matrix is discretized using a nested-element approach, whereby the matrix elements which are closest to the fractures have the smallest volumes and nodal distances. Thus the rock is well-discretized in the regions where the thermodynamic properties are likely to change more rapidly and coarsely discretized away from the fractures, where changes will occur more slowly. This reduces the overall number of elements and makes the mesh more numerically tractable.

To reduce the number of elements even further and to allow the model to handle problems on a larger scale, a semi-analytic approach to calculate the flux between a fracture and an unsaturated rock block has been developed. The boundary-layer method is used to find simple, closed-form solutions to the governing partial differential equation of 1-dimensional imbibition into both a semi-infinite block and a spherical block. The solutions have been tested against numerical codes and found to be very accurate. The accuracy of using the semi-analytic approach for blocks with irregular geometries is being evaluated.

Models of Unsaturated Flow in a Fractured Porous Medium

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LBL-USGS Program

Introduction

Two approaches are being developed to handle the problem of unsaturated flow in a fractured porous medium:

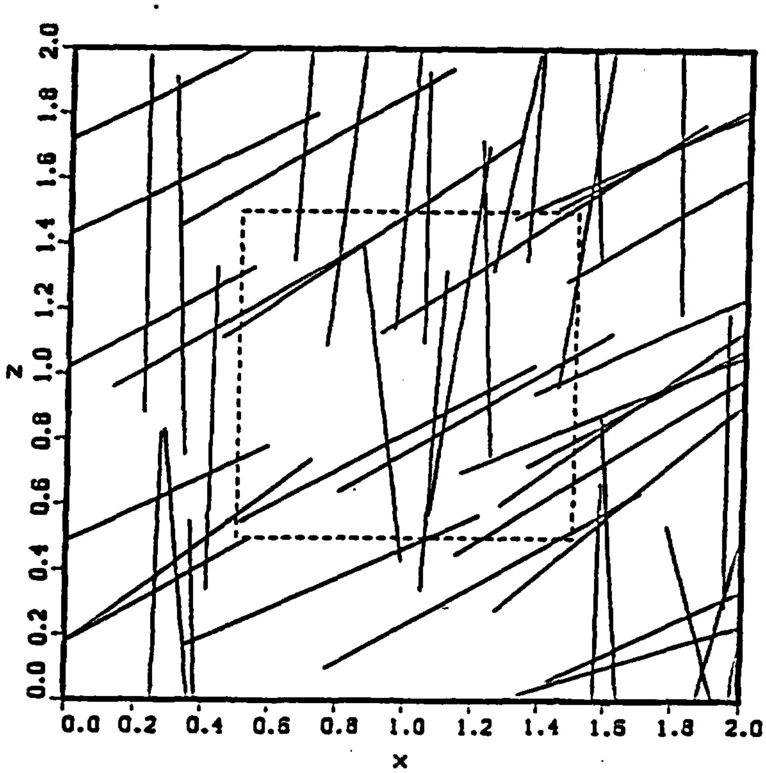
- Programs which discretize both the fracture network and the rock matrix in 2- and 3-dimensional systems.
- Semi-analytical treatment of fluid imbibition from a fracture to the rock matrix.

Application of Models

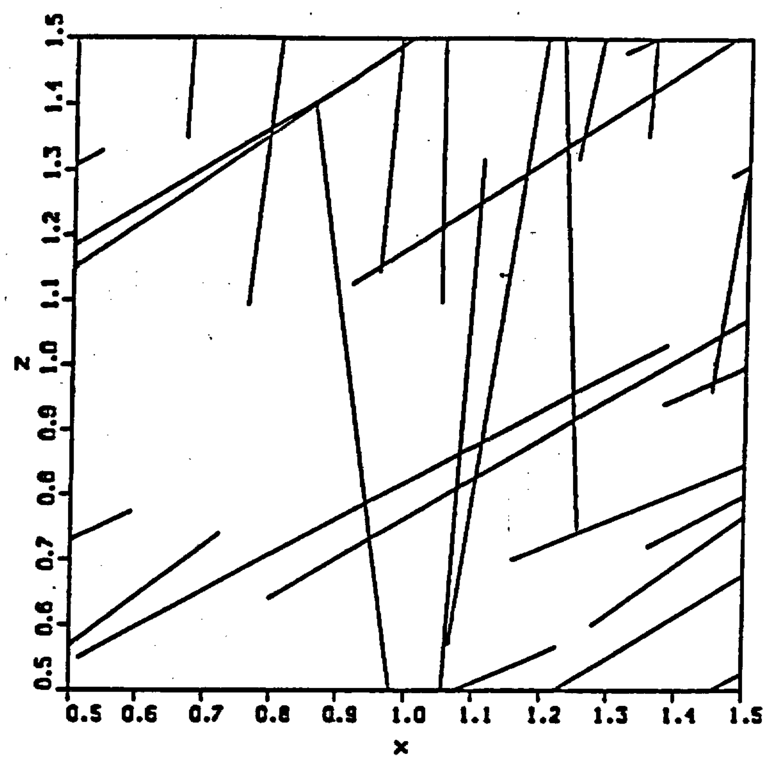
- To design and interpret the results of hydrological prototype tests and exploratory shaft tests.
- To assist in large-scale characterization of a fractured porous system, such as Yucca Mountain.
- To perform theoretical studies of unsaturated flow.

Two-Dimensional Fracture/Matrix Mesh Generator

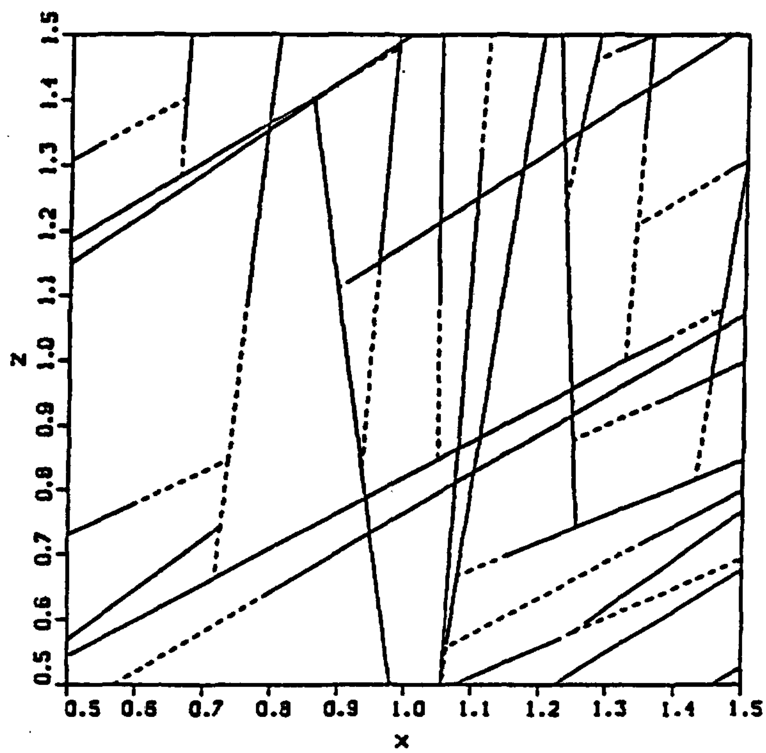
The program automatically discretizes both fractures and rock matrix in an arbitrarily-shaped, two-dimensional, saturated or unsaturated, fractured porous medium.



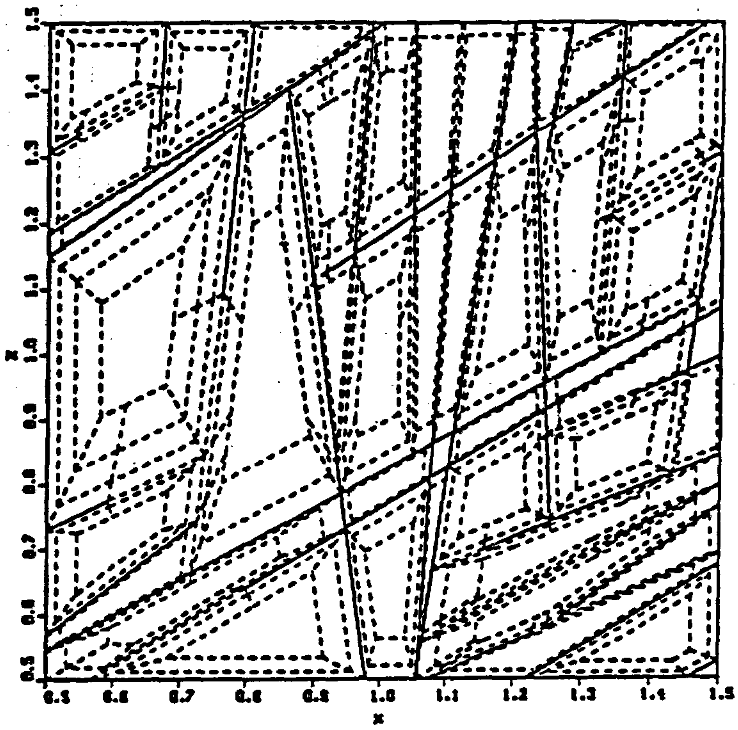
Random Fracture Network



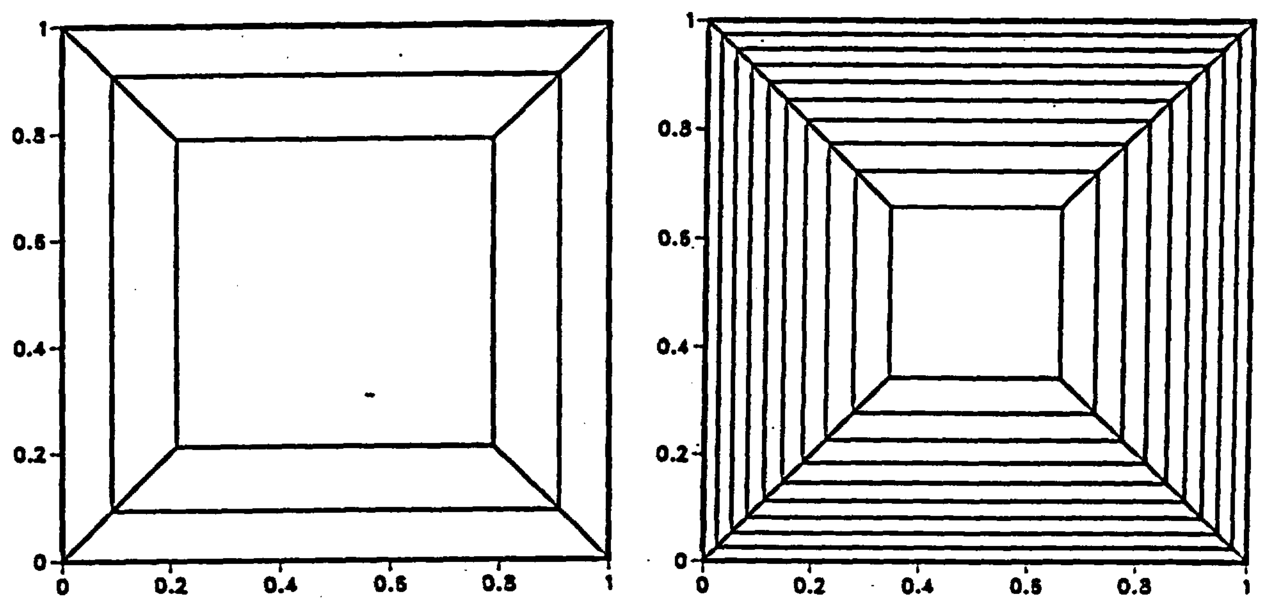
Fractures and Fracture Extensions



Fully-Discretized System



Accuracy of the Gridding Method



Three-Dimensional Fracture/Matrix Mesh Generator

The program discretizes both fractures and rock matrix in a three-dimensional block containing a network of fractures.

- The program is a tool which will be used for the analysis of lab and field tests related to the unsaturated zone.
- The output of the program will be tailored to integrated finite-difference codes for calculations of heat, mass, and chemical transport.

Approach

- Fractures are rectangular or regular polygonal planar features.
- Positions of fracture centers are either specified by the user or randomly distributed throughout the generation region.
- Other fracture parameters are either specified by user or have a specified distribution, such as normal, lognormal, exponential, or uniform.

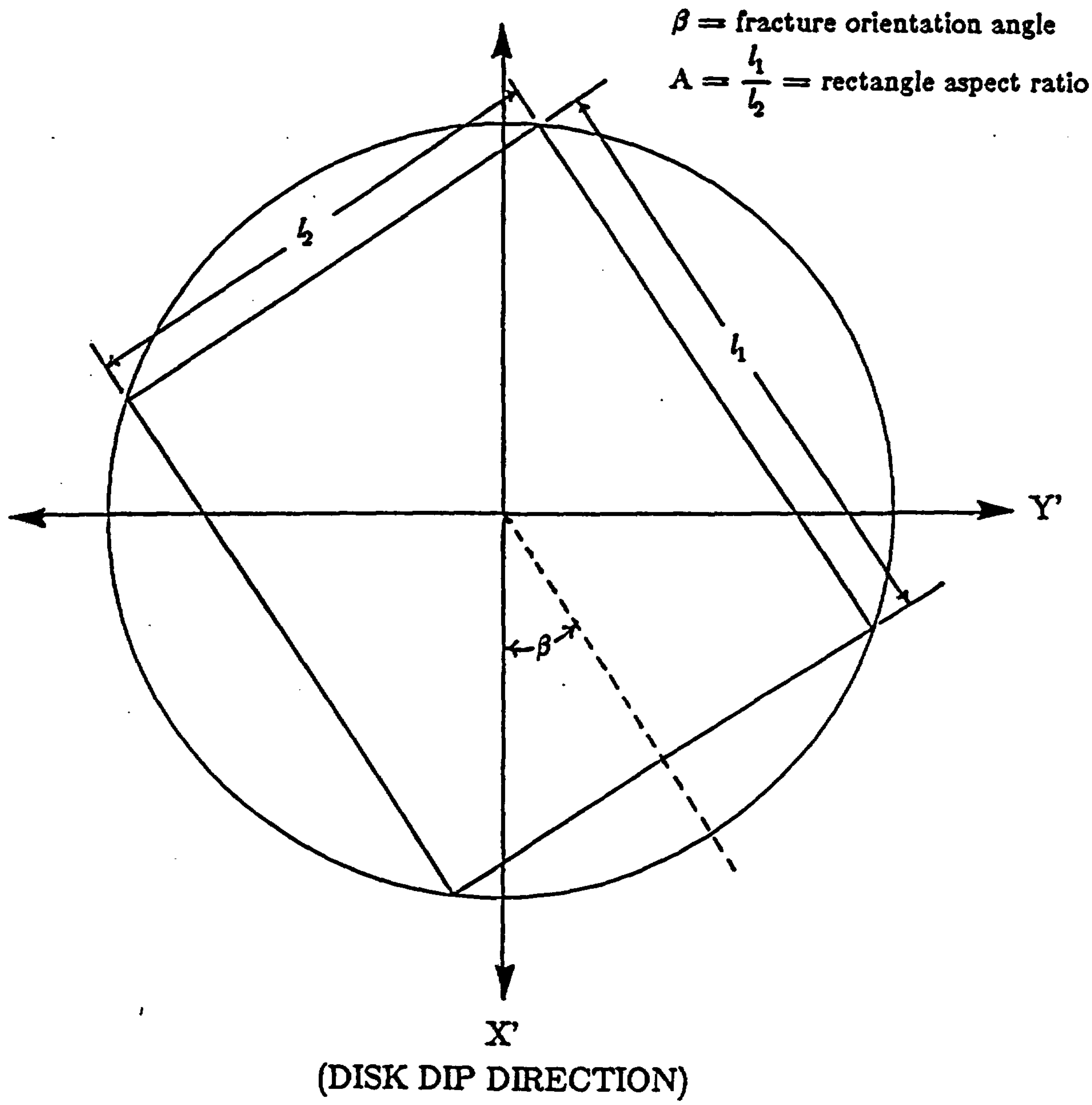
Reasons for Choosing Polygonal and Rectangular Fracture Shapes

- more general representation of fractures than disks or mosaics
- Distinct rock blocks can be formed on any scale and with any shape
- fractures are bounded or unbounded, depending on fracture length and size of flow region
- relative computational ease in extension to matrix discretization

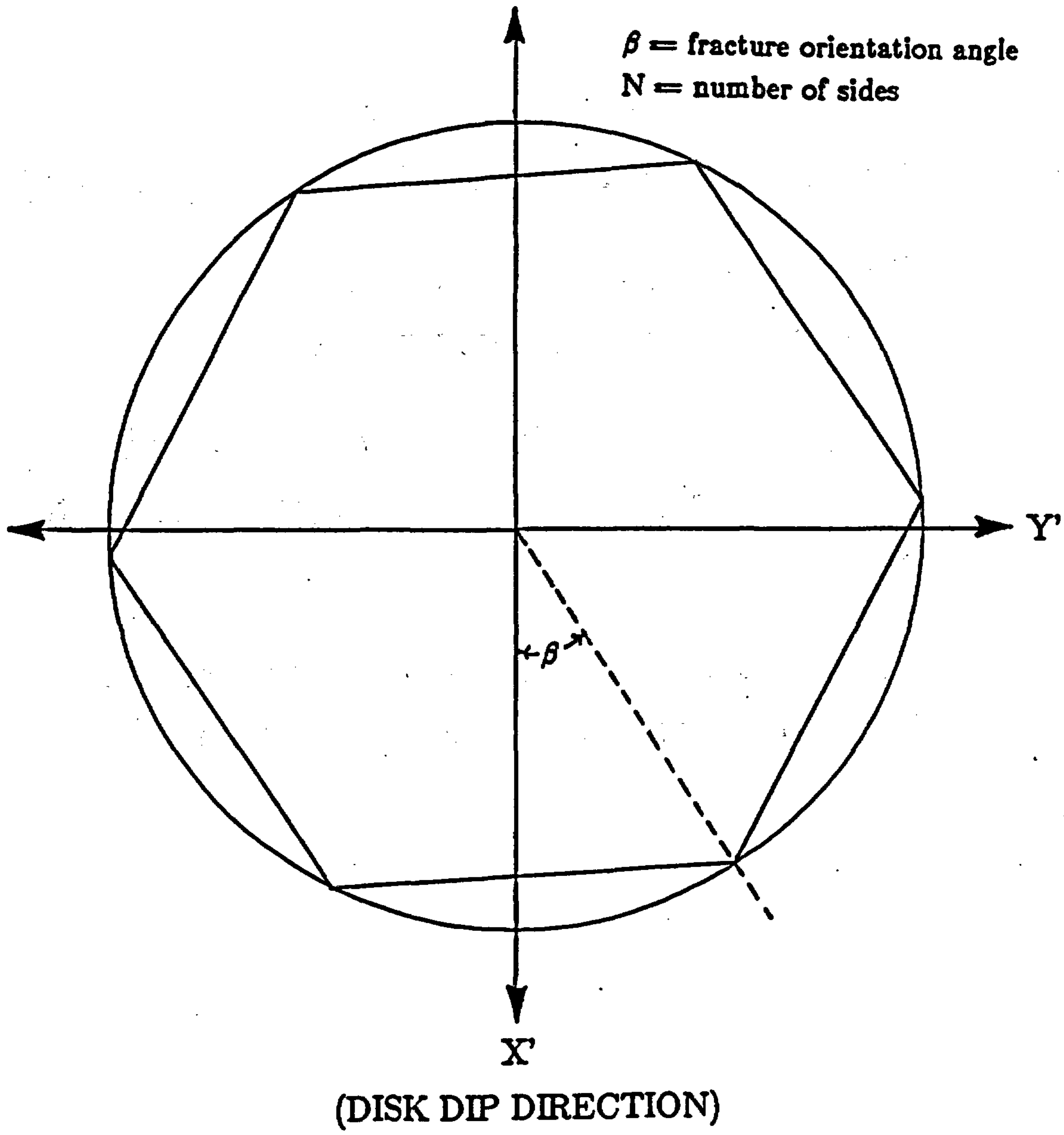
Disadvantages of Model

- using a disk representation would result in a curved boundary which is more realistic
- fractures almost always terminate in intact rock
- fractures are always planar; they do not react to presence of nearby fractures or changes in the stress field

Rectangular Fracture



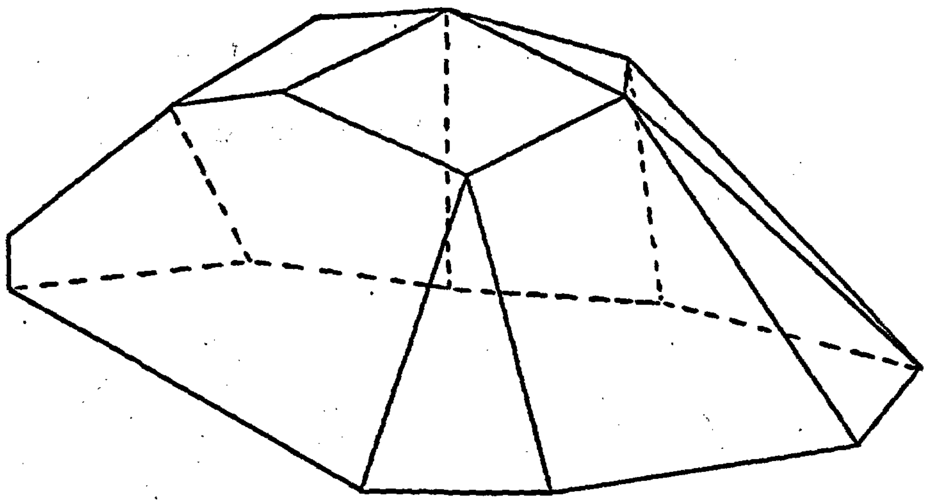
Regular Polygonal Fracture



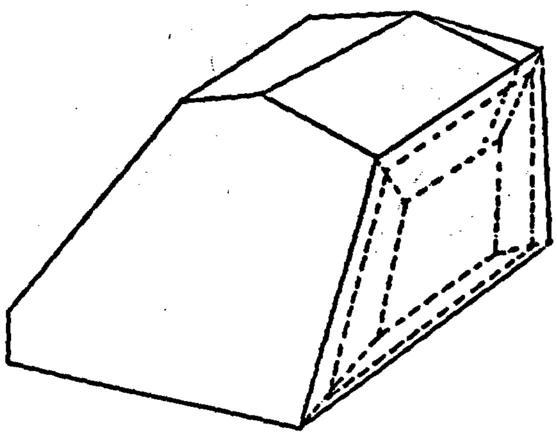
Discretization Method

- Form enclosed rock blocks using real fractures and imaginary fractures (fracture extensions).
- Define radial lines from corners of each block side to center of gravity of block.
- Define planes parallel to rock block sides, spaced so that small nodal distances occur close to fractures.
- Calculate nodal position of each element, interface area, and nodal. connection lengths

Example of a Rock Block



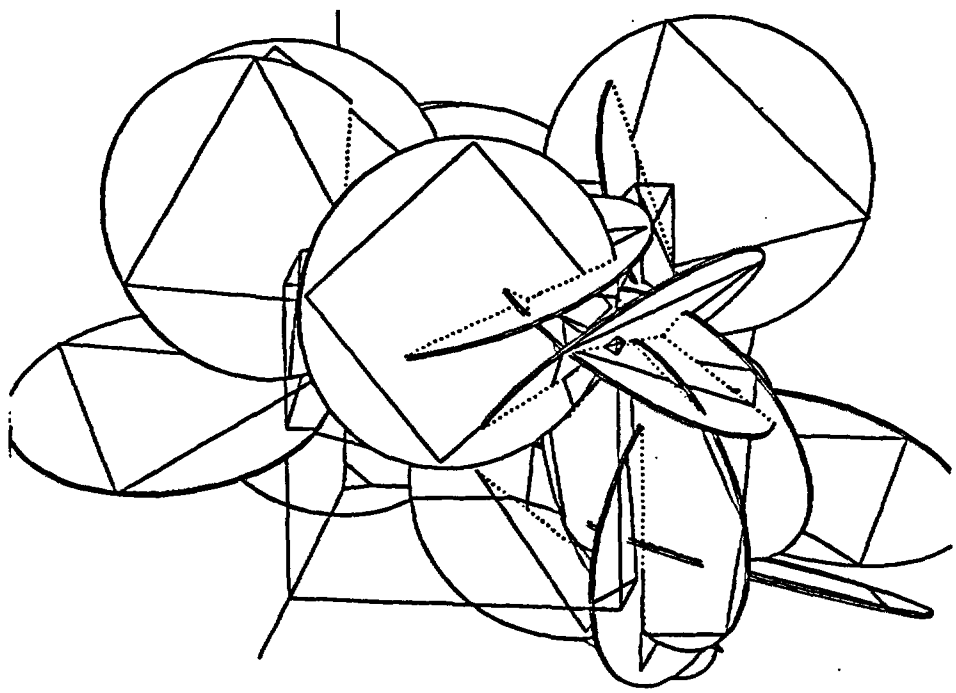
Rock block composed of real and imaginary fractures.

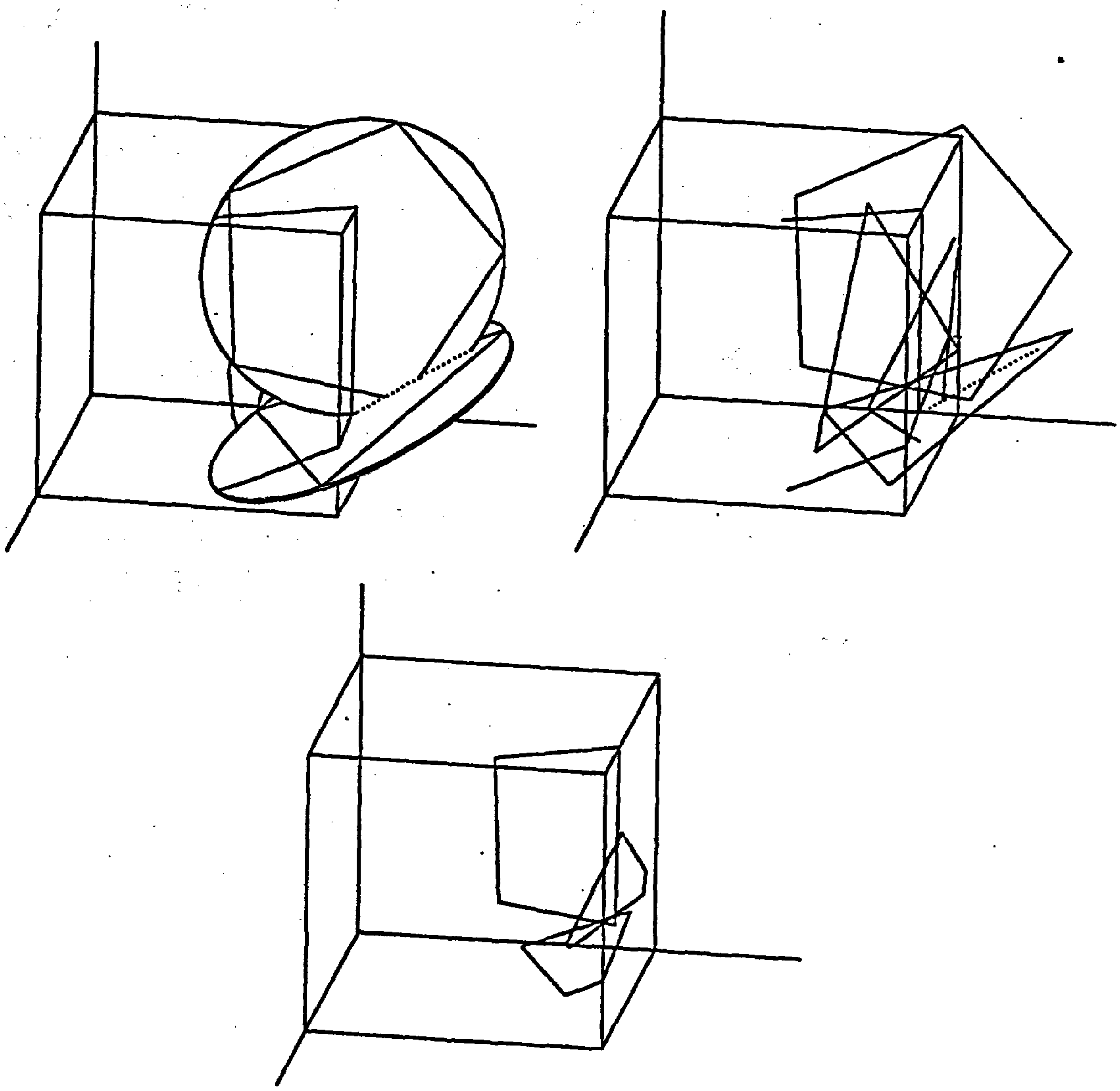


Cross-section showing matrix discretization.

Fracture Truncation at the Flow Region

- fracture intersections and fracture truncation at the edges of a cube-shaped boundary are calculated



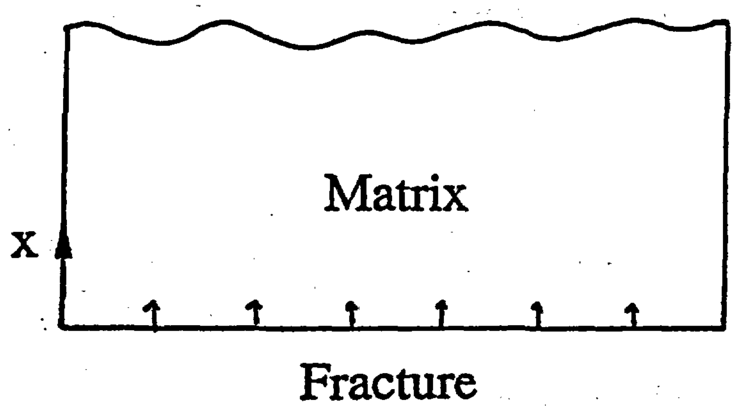


Semi-Analytical Treatment of Unsaturated Flow in Fractured Rock

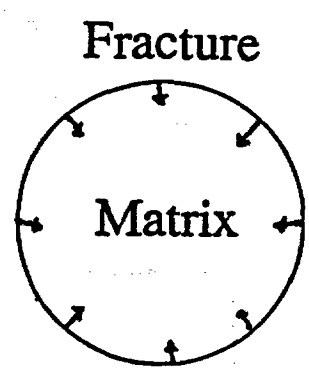
- Replace flow between fractures and matrix with an analytical expression which can then be used as a source/sink term.
- Only the fractures will be explicitly discretized in the numerical simulations.
- The number of grid blocks will be reduced, thereby greatly reducing the CPU time needed for a simulation.

Two Idealized Geometries Have Been Considered

- Flow into a semi-infinite block



- Flow into a sphere



Formulation of Problem for 1-D Flow

Governing equation for 1-D unsaturated flow:

$$\frac{\partial}{\partial x}\left[\beta k_r(\psi)\frac{\partial \psi}{\partial x}\right] = G(\psi)\frac{\partial \psi}{\partial t}$$

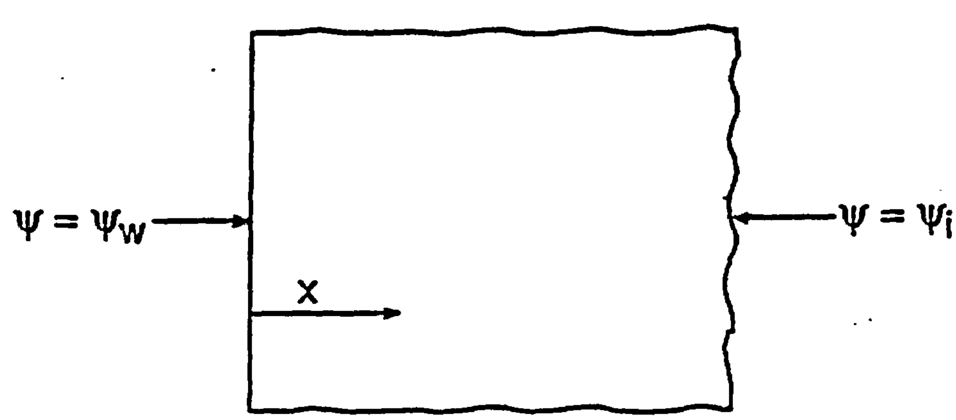
Van Genuchten form of the characteristic curves:

$$S(\psi) = S_r + (S_s - S_r)[1+(\alpha\,|\,\psi\,|\,)^n]^{-m}$$

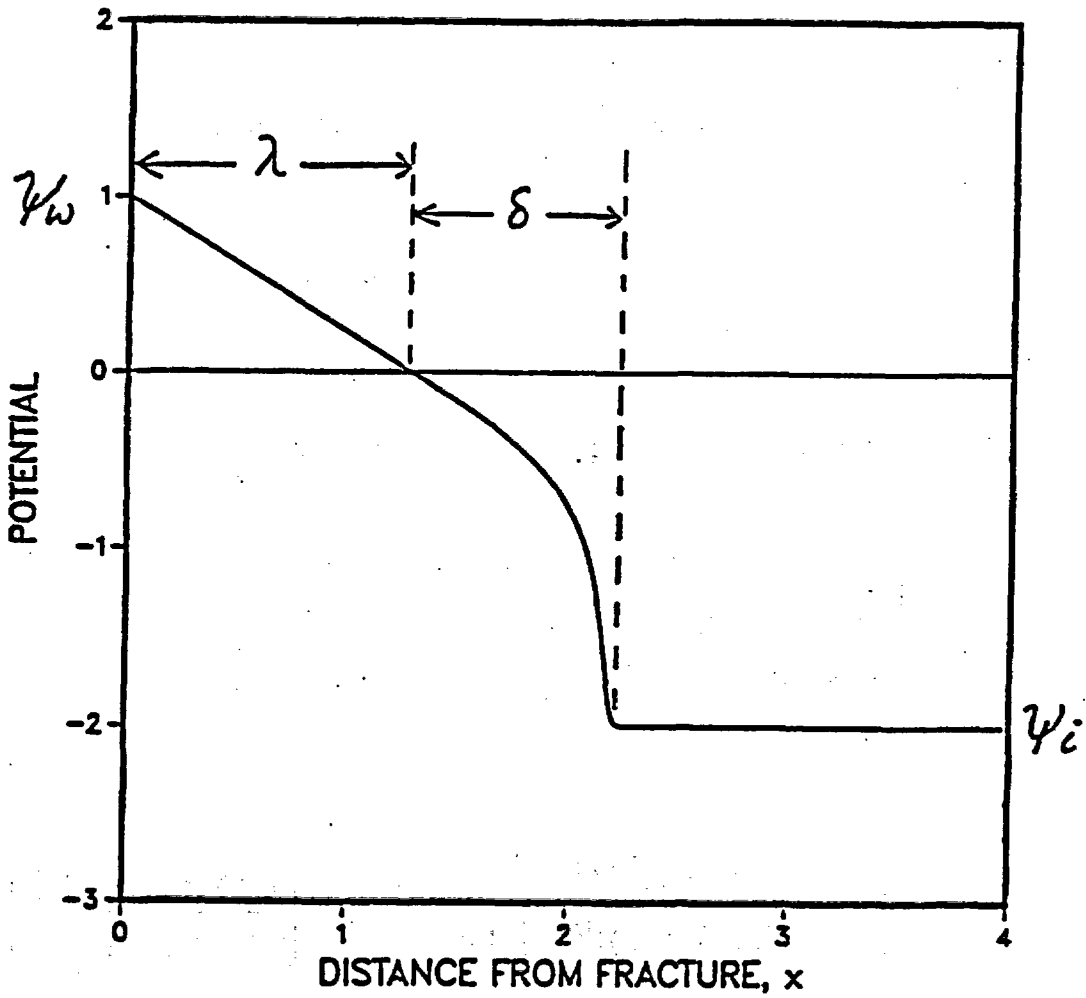
$$k_r(\psi) = \frac{\{1-(\alpha\,|\,\psi\,|\,)^{n-1}[1+(\alpha\,|\,\psi\,|\,)^n]^{-m}\}^2}{[1+(\alpha\,|\,\psi\,|\,)^n]^{m/2}}$$

Initial and boundary conditions:

$$\psi(x = 0, t) = \psi_w$$
$$\psi(x, t = 0) = \psi_i$$
$$\lim_{x\to\infty}\psi(x, t) = \psi_i$$



APPROACH: Boundary-Layer or "Integral" Method



Boundary-Layer Solution for 1-D Flow

Assumed saturation and pressure profiles:

$$\psi = \psi_w \,[1-(x/\lambda)] \qquad \text{for } \; 0<x<\lambda$$

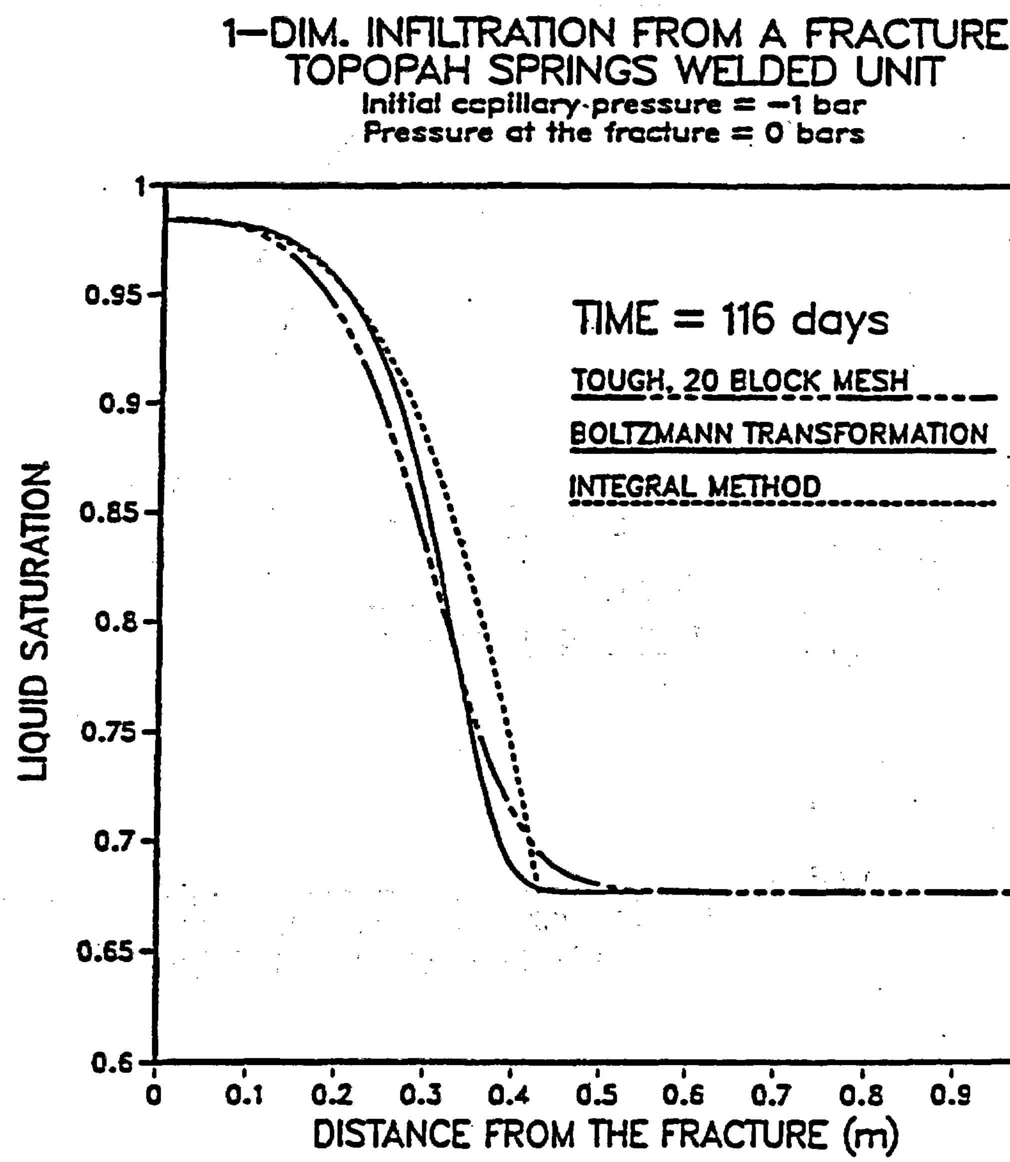
$$S = S_s + (S_i - S_s)\left[\frac{x-\lambda}{\delta}\right]^n \qquad \text{for } \; \lambda < x < \lambda + \delta$$

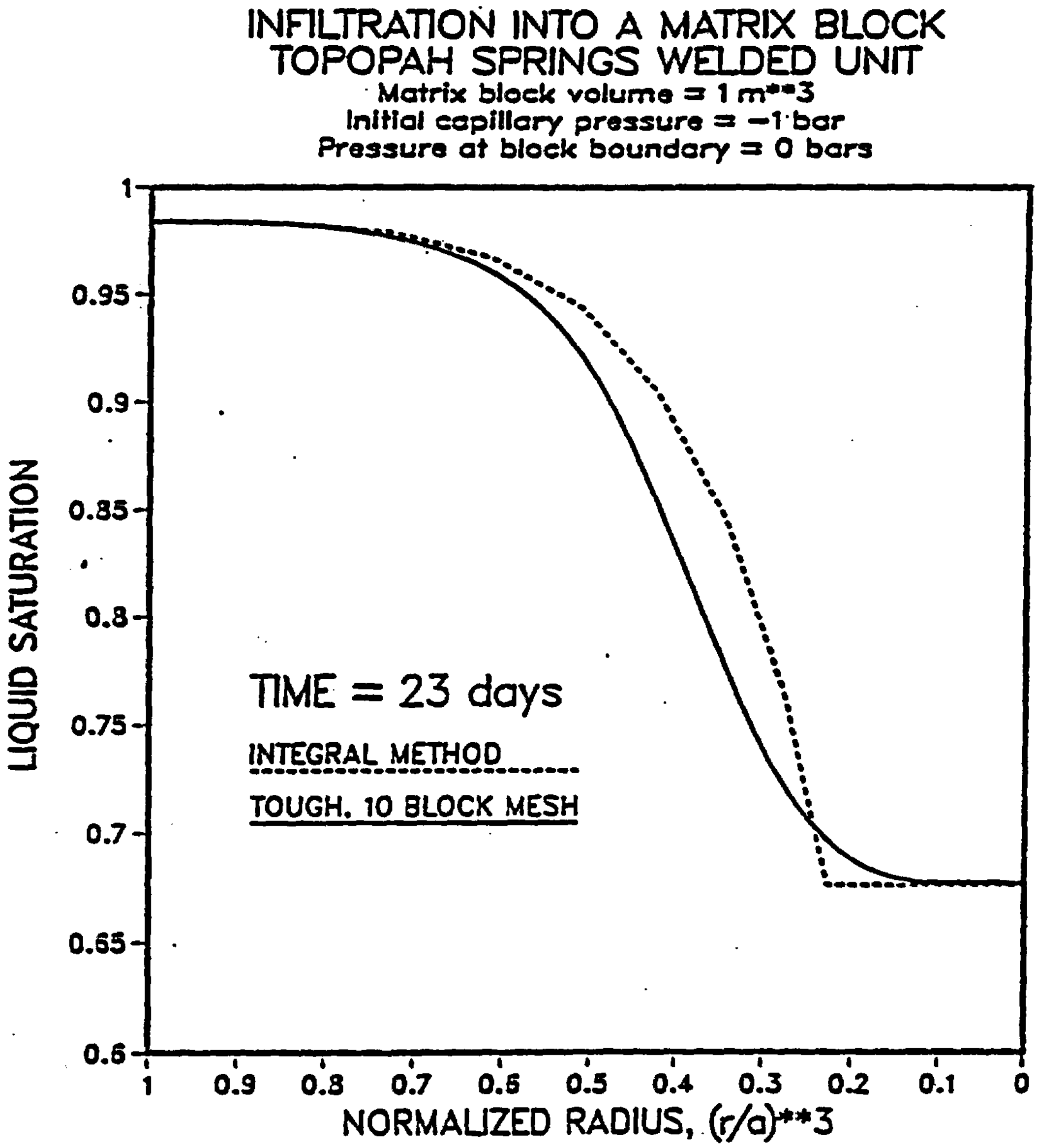
$$S = S_i \qquad \text{for } \; x > \lambda + \delta$$

Insert profiles into governing PDE and integrate:

$$\delta = \left[\frac{2kt}{\alpha\mu\phi}\frac{(S_s-S_i)^{-1+1/n}}{[m(S_s-S_r)]^{1/n}}\left\{\frac{n}{n+1} + (\alpha\psi_w)\left[\frac{m(S_s-S_r)}{(S_s-S_i)}\right]^{1/n}\right\}^{-1}\right]^{1/2}$$

$$q = \left[\frac{k\phi}{2\alpha\mu t}\frac{(S_s-S_i)^{1+1/n}}{[m(S_s-S_r)]^{1/n}}\left\{\frac{n}{n+1} + (\alpha\psi_w)\left[\frac{m(S_s-S_r)}{S_s-S_i}\right]^{1/n}\right\}\right]^{1/2}$$

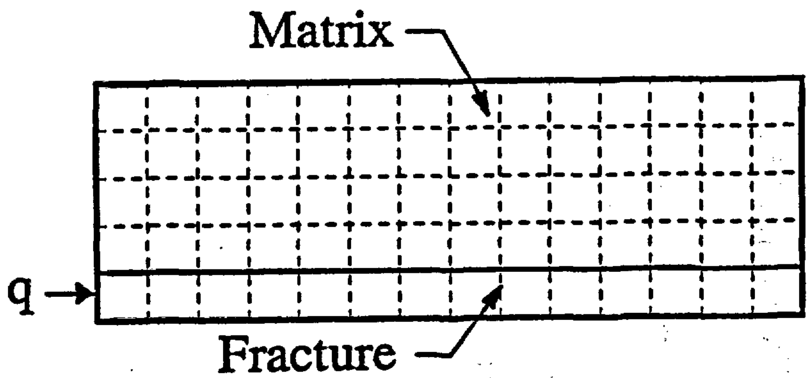

1—DIM. INFILTRATION FROM A FRACTURE
TOPOPAH SPRINGS WELDED UNIT
Initial capillary-pressure = −1 bar
Pressure at the fracture = 0 bars
TIME = 116 days
TOUGH, 20 BLOCK MESH
BOLTZMANN TRANSFORMATION
INTEGRAL METHOD
LIQUID SATURATION
DISTANCE FROM THE FRACTURE (m)
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1



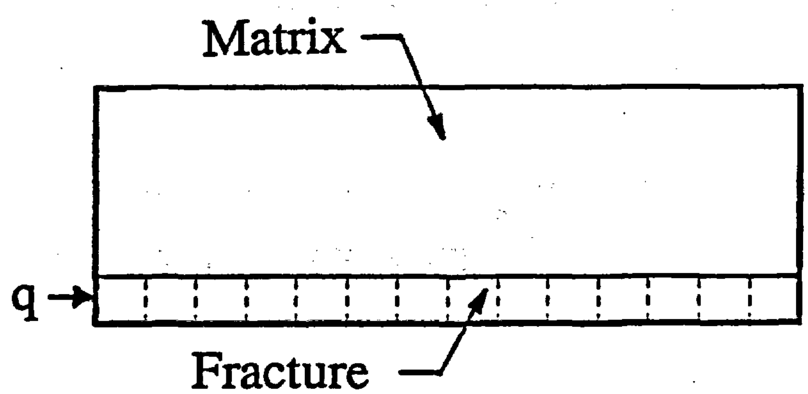
INFILTRATION INTO A MATRIX BLOCK
TOPOPAH SPRINGS WELDED UNIT
Matrix block volume = 1 m**3
Initial capillary pressure = −1 bar
Pressure at block boundary = 0 bars
LIQUID SATURATION
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
NORMALIZED RADIUS, (r/a)**3
TIME = 23 days
INTEGRAL METHOD
TOUGH, 10 BLOCK MESH

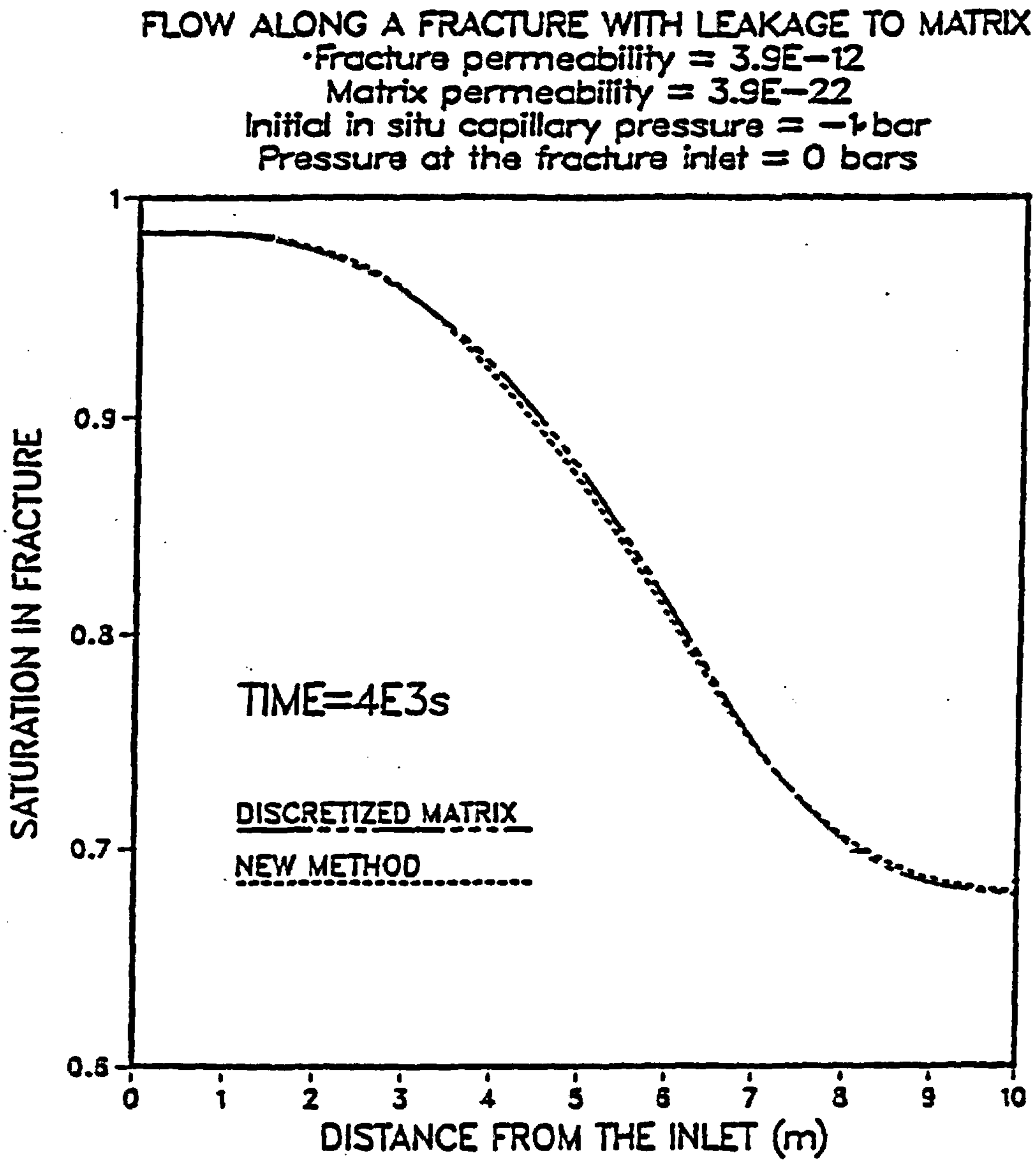
Infiltration into Matrix from a Moving Front in the Fracture

- Fully-gridded case



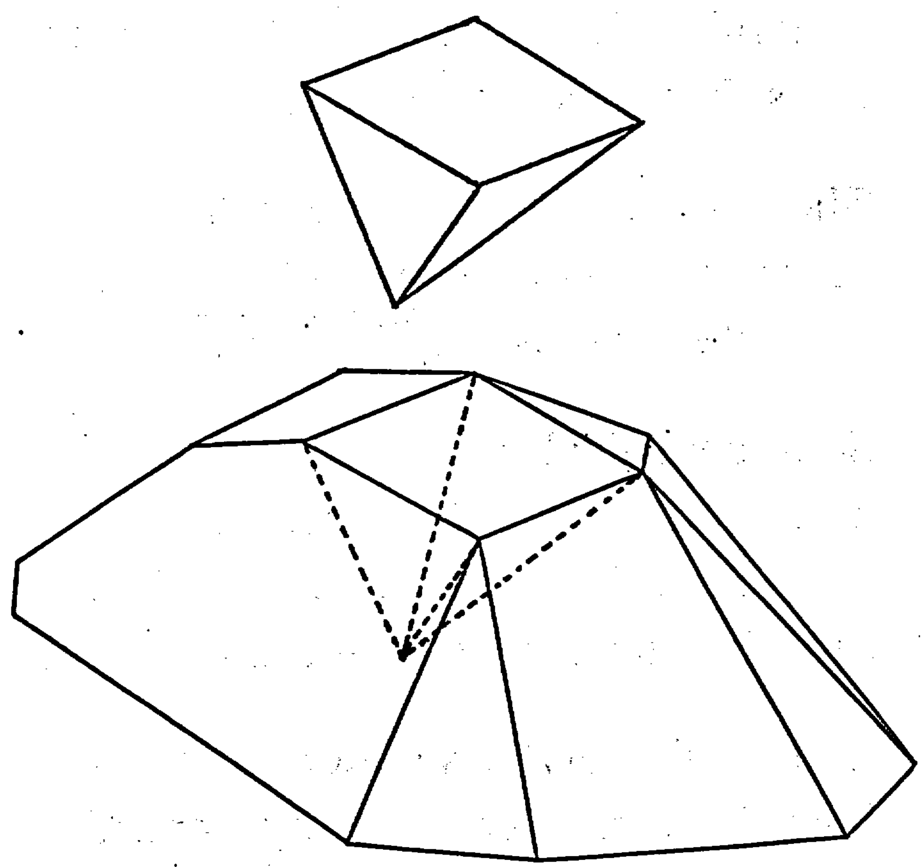
- Semi-analytic solution




FLOW ALONG A FRACTURE WITH LEAKAGE TO MATRIX
·Fracture permeability = 3.9E−12
Matrix permeability = 3.9E−22
Initial in situ capillary pressure = −1 bar
Pressure at the fracture inlet = 0 bars
SATURATION IN FRACTURE
1
0.9
0.8
0.7
0.6
TIME=4E3s
DISCRETIZED MATRIX
NEW METHOD
0
1
2
3
4
5
6
7
8
9
10
DISTANCE FROM THE INLET (m)

Extension to Irregular Geometries

"pyramid assumption"



Summary

- Fracture/matrix mesh generators are being developed to discretize both 2-D and 3-D fractured porous systems, allowing the use of integral finite-difference codes to solve for the mass, heat, and chemical transport in the system.

- The approximations made in the mesh generating programs have been found to be reasonably accurate for most applications.

- Semi-analytical solutions for fluid flow between a fracture and the rock matrix have been developed for the cases of 1-D imbibition into a semi-infinite body and into a spherical block.

- The semi-analytic solution allows for large savings in computer time by modeling the rock matrix as a source or sink.

GAMMA- AND X-RAY TOMOGRAPHY STUDIES

Silvio Crestana[1,2] and D. R. Nielsen[1]

[1]University of California-Davis and [2]UAPDIA-EMBRAPA-Brazil

Presented at NRC Workshop IV -December 1988, Tucson, Arizona

Abstract

The advent of the first commercial medical X-ray computed tomograph (CT) 15 years ago gave rise to a true revolution in radiology, particularly in medical diagnosis radiography. Although the use of tomography in medicine has been successively increased in the last 15 years, only recently it has been successfully used for rock-soil-water-plant related studies (Petrovic et al., 1982; Hainsworth and Aylmore, 1983; Crestana et al., 1985; Vinegar, 1986, and Anderson et al., 1988).

We have obtained results showing the appropriateness of CT to measure soil bulk density, soil water content in 2- and 3-dimensions, as well as related measurements for transient flow (Crestana, 1985; Crestana et al., 1985, 1988a). Three-dimensional measurement of transient flow from drip irrigation in a soil column and seed germination growth and uptake of water by roots (Crestana, 1985; and Crestana et al., 1988a) has been achieved. Several results involving soil systems like plant, seeds, insects and cone penetrometer interactions have also been presented (Tollner et al., 1987). Using a third-generation commercial X-ray computerized tomograph, several non-swelling soil columns of different initial water contents and bulk densities were scanned to obtain 2-dimensional images (Crestana et al., 1988b). The infiltration process was capable of being monitored every 6·7s. Water content distribution as a function of position and time allowed the calculation of the soil-water diffusivity. A comparison of the data from infiltration and the solution of Richards' equation has demonstrated the utility of the method.

Two limitations of the CT technique exist: the complexity and the high cost of commercial tomographs. We were able to design and build for the first time a simple and inexpensive X- and γ-ray CT micro-scanner dedicated to soil science investigations (Crestana, 1985; Crestana et al., 1986, 1988a; Cruvinel, 1987; and Cesareo et al., 1988). Subsequently, we have successfully used the instrument in a variety of measurements described briefly in the following paragraph.

Undisturbed soil clods submitted to successive plowing processes in the field were scanned using the CT micro-scanner (Vaz et al., 1988). It was possible to observe and measure a thin compacted layer present in the clods. One of the advantages of the CT micro-scanner over the γ-ray absorption apparatus is the possibility to perform 2- and 3-dimensional scans of soil samples (non-disturbed) independent of the geometry and the shape of each sample. Our CT micro-scanner allows the use of several beam energies and different radiation sources stemming

from different istopes or X-ray fluorescence. We have demonstrated that the use of 30 to 40 Kev is the best energy for water-content resolution rather than that of 60 Kev supplied commercially. The technique of differential tomography (DCAT) was also employed to quantify water draining in soil, taking advantage of the photoelectric discontinuity of Iodine when we employed the radiation of Barium (32 Kev) or Cerium (34.5 Kev) as secondary targets of an X-ray source. The use of Thulium (59.3 Kev) in the soil as a tracer allows us to enhance the soil-water images when we employed a source of Americium (59.6 Kev). In conclusion: fluorescent radiation, tracers, CT, and DCAT provides new exceptional possibilities to study basic and applied soil-rock processes such as absorption and redistribution of water, nutrients or pollutants, the uptake of water-solutes by plant roots as well as high resolution 2- and 3-phase system measurements in fractured and cracked porous media like rocks and swelling soils.

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--Anderson et al., 1988. Soil Sci. Soc. Am. J. 52:35-40.

--Crestana, S., 1985. Ph.D. Thesis. USP-SP-BRAZIL.

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SOLUTE MOVEMENT IN DUAL-POROSITY MEDIA

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ABSTRACT

Solute transport models based on the classical (Fickian) advection-dispersion equation (ADE) have been, and will remain, important tools for predicting the movement of solutes in soil and aquifer systems. Unfortunately, predictions obtained with these ADE type models are often of limited value when dealing with heterogeneous field soils. Small-scale (local) and large-scale (global) heterogeneities occur in soils because of the problem of preferential flow through soil macropores, and because of soil spatial variability (notably in the unsaturated hydraulic properties) across the landscape. Prefential flow stems from the presence of decayed root channels, drying cracks in fine-textured soils, worm and gopher holes, voids in naturally aggregated soils, fractured unsaturated rock, or other types of macropores. Preferential flow often also results from wetting front instabilities caused by hydrophobicity and/or soil layering.

Increasingly complex mathematical models have been developed over the years to deal with preferential flow in macroporous field soils. A common feature of these models is the assumption that dissolved solutes move by advection (convection) and dispersion through well-defined pores and cracks, while solute transfer between liquid-filled macropores and the soil micropores occurs by diffusion. A large number of such geometry-based two-region models currently exist, alternatively termed also mobile-immobile, bi-continuum, and dual-porosity (or double-porosity) models. Analytical and numerical solutions have been derived for a variety of agggregate geometries, including spherical, cylindrical and rectangular aggregates. While geometry-based models are conceptually pleasing and have resulted in improved predictions, the question remains whether or not such models are too complicated for routine use. They

require a large number of transport parameters which are often difficult to measure independently, especially in the field. Some of these parameters are also variable in time and space, especially during transient unsaturated flow involving alternate wetting and drying cycles. In addition, water in a macroporous soil may not necessarily flow in a manner that is consistent with the macropore network, e.g., because of flow channeling inside the macropores, wettability problems, or because of macropore discontinuities.

As an alternative to geometry-based models, dual-porosity type approaches may be formulated assuming first-order mass transfer between mobile and immobile liquid regions. These types of lumped first-order approaches are less parameter-intensive, yet include the basic processes responsible for physical non-equilibrium during transport in structured soils. The approach generally assumes that field-tracer experiments can be carried out for calibration purposes. An advantage of the lumped approach is that the method can be effectively included into relatively simple management-oriented models. Moreover, equations have been developed that accuractely predict the previously unknown mass transfer coefficient from readily observable field data, including aggregate geometry, aggregate size, and the solute diffusion characteristics of the medium. An additional advantage is that the lumped mobile-immobile water flow approach can be readily incorporated into stochastic formulations (e.g., transfer function type models) of solute transport in spatially variable field soils.

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Pore Structure Properties of Tuff:
A Preliminary Study of Experimental Methodology

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University of New Mexico
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Sandia National Laboratories

Why Study Pore Structure?

1. Matrix flow
2. Retardation
3. Fracture/Matrix interface

Pore Structure Analysis

1. Mercury porosimetry
2. Nitrogen adsorption
3. Microscopy
4. SAXS/SANS
5. CAT Scanner
6. NMR relaxation
7. MRI

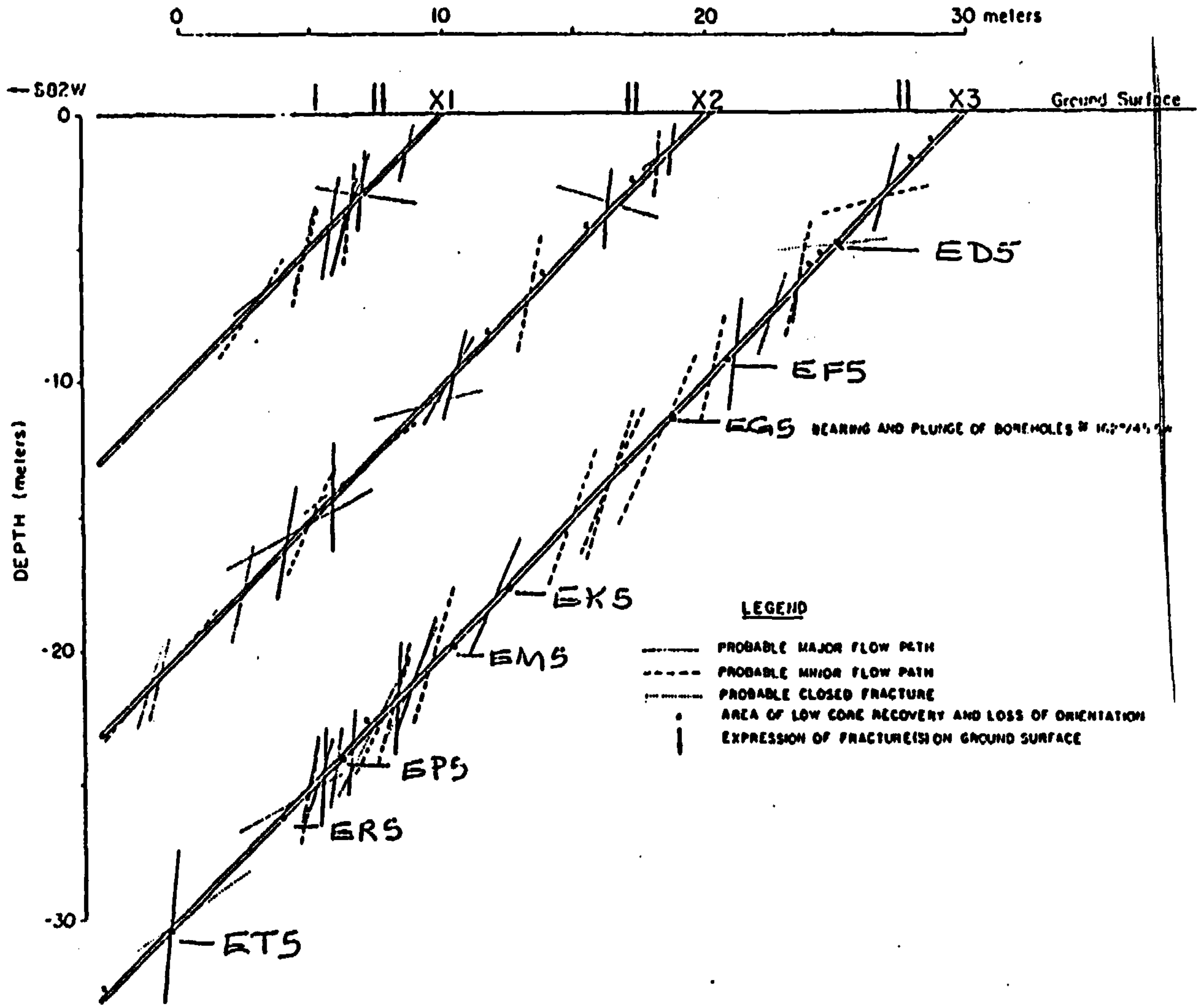


Figure 1 Cross-section of Apache Leap borehole indicating core sample location.

Mercury Porosimetry
Advantages

1. Fast
2. Wide pore size range
3. Reproducible
4. Widely applied

Mercury Porosimetry - Disadvantages

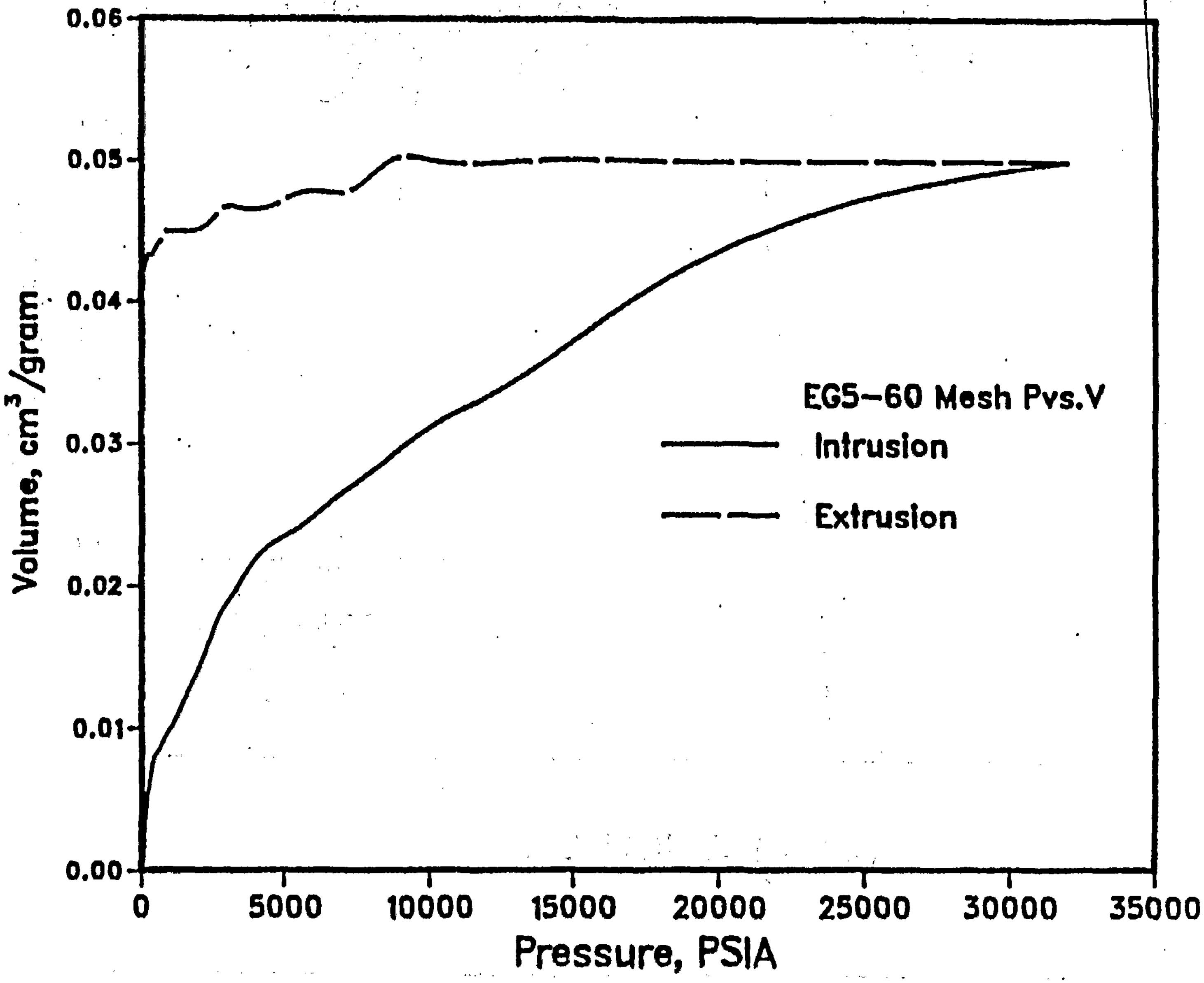
1. Network / Percolation effects

2. Assumed Pore Shape

3. Sample Compression

4. Dry Materials

5. Contact Angle / Surface Tension Uncertainty



EG5-60 Mesh Pvs.V
Intrusion
Extrusion
Volume, cm³/gram
Pressure, PSIA
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0
5000
10000
15000
20000
25000
30000
35000

134

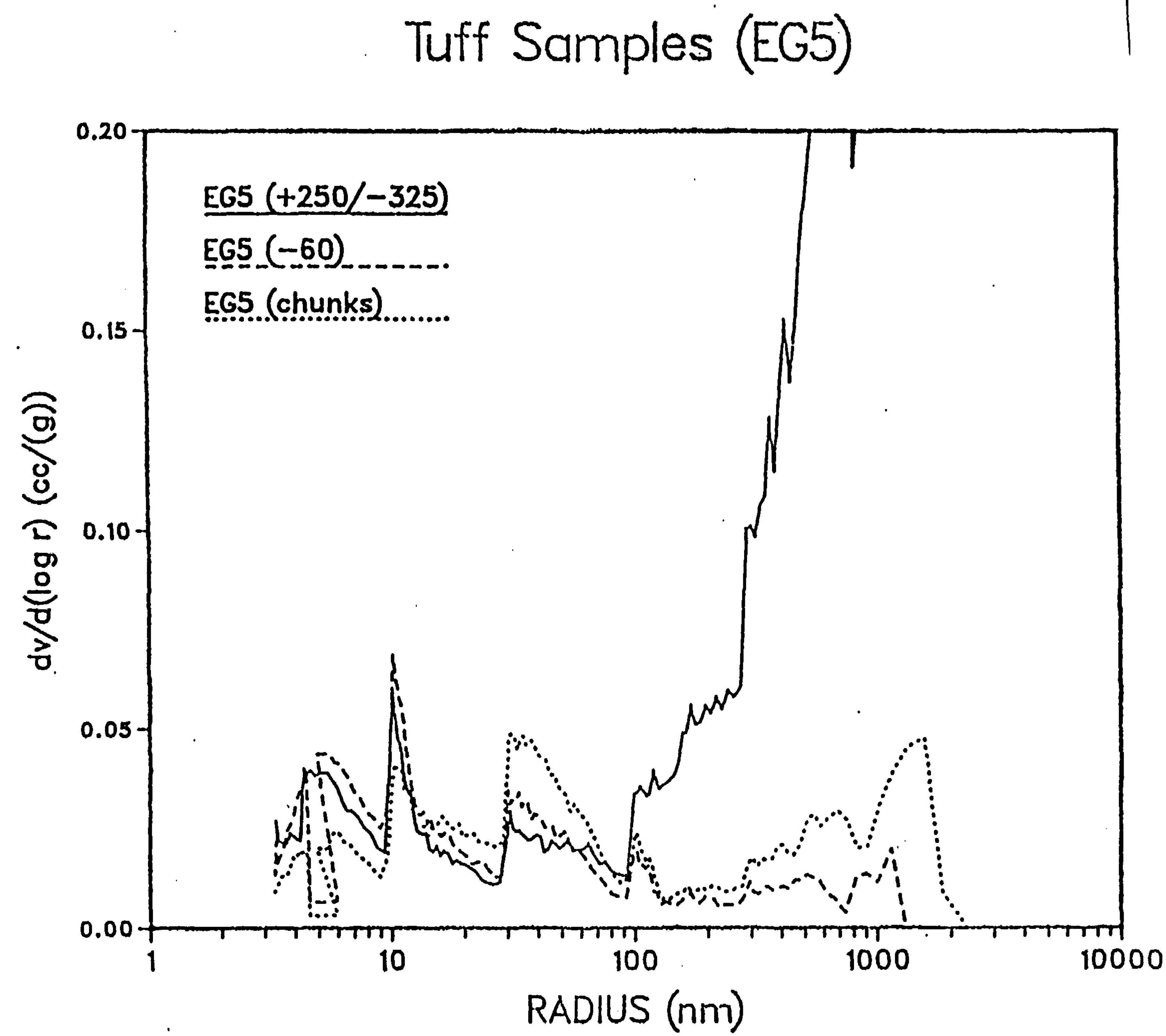


Figure . Effect of particle size on mercury porosimetry pore size distributions (EG5)

Pore Volume - Mercury Porosimetry

Sample	Pore Volume (cc/g)
EG5 (−250/+325)	0.31
EG5 (−60/+140)	0.050
EG5 (chunks)	0.062
SNL (−250/+325)	0.35
SNL (chunks)	0.077

Nitrogen Condensation Advantages

1. Very accurate (1–10nm)
2. Reproducible
3. Widely applied

Nitrogen Desorption - Disadvantages

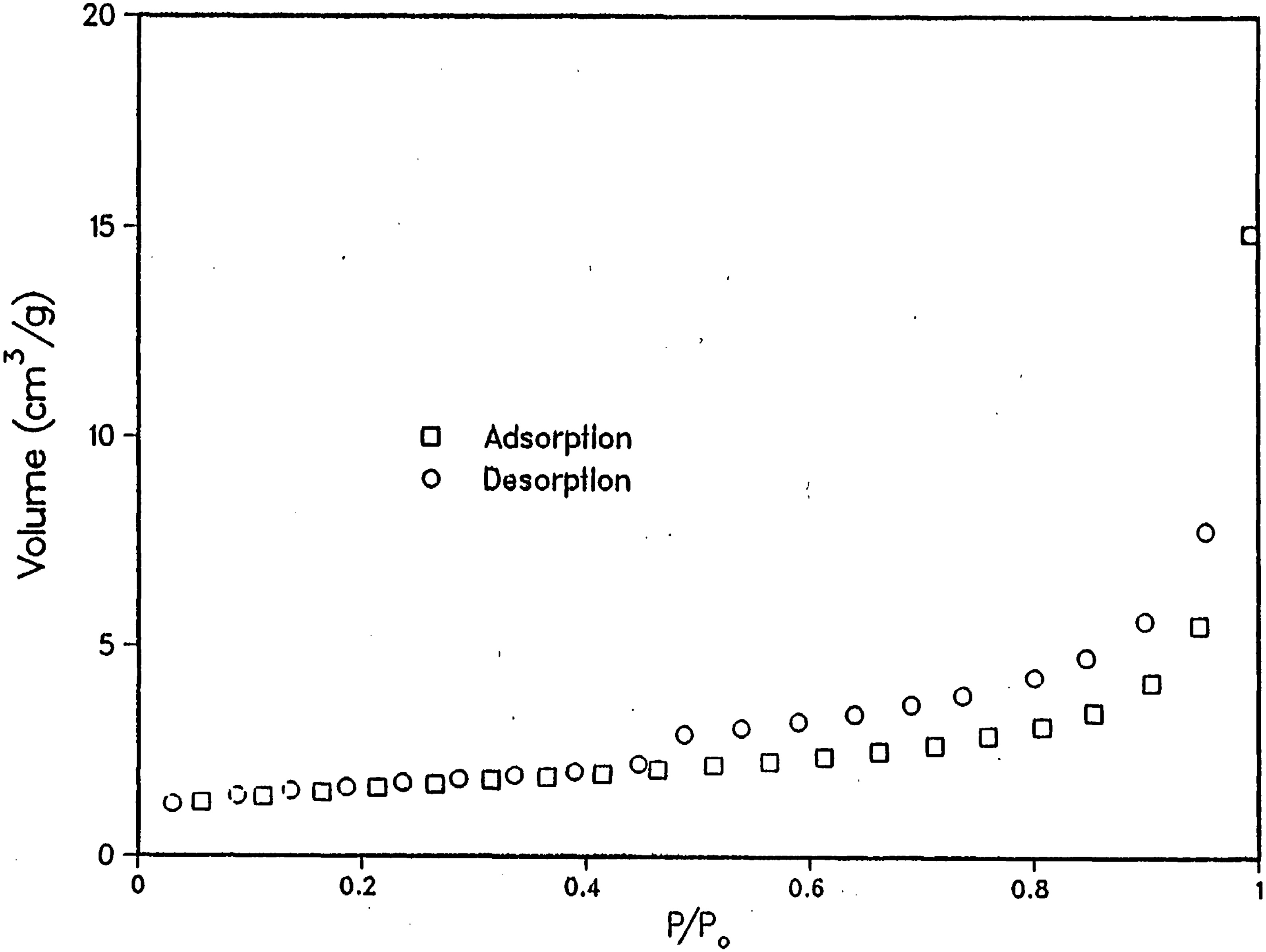
1. Network / Percolation effects

2. Assumed Pore Shape

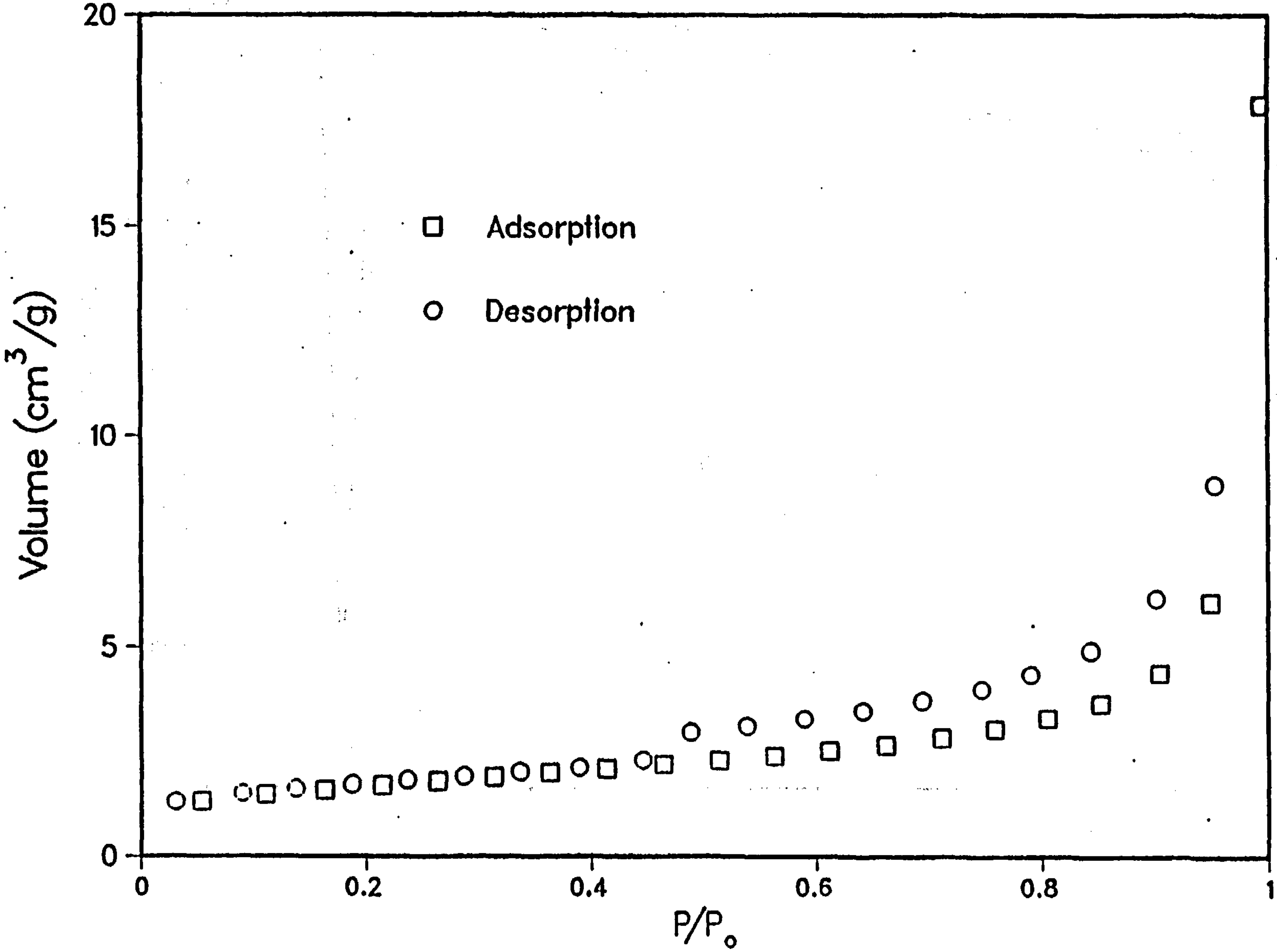
3. Dry Materials

4. Time Consuming

5. Adsorbed Film Correction



Fig[illegible] 5A. [illegible]sor[illegible]n/d[illegible]pti[illegible] iso[illegible]ms f[illegible] EK5


20
15
10
5
0
Volume (cm^3/g)
0
0.2
0.4
0.6
0.8
1
P/P$_o$
Adsorption
Desorption

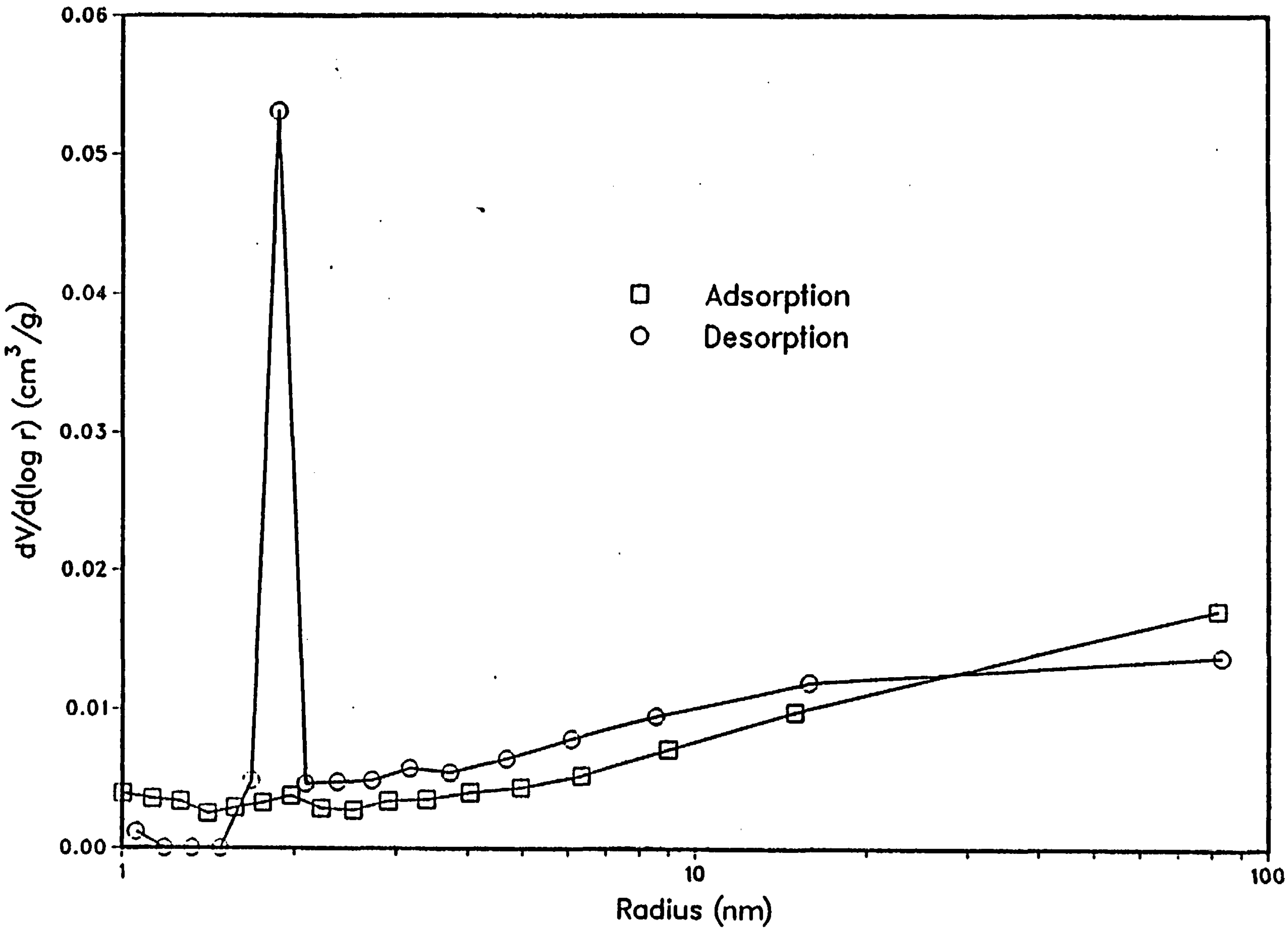


Figure 6A. Pore size distributions for EK5.

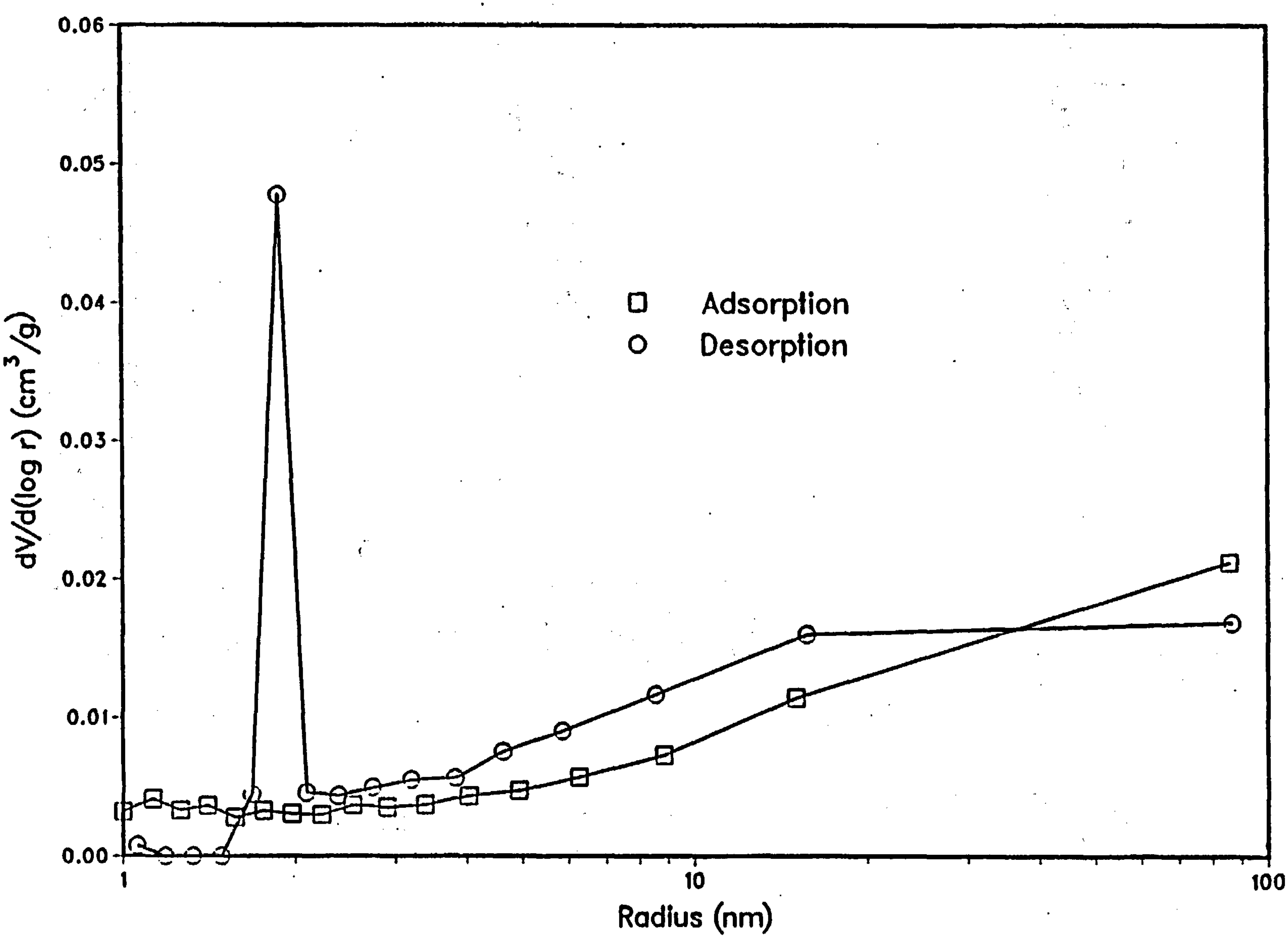


Figure 6B. Pore size dsitrbutions for ET5.

Surface Area(-250/+325)

Sample	Nitrogen(m^2/g)	Mercury(m^2/g)
ED5	5.1	9.0
EF5	5.4	6.6
EG5	4.4	8.6
EK5	5.4	7.6
EM5	4.6	7.2
EP5	4.9	7.8
ER5	4.9	6.2
ET5	5.7	9.4
SNL	1.8,2.1	3.2

Pore Volume - Comparision

Sample	Nitrogen(cc/g)	Mercury(cc/g)
EK5	0.023	0.40
ET5	0.028	0.38

Surface Area - Particle Size Effect

Sample	Nitrogen (m^2/g)	Mercury (m^2/g)
EG5(−250/+325)	4.4	8.6
Eg5(−60/+140)	----	8.3
EG5(chuncks)	----	5.6
SNL(−250/+325)	1.8,2.1	3.2
SNL(chunks)	----	1.8

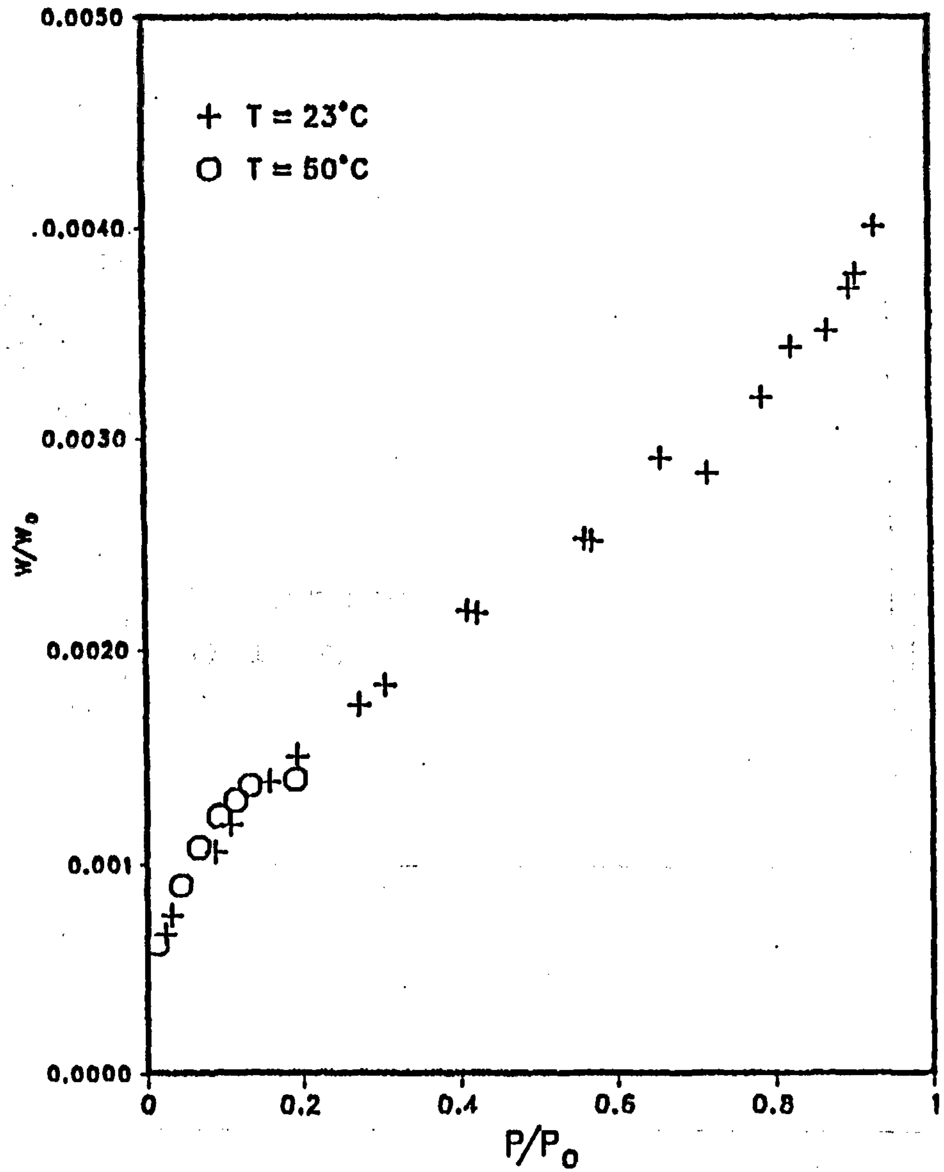


Figure 7 Water adsorption isotherms for EK5.

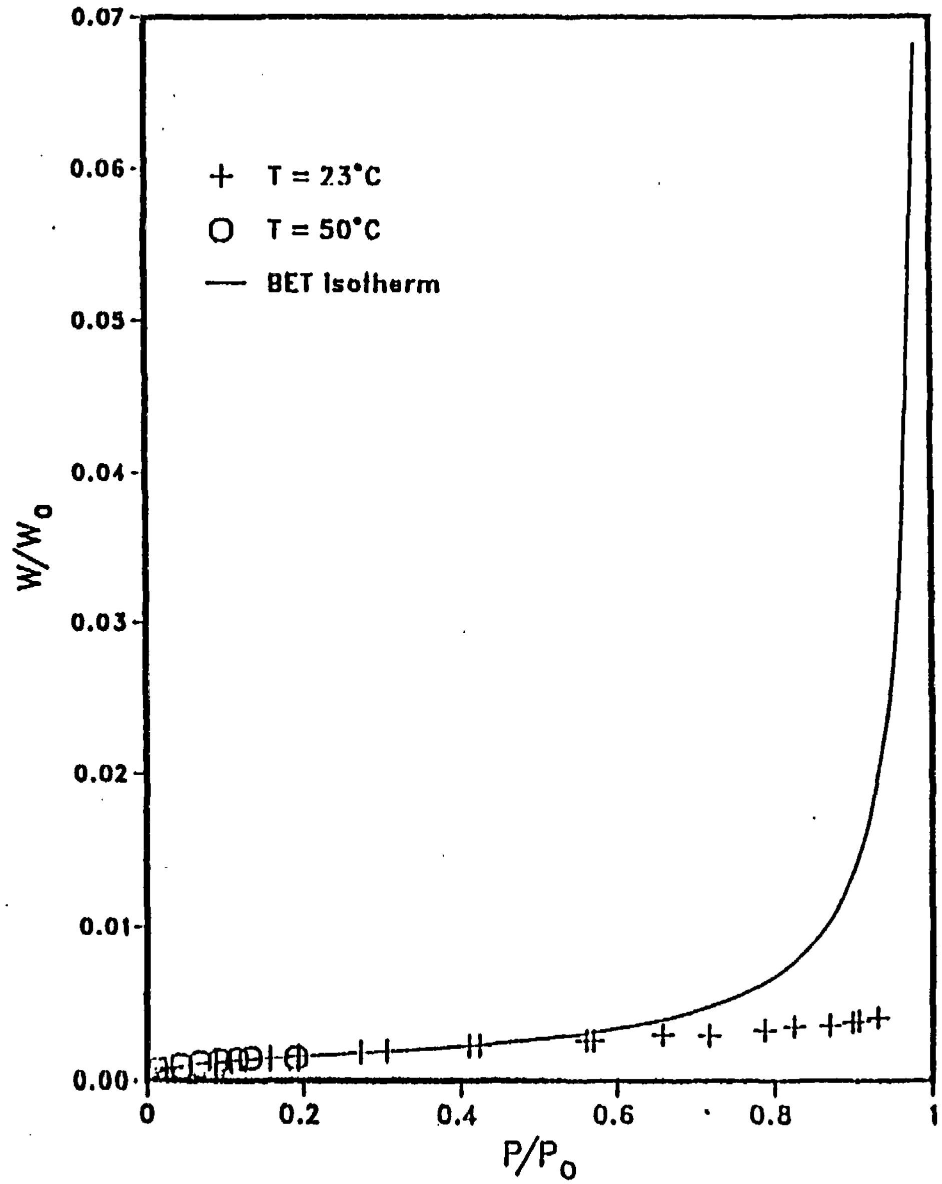


Figure 9 Comparison of measured water uptake and BET isotherm.

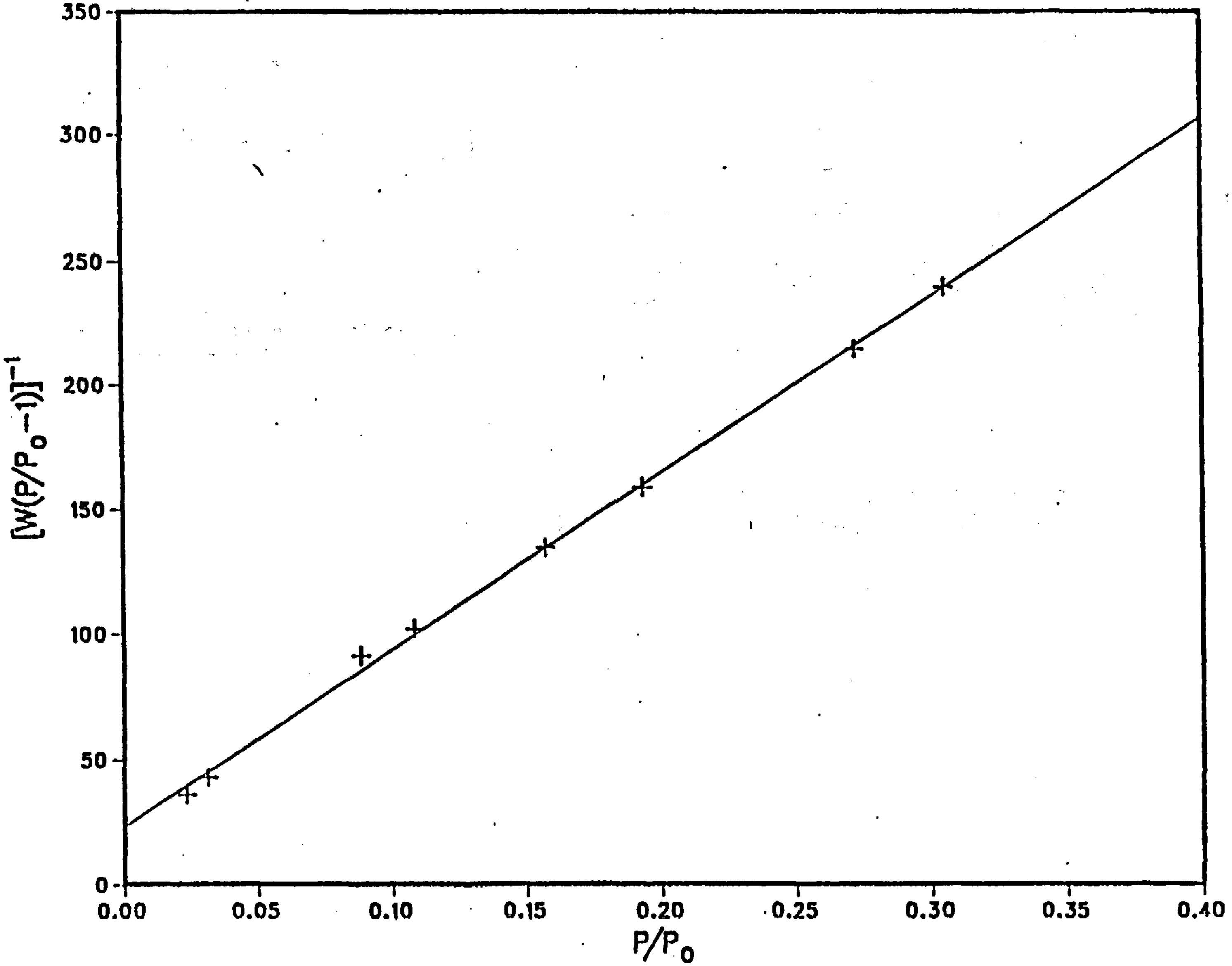


Figure 8 BET plot of water adsorption at 296 K on EK5.

Water Adsorption

Sample: EK5

	Surface Area(m^2/g)	C
Nitrogen (77 K)	5.4	>100
Water (296 K)	4.9	30

SCALING OF MATRIC HYDRAULIC PROPERTIES

A. W. WARRICK

NRC Workshop IV
December 1988
Tucson, Arizona

Abstract

Scaling is the quantification of heterogeneity of observations or processes from site to site. The advantage sought is to lump variability associated with a given site into a single parameter (or at least to reduce the necessary number of parameters).

Several approaches are used (see Tillotson and Nielsen, 1984; Sposito and Jury, 1985). The "original" form was based on similitudes of the microscopic system. If the medium is "similar" then the pressure head h for any constant degree of saturation is inversely proportional to the scaling length; the hydraulic conductivity is directly proportional to the square of the same scaling length. Expanded analyses relax the constraint of true similarity. A functional form is assumed for the "average" and the equivalent of the scaling length is chosen by "best-fitting" the assumed functions to the experimental data. The "characteristic lengths" lose their strict interpretation and are simply called "scaling coefficients." In fact, the scaling coefficients for the different hydraulic functions are no longer required to be identical. Examples are given in Warrick et al. (1977) and Warrick and Nielsen (1980).

For the ALTS data, scaling was applied to the moisture characteristics and the permeability data. For the moisture characteristics, the scaling coefficients were "best fit" by minimizing the sum of squares:

$$SS = \Sigma_{r,i} (\log \hat{h}_{r,i} - \log \alpha_r h_{r,i})^2 \qquad [1]$$

where

$$\hat{h} = (S^{[n/(n-1)]} - 1)^{(1/n)} \qquad [2]$$

following "van Genuchten's" relationship. The sites are indexed by r and the measurement suctions are $h_{r,i}$. Minimization of Eq. 1 for a given n results in alphas given by

$$\log \alpha_r = (1/I)(\Sigma_{r,i} \hat{h}_{r,i} - \Sigma_{r,i} h_{r,i}) \qquad [3]$$

The algorithm used first specified n and then solved for the alpha's and SS until the minimum SS was determined.

Laboratory results consisted of degree of saturation for 6 pressure increments on the 105 "big" cores along with all of the results for the "small" cores for which the suction exceeded 10 bars. The large core results were determined on pressure plate measurements; the small core results were based on psychrometric measurements.

Results include the scaled moisture retention relationships. The SS in Eq. 1 was 118 (for 1211 observations) compared to 164 when an average scaling coefficient is used. (The mean and variance of log alpha was -1.9 and 0.0387; the best and worst mean square error for individual sites were 0.103 and 0.787, respectively). The result obtained if only the large core results are used is more or less equivalent to those by fitting individual n and alpha for each core. The resulting alpha values are well approximated by a log normal distribution.

Scaling coefficients were also determined based on saturated conductivities of the 105 large cores and air permeabilities of the large cores. Results were less impressive. Perhaps this can be explained by the fact that in these cases the scaling coefficient was for only 1 data point, whereas for the moisture characteristics each scaling coefficient was based on generally 10 or more data points. Outliers were not removed.

Synthetic moisture characteristics were generated by choosing random alpha and error components based on

$$\log h_{r,i} = \log (\hat{h}_{r,i}/\alpha_r) + \epsilon_{r,i} \qquad [4]$$

where alpha was taken from a random log normal distribution and epsilon from a normal random population with zero mean and variance of (118/1211) based on the original fit. The results are qualitatively similar to the input values except for the low suction ranges where the original data tended to be more dispersed.

The overall results are that scaling results are promising for the moisture characteristic results, but are less impressive for the permeability. Alternative fitting criteria should be examined as to whether outliers near the wet end could be dealt with more effectively.

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AWW

SCALING OF MATRIC HYDRAULIC PROPERTIES

A. W. WARRICK
December 1988

Introduction

What is it?
Quantification of similarities of observations or processes from site to site

Why?
Express variability into a single parameter (or at least reduce necessary number of parameters)

How?
Microscopic similitude analysis ("Original")

*Expanded similarity analysis (Assume functional forms and use the best fit)

AWW 2

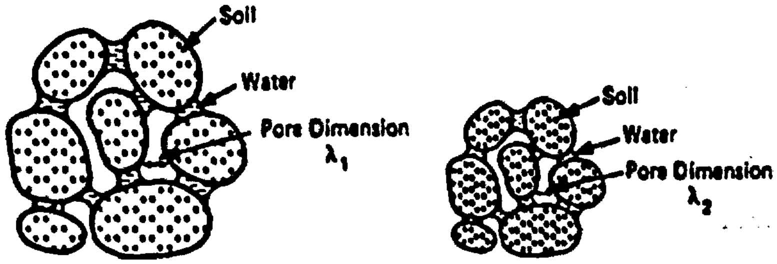


FIG. 6. Schematic illustration of scale similarity in soils.

Consequences with respect to h vs. S and K vs. S

$$h_1/h_2 = \lambda_2/\lambda_1$$

$$K_1/K_2 = (\lambda_1/\lambda_2)^2$$

Therefore

$$(\alpha\ h) = \text{function\_1}(S)$$

$$(K/\alpha^2) = \text{function\_2}(S)$$

where function_1 and function_2 are independent of location. (Note if consider saturated only then function_2(S) is a constant)

If have true similarity the alpha's from h's are the same as alpha's from K's, otherwise generally are fit independently.

/JW'

<u>Background examples</u>

Panoche K and h
   20 locations x 6 depths
   (over 150 hectares and
            30, 60, .. 180 cm)

   function 1 = (4th order polynomial)/S

   function 2 = 3rd order polonomial

See Fig. 2, 3, 9, 10 from 1977 paper

Scaling infiltration
   Write dimensionless Richards' Eq.
   Express Philip's solution in terms
   of scaled variables resulting in one
solution for all alpha's

See Table 13.4 and Figure 13.5 of 1980
paper

AMW 4

ALTS Moisture Characteristics

Large core (pressure plate)
105 "locations", 5 suctions
Small core (psychrometer)
105 "locations", 7-14 suctions
(Used only suctions > 1000 kPa)

Criterion used:

Minimize

$$SS = \Sigma_{r,i} \left(\log \hat{h}_{r,i} - \log \alpha_{r,i} \right)^2$$

where

$$\hat{h} = \{ S^{[n/(n-1)]} - 1 \}^{(1/n)}$$

("van Genuchten's" relationship)

For given n have

$$\log \alpha_r = (1/I)(\Sigma_{r,i} \hat{h}_{r,i} - \Sigma_{r,i} h_{r,i})$$

AWW 5

Algorithm:

Specify several n values
Calculate set of alpha's and
resulting SS for each n
Choose single n giving best SS

See results for
$S_{r,i}$ vs. $\hat{h}$ and
(mean α $h_{r,i}$)
* ~~$\alpha_{r,i}$ vs. $h_{r,i}$)~~
1:1 plots (2 of them)
Frequency distribution of alphas

ALTS Saturated K's (Big cores)

$\alpha_r = K_r^{0.5}$

See frequency distribution of log K

AWW 6

Deconvolution

$$\log \hat{h}_{r,i} = \log h_{r,i} - \log \alpha_r + \epsilon_{r,i}$$

Procedure:

Generate log normal alphas and use epsilon log normal. Use epsilon normal random with zero mean and variance based on r.m.s.

See synthetic h vs. S

Conclusions

The chosen moisture characteristics scale reasonably well

The chosen conductivities did not scale very well

Need to look at some other best-fitting criteria for alpha's. Also, may want to delete some outliers on K.

AWW 7

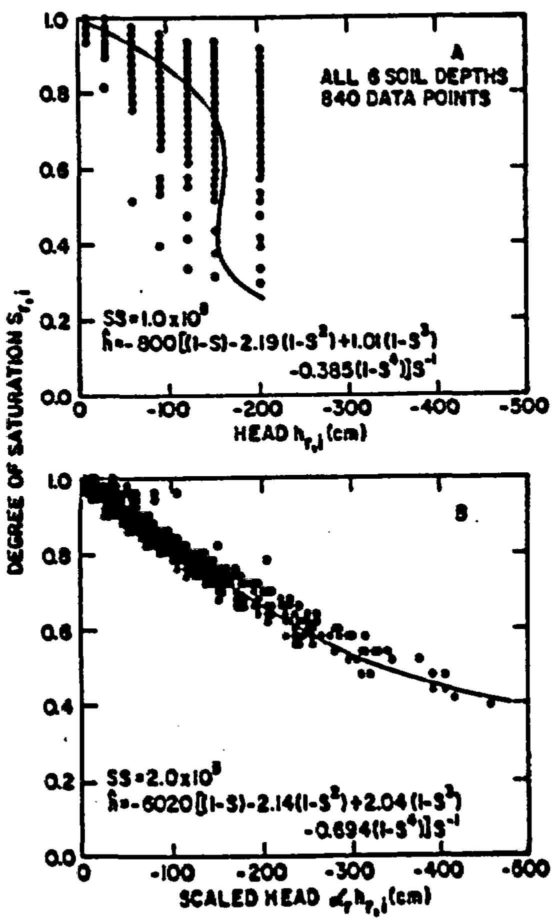


Fig. 2. Soil water characteristic data for six depths of Panoche soil: (*a*) unscaled and (*b*) scaled.

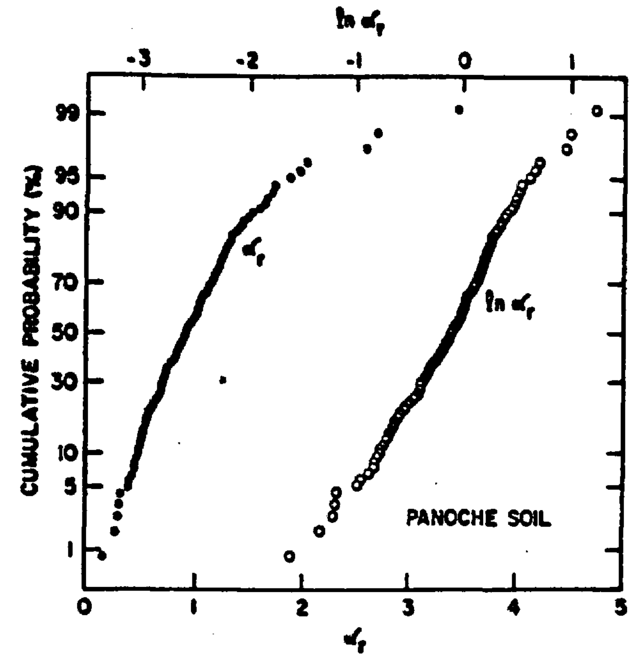


Fig. 3. Probability plots of α_r and ln α_r calculated from soil water characteristic data for all six depths of Panoche soil.

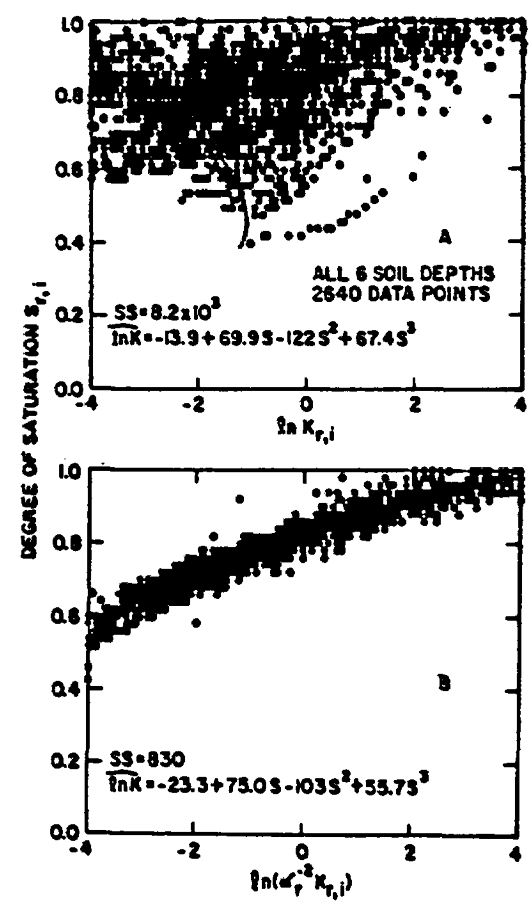


Fig. 9. Hydraulic conductivity data for all six depths of Panoche soil: (*a*) unscaled and (*b*) scaled.

AWW 8

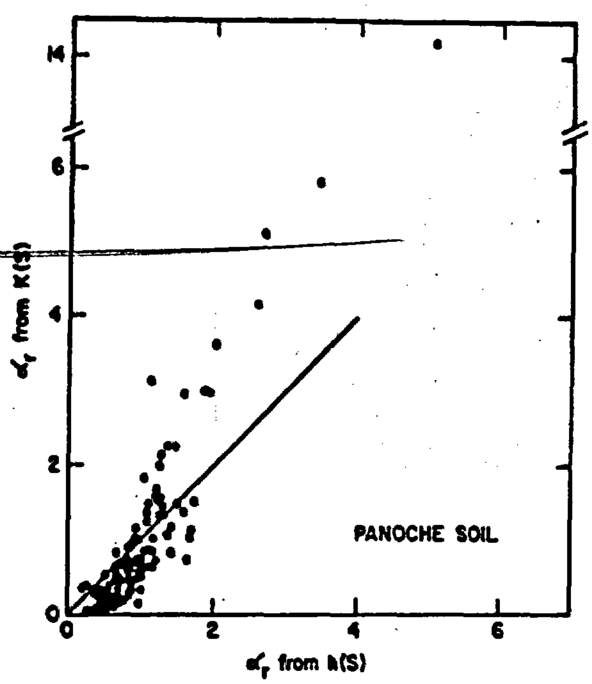


Fig. 10. Values of α_r calculated from hydraulic conductivity data versus those calculated from soil water characteristic data for all six depths of Panoche soil.

Table 13.4
VALUES FOR λ, χ, AND ψ*

s	λ	χ	ψ
0.939	0.0	0.0	0.0
0.867	18.4	4.92	0.778
0.798	22.8	4.15	0.607
0.728	24.2	3.79	0.592
0.657	24.8	3.63	0.591
0.587	25.1	3.55	0.591
0.517	25.3	3.50	0.592
0.446	25.5	3.47	0.592
0.376	25.5	3.45	0.592
0.305	25.6	3.44	0.592
0.235	25.6	3.43	0.592
0.164	25.6	3.43	0.592
0.0939	25.6	3.43	0.592
0.0235	25.6	3.43	0.592
0.0	∞	3.43	0.592

* After Warrick and Amoozegar-Fard, 1979.

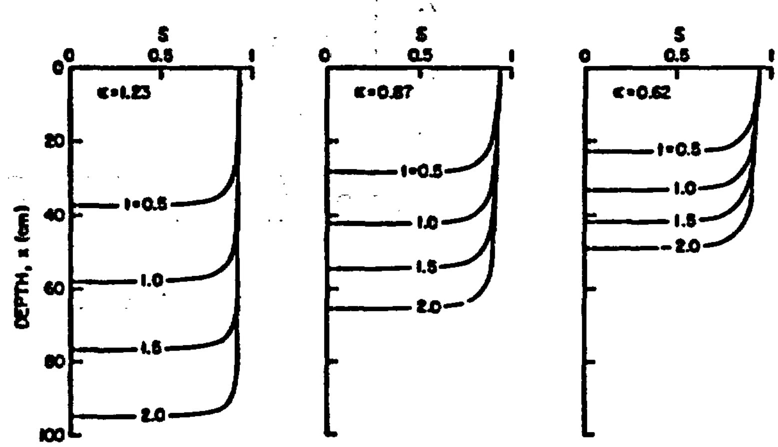
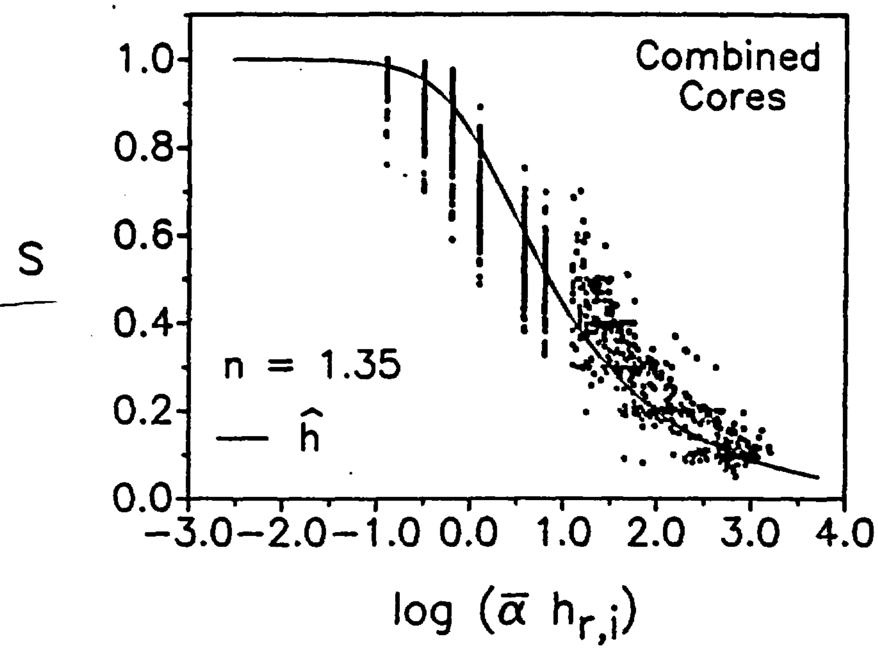
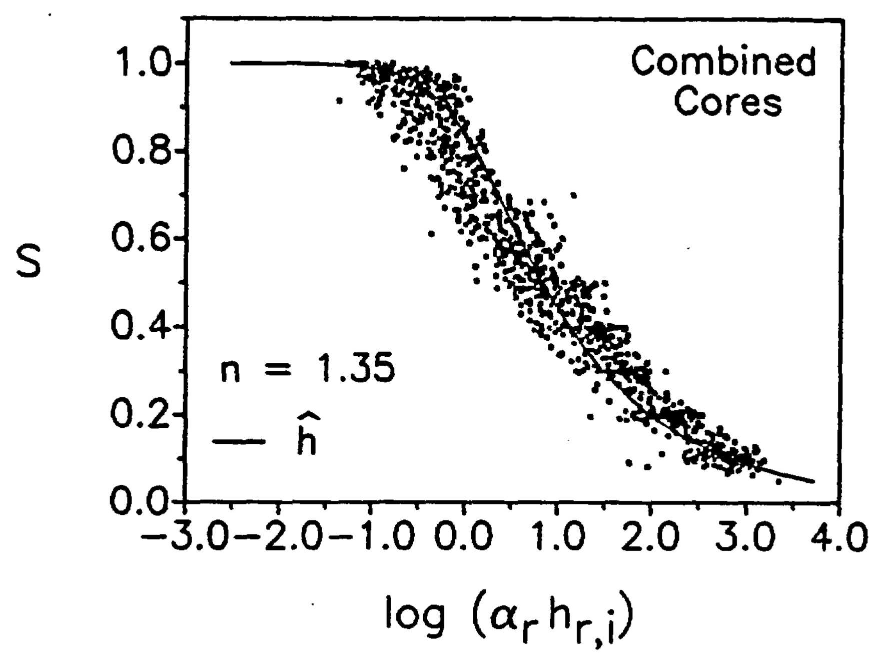
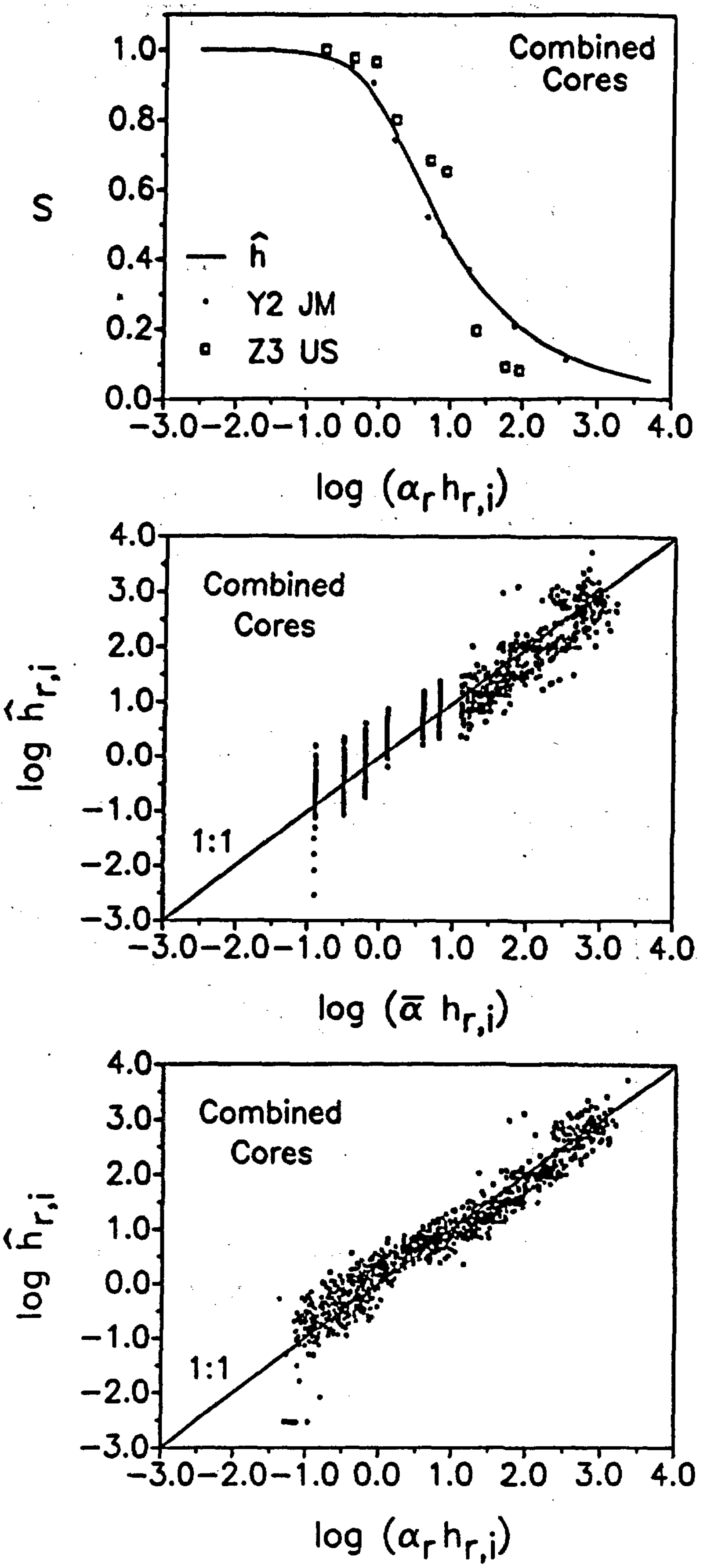


Fig. 13.5. Moisture profiles for α = 1.23, 0.873, and 0.618 (75, 50, and 25 percentile values, respectively). The distribution of α is shown as Fig. 13.1b. (After Warrick and Amoozegar-Fard, 1979.)


Combined
Cores
S
n = 1.35
— $\hat{h}$
1.0
0.8
0.6
0.4
0.2
0.0
−3.0 −2.0 −1.0 0.0 1.0 2.0 3.0 4.0
$\log\,(\bar{\alpha}\ h_{r,i})$


Combined
Cores
S
n = 1.35
— $\hat{h}$
1.0
0.8
0.6
0.4
0.2
0.0
−3.0 −2.0 −1.0 0.0 1.0 2.0 3.0 4.0
$\log\,(\alpha_r\, h_{r,i})$

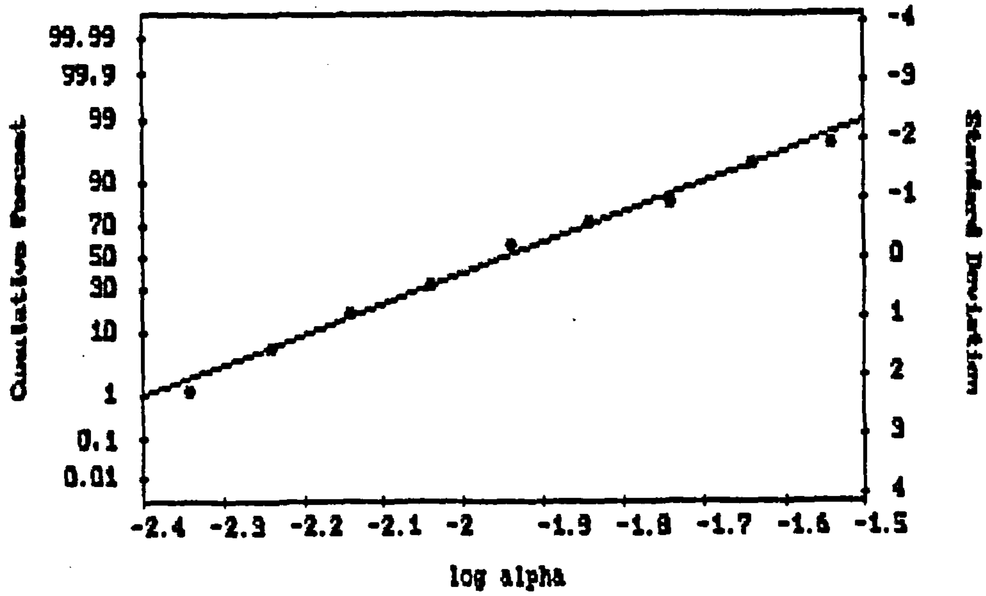
AMW 10



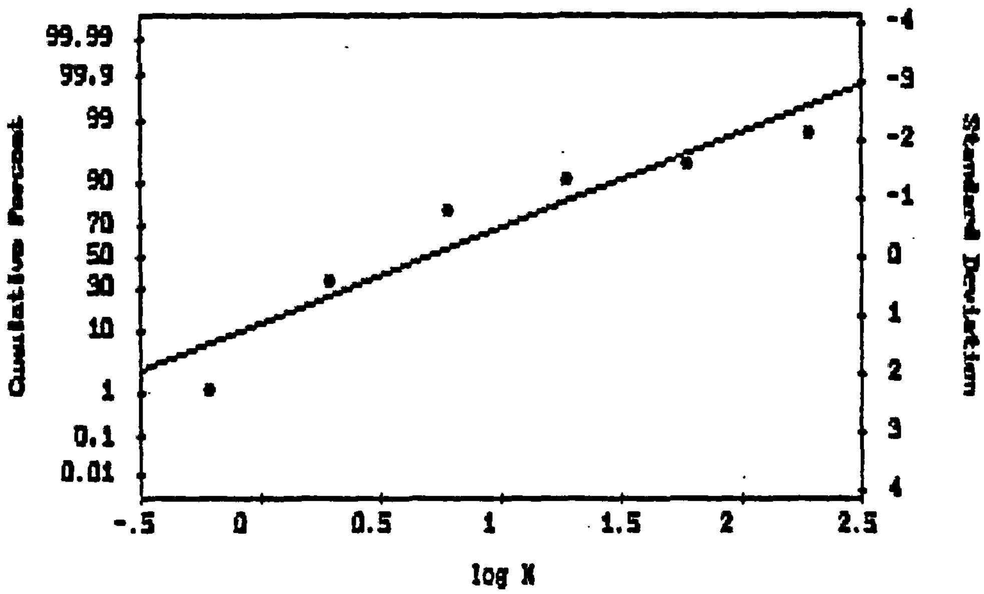
Combined Cores
S
$\hat{h}$
Y2 JM
Z3 US
1.0
0.8
0.6
0.4
0.2
0.0
−3.0 −2.0 −1.0 0.0 1.0 2.0 3.0 4.0
log ($\alpha_r h_{r,i}$)
Combined Cores
log $\hat{h}_{r,i}$
1:1
4.0 3.0 2.0 1.0 0.0 −1.0 −2.0 −3.0
−3.0 −2.0 −1.0 0.0 1.0 2.0 3.0 4.0
log ($\bar{\alpha}$ $h_{r,i}$)
Combined Cores
log $\hat{h}_{r,i}$
1:1
4.0 3.0 2.0 1.0 0.0 −1.0 −2.0 −3.0
−3.0 −2.0 −1.0 0.0 1.0 2.0 3.0 4.0
log ($\alpha_r h_{r,i}$)

AWW 1

ALTS Moisture Characteristics



ALTS Saturated K



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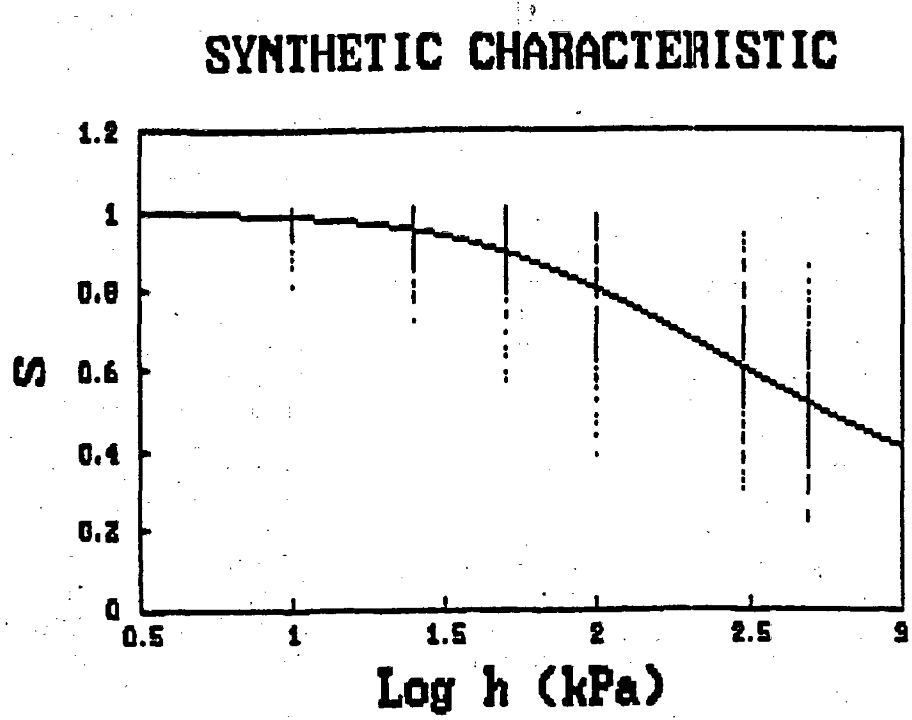

Characterization of Fracture Networks for Fluid Flow Analysis

Jane C.S. Long, Kevin Hestir, Amy Davey, Ernest L. Majer, John Peterson, Kenzi Karasaki

Introduction

With the advent of problems such as the storage of nuclear waste and production from fractured oil reservoirs, characterization of fracture networks in rock has been the focus of increasing study. The goal of much of this work is to develop a numerical model which can be used to predict the flow and transport of fluids through rock. Building such models is difficult because fracture networks are complex, three-dimensional systems.

One approach to the problem has been to attempt to build a statistical model of the network based on sampling fracture data in outcrops and boreholes. In building the fracture network up from such small scale data, we do not get a good statistical sample of unusual features. Consequently, it is very difficult to come up with a model which includes the effect of in frequent features, for example fracture zones. However, it is the fracture zones that often dominate the behavior of the fracture network. We do measure many fractures which do not have a large role in fluid flow. This results in developing a fracture network which is far too dense to explain observed non-continuum behavior. Such models predict millions of fractures in volumes of rock with the dimensions of tens of meters. From the hydrologic point of view, this model is wrong. Hence the "building up" approach fails to give us the dominant behavior of the network.

New Perspectives

We are proposing a new multi-tiered approach to developing fracture network models. In this approach, we first identify the fracture zones using geophysics and geology. Then, we conceptualize the zones using geomechanics and geology and develop an initial model of the fractured rock. This model becomes the basis for inverse hydrologic analysis.

We present several preliminary examples of ongoing research from two field sites, the Grimsel Test Facility in Switzerland under investigation by the DOE-Nagra Cooperative project and the Stripa Mine in Sweden under investigation by the Stripa project.

Examples of Field Data Analysis

The first example comes from the Grimsel test facility in Switzerland. Here, LBL and Nagra are jointly pursuing an experiment called the FRI experiment. The site of the experiment is shown in Figure 1 in plan view. At this site, there is a sub-vertical shear zone which transects the rock between two parallel horizontal drifts. Two holes have been drilled on either side of the zone, between the two drifts. In addition, many small holes have been drilled along the drift walls between the two holes. From these holes LBL performed four-sided cross-hole seismic measurements resulting in the P-wave slowness tomogram shown in Figure 2. In this tomogram dark zones represent slower velocities than light zones. The tomography shows the shear zone quite clearly.

The next step is to estimate the hydrologic features which control the behavior of well tests performed in the boreholes. Water injected into the shear zone from borehole 87.001 will not be restricted to flowing in the plane of the tomogram. Most likely, water will flow in the plane of the shear zone. So, once the zone is identified the hydrologic information must be used to find an equivalent hydrologic network in the plane of the zone. For an example of this, we turn to the Stripa Mine in Sweden.

At the Stripa mine, SGUab has performed radar tomography and identified several fracture zones for the Stripa Project. The zone called RB, cuts three parallel boreholes, N2, N3, and N4 and thus is similar to the geometry of the FRI zone.

First we propose a base geometry for hydrologic conductors called a template. In this case, we have chosen one of the simplest possible geometries, a square grid of conductors in the plane of the fracture zone, where not all the elements of the grid are present. Figure 3 shows such a grid where the pumped well, N3 was centrally located between N2 and N4. We anticipate that future investigations of shear zone morphology will provide a more sophisticated template for conductors. We now simulate a well test in the pattern of hydrologic conductors. The results of the well test show that N4 is more connected to N3 than is N2 because N3 responds before N2. Given real well test data from N3 we could adjust the pattern shown in Figure 3 so that it better matched the hydrologic data. In fact such "adjustment" constitutes performing hydrologic inversion.

Two inversion techniques are envisioned for finding an equivalent fracture network. In the first technique we note that flow to a well through a porous media or a very well connected fracture network is either two- or three-dimensional. However, in a partially connected fracture network, the flow may not have a integral dimension.

Barker (1988) has developed a solution for the well test equation which treats dimension as a variable. From this solution, he can develop type curves for partial dimension. Physically, such partial dimension is the result of the degree of connectivity in the network, ie the percentage of bonds to fill in the lattice template (Long and Witherspoon, 1985).

As an example, we have numerically modeled a well test in a system of theoretical fractal dimension equal to 1.465 (Figure 4). When the numerical results are fit to Barker's curves they give a partial dimension of 1.40. The difference may be due to the fact that the numerical example is only "fractal" between an upper and lower limit. It remains to relate the connectivity of a random fracture network to its fractal dimension. If this can be done, the Barker solution can be used to find connectivity and therfore the percentage of bonds to fill.

A second possible technique is a structured way to make changes in the model of the fracture system such that it behaves more like the real system. In this technique, we model hydraulic tests and compare the results with the field results. Then we change the model by adding or deleting a conductor. We remodel the hydraulic test and see if the results fit the pump test data better. If so, then we keep the change. If the change makes for a worse fit, we keep the change with a probability equal to:

$$P = e^{(E_1 - E_o)/T}$$

where E is equal to the square difference between the prediction and the measurement, o refers to the previous iteration, 1 refers to the present iteration, and T is a factor that decreases geometrically with the number of iterations. This technique allows one to get closer to a global minimum difference between measurements and model results instead of getting caught in a local minimum.

Any hydraulic test that can be modeled can be used to calculate E. Figure 5 shows an artificial example of the change in E with each iteration based on well tests in a partially filled grid. Tracer tests data probably provide a more ideal type of data to use. However, the technique is computationally intensive which may be a limitation.

Conclusion

The above approaches are still under development. Together, they form the basis of a new methodology for characterizing fractured rock. In following this methodology, we could produce a variety of systems which all fit the data. It is unlikely that any of these solutions are unique. Therefore, if we can determine a system which behaves like the real system for our test cases, is that good enough? Of course the answer to the question depends on the application but it is clear that this is an area which itself deserves research.

Acknowledgments

This work was funded U.S. DOE under Contract NO. DE-AC03-76SF00098 through the Repository Technology Program. Much of the work is fostered through cooperation with Nagra, Nationale Genossenschaft für die Lagerung radioaktiver Abfälle and the Stripa Project. The authors are indebted to Charles McCombie, Piet Zuidema, Peter Blümling, Caroline Wittwer and Gerd Sattel among many others at Nagra; John Barker of BGS, Ollie Olsson, and Borje Niva of SGUAB and the Stripa Project.

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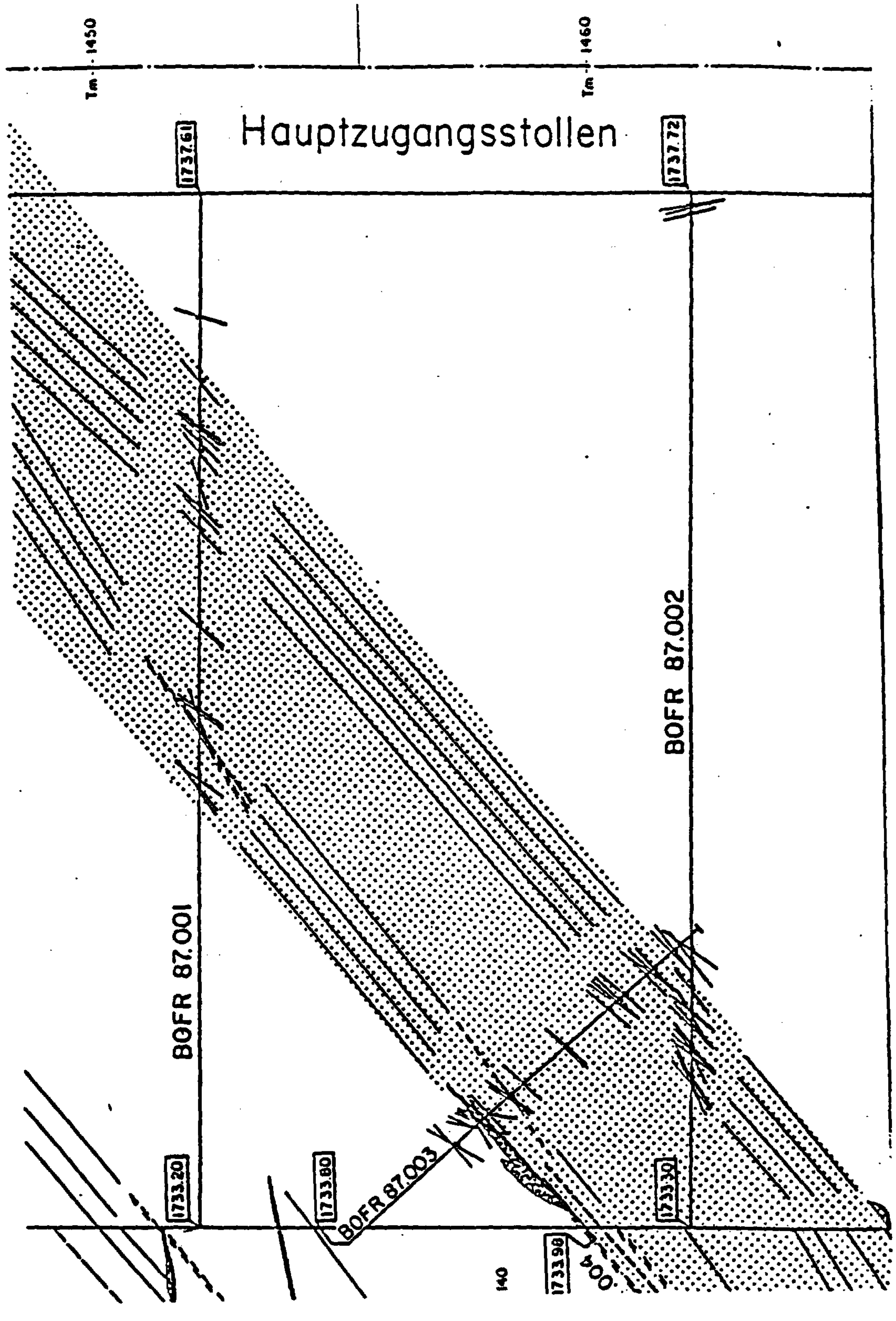


Figure 1. Plan view of the FRI experiment site showing the trace of the sub-vertical shear zone crossing between two parallel horizontal drifts.

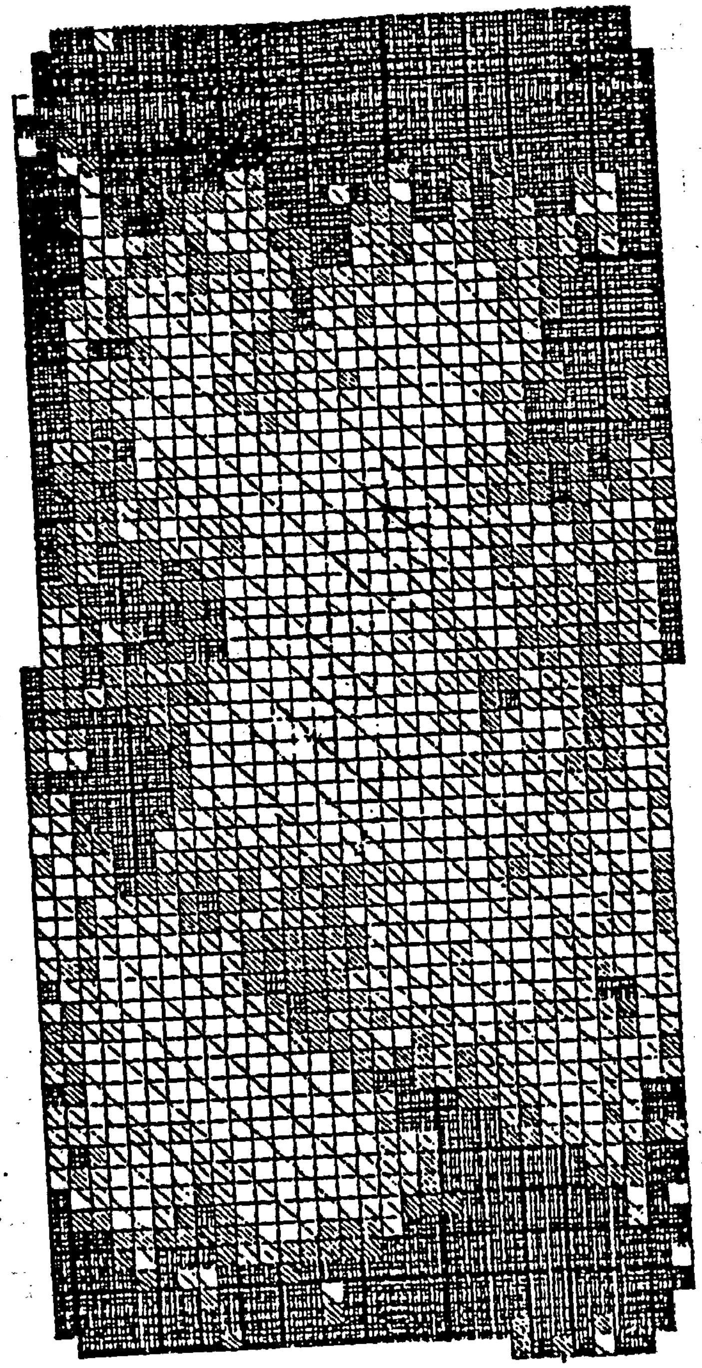


Figure 2. Tomographic results for the FRI zone.

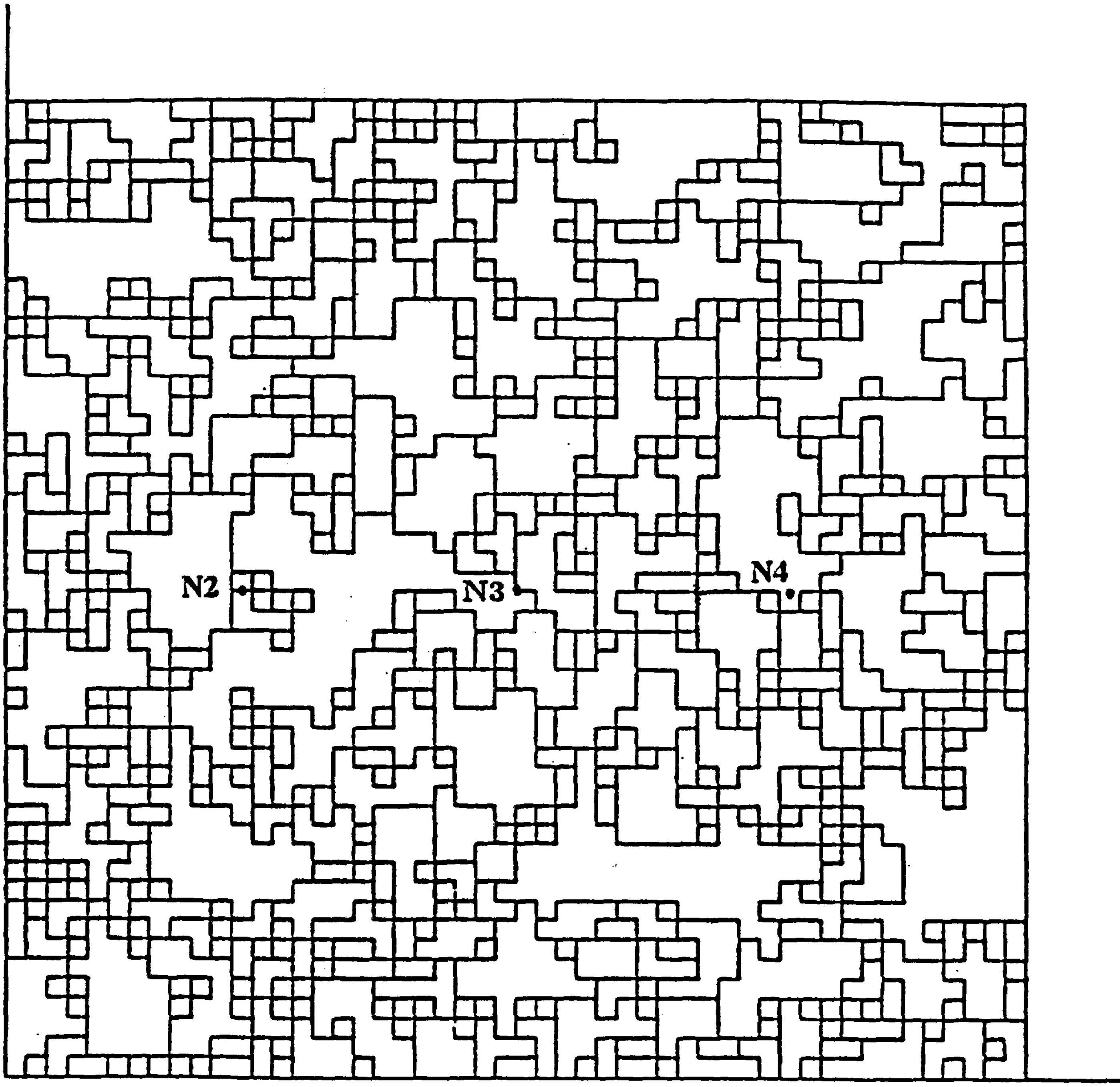
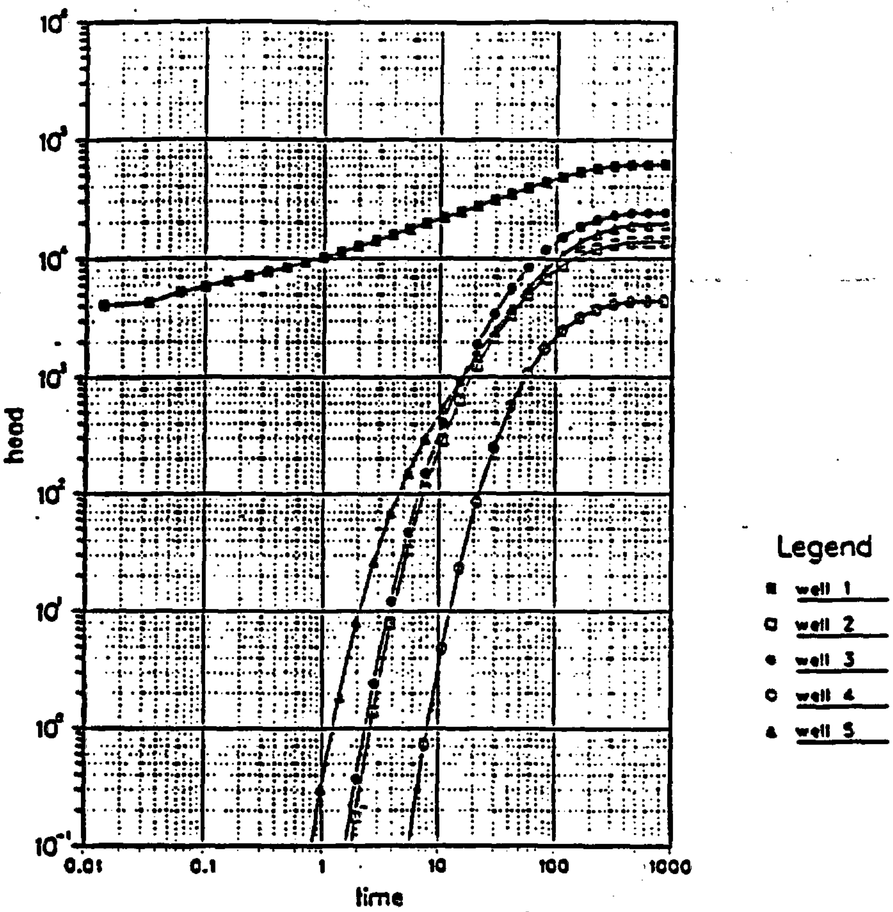


Figure 3. Pattern of hydrologic conductors resulting from analysis of radar slowness tomograms.



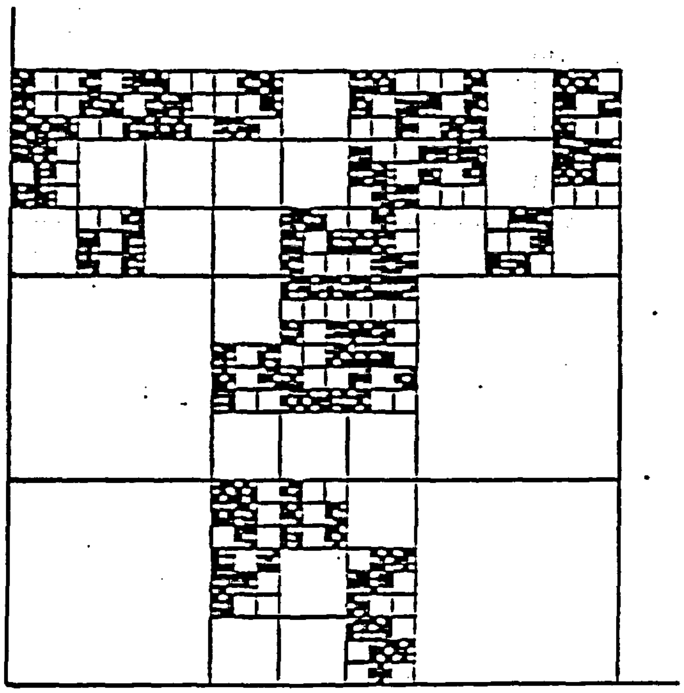


Figure 4. Well test results in a fractal network.

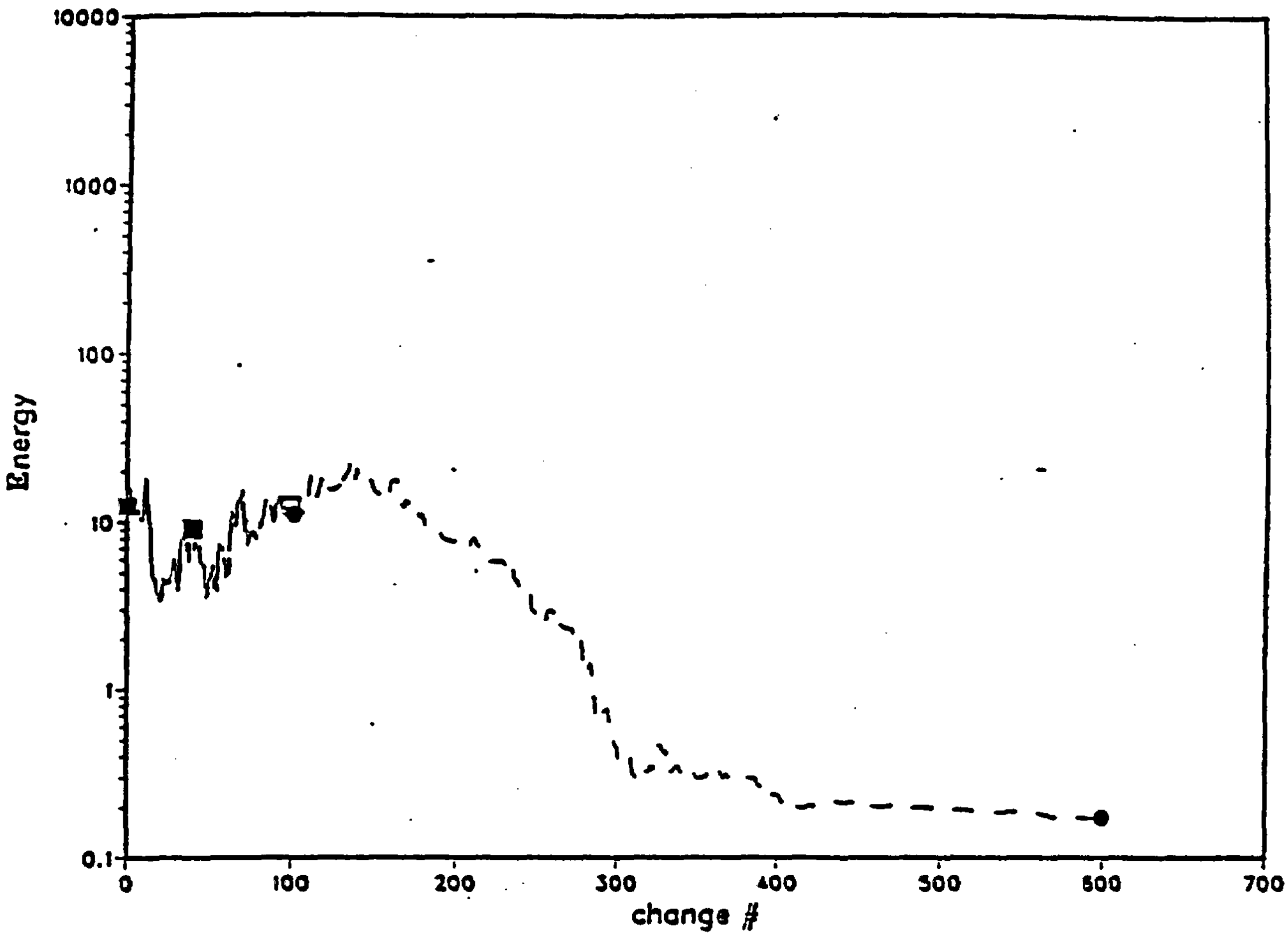


Figure 5. Example of the change in error, E with iteration towards a model which better matches field data.

APPLICATIONS OF FRACTALS TO PARAMETER ESTIMATION

Scott W. Tyler
Stephen W. Wheatcraft
Gregory A. Sharp
NRC Workshop IV
December 1988
Tucson, Arizona

In recent years, fractal mathematics have been used to quantify many natural processes. In this presentation, we describe several applications of fractal geometry and mathematics to the problems of flow and transport in heterogeneous soil and aquifer materials. These include:

1. Scale-dependent dispersion in 1-D flow systems.

2. Transport in 2-D fractal heterogeneous aquifers.

3. Soil water retention estimation.

The concepts of fractal geometry revolve around the use of scale-invarient transformations. Such transformations appear to accurately represent many natural processes in which variability (heterogeneity) is present over a wide range of scale. For example, a coastline appears to be highly irregular when viewed from an aircraft at 30,000 feet. As the aircraft descends, irregularities (small embayments, estuaries, etc.) become discernible which were not visible at higher altitudes. Upon landing on the shoreline, additional detail can be found. Such a thought experiment may be carried down to the microscopic or perhaps even the molecular scale. The measured length of the coastline therefore becomes a function of the scale of observation and has been shown to obey a power law (fractal) scaling of the form:

$$L(\epsilon) = A\ \epsilon^{1-D}$$

where ϵ represents the scale of the observation, D is the fractal dimension and A is a constant.

Power law or fractal scaling concepts have been applied to a wide variety of geologic and hydrologic processes. Hewitt (1986), Adler (1985, 1987, 1988) and Katz and Thompson (1985) have applied fractal concepts to multiphase transport, permeability, and rock porosity, respectively. Analysis of fracture spacing and soil physical processes by Barton and Larson (1985) and Burrough (1983a, 1983b), respectively have shown that fractal concepts can be used to predict behavior over a wide range of scales. For a more complete description of fractal applications, the reader is referred to Feder (1988).

In our work we have concentrated on applications of fractals to descriptions of hydraulic properties of aquifers and soils. In a simple analysis of one-dimensional dispersion in saturated heterogeneous media (Wheatcraft and Tyler, 1988), we developed an analytic expression to describe the growth of field-measured dispersivity A_M of the form:

$$A_M = Cx^{2D}$$

Where D is the fractal dimension of the heterogeneity and x is the mean displacement of the tracer plume. This relation suggests that the dispersivity will grow faster than distance traveled by the centroid of tracer plume. Such non-linear behavior is in contrast to traditional and stochastic theories and is born out in many tracer tests (Gelhar et al., 1985).

To investigate transport behavior in two-dimensional domains, tracer experiments were conducted numerically in fractal geometry (Sharp, 1988). Conductivity fields of various scales were developed around the geometry of Serpinski carpets whose fractal dimension can easily be estimated. Our objective was to determine the relationship between the fractal dimension of the geometric pattern and the dimension of the tracer paths. The results of these numerical experiments showed that dispersivities predicted by the classical advective-dispersion equation grow in a power-law scaling manner as predicted by our earlier one-dimensional results however, the growth (as measured by the fractal dimension) is much lower than the dimension of the conductivity field.

We have also applied fractal concepts to the estimation of soil water retention properties using the method proposed by Arya and Paris (1982). We have shown that the Arya and Paris model is based upon fractal mathematics and as a result, arbitrary curve fitting parameters in the model represent the fractal dimension of pore traces in the soil. A simple method has been developed based upon the fractal dimension of the particle-size distribution to estimate the pore trace dimension allowing for the rapid estimation of retention properties from basic soil survey information (Tyler and Wheatcraft, 1989).

The application of fractal mathematics to a wide range of geologic and hydrologic processes suggests a new approach to analysis of spatial variability in soil and aquifer properties. These approaches imply a much longer range of correlation than is traditionally used in geostatistical analysis. Time and analysis of field data collected over a wide range of scales are required before these concepts can be shown to be universal.

ACKNOWLEDGMENTS

This work was funded by the Nevada Agency for Nuclear Projects/Nuclear Waste Projects Office under Department of Energy grant number DE-FG08-85-NV10461. The opinions expressed in this paper do not necessarily represent those of the State of Nevada or the U.S. Department of Energy.

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*These references represent only a subset of the work of P.M. Adler and C.G. Jacquin on the subject of fractals.

APPLICATIONS OF FRACTALS TO PARAMETER ESTIMATION

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STEPHEN WHEATCRAFT

GREGORY SHARP

DESERT RESEARCH INSTITUTE

HYDROGEOLOGIC APPLICATIONS

MULTIPHASE TRANSPORT - HEWITT(1986)

PERMEABILITY - ADLER(1985,1987)

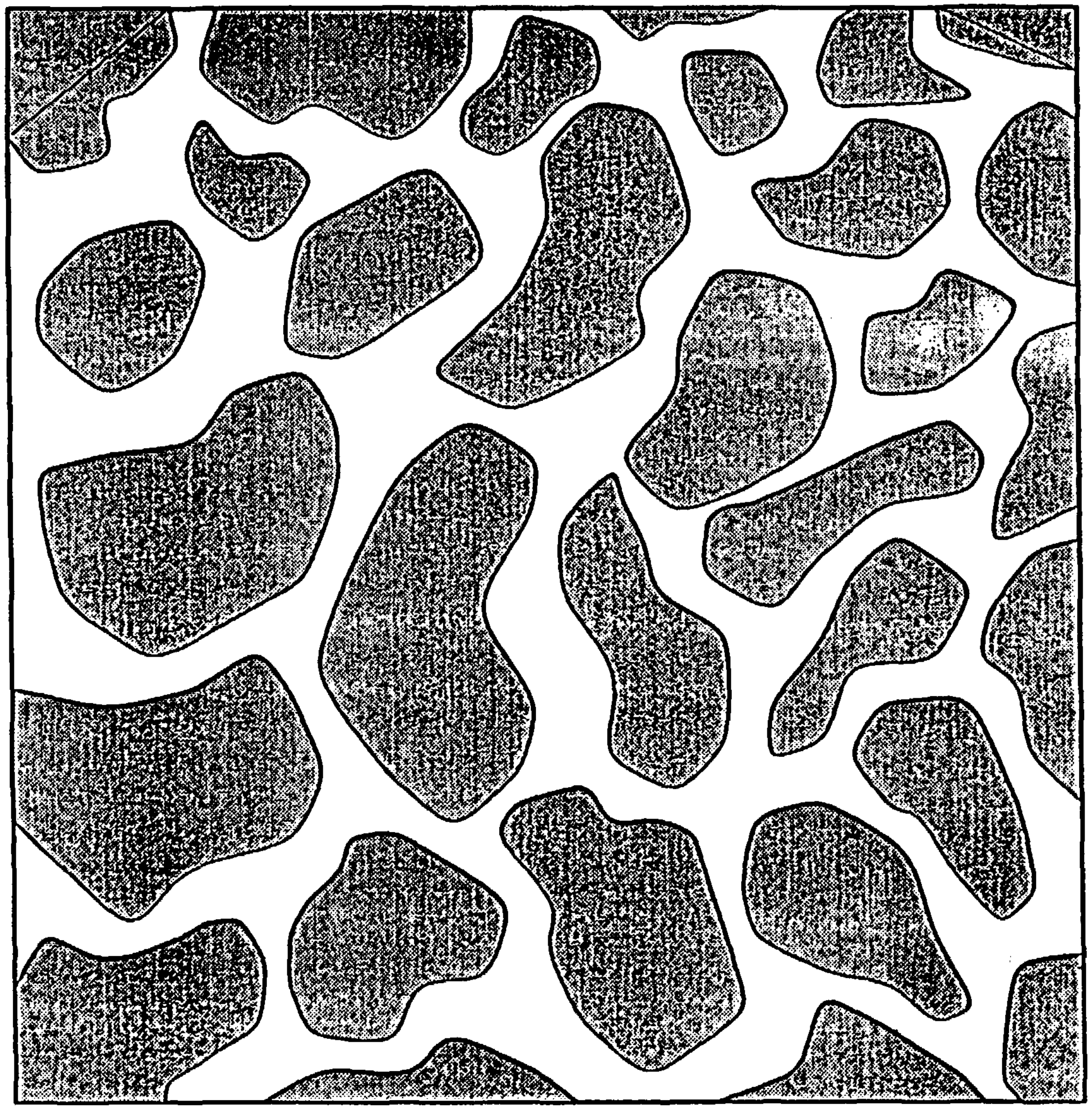
POROSITY - KATZ AND THOMPSON(1985)

FRACTURES - BARTON AND LARSON(1985)

SOIL PROPERTIES - BURROUGH(1983)

DISCUSSION TOPICS

- **INTRO TO FRACTAL SCALING**
- SCALE-DEPENDANT DISPERSIVITY (1-D)
- DISPERSION IN SYNTHETIC MEDIA (2-D)
- FRACTAL SOIL-WATER RETENTION
- FUTURE DIRECTIONS



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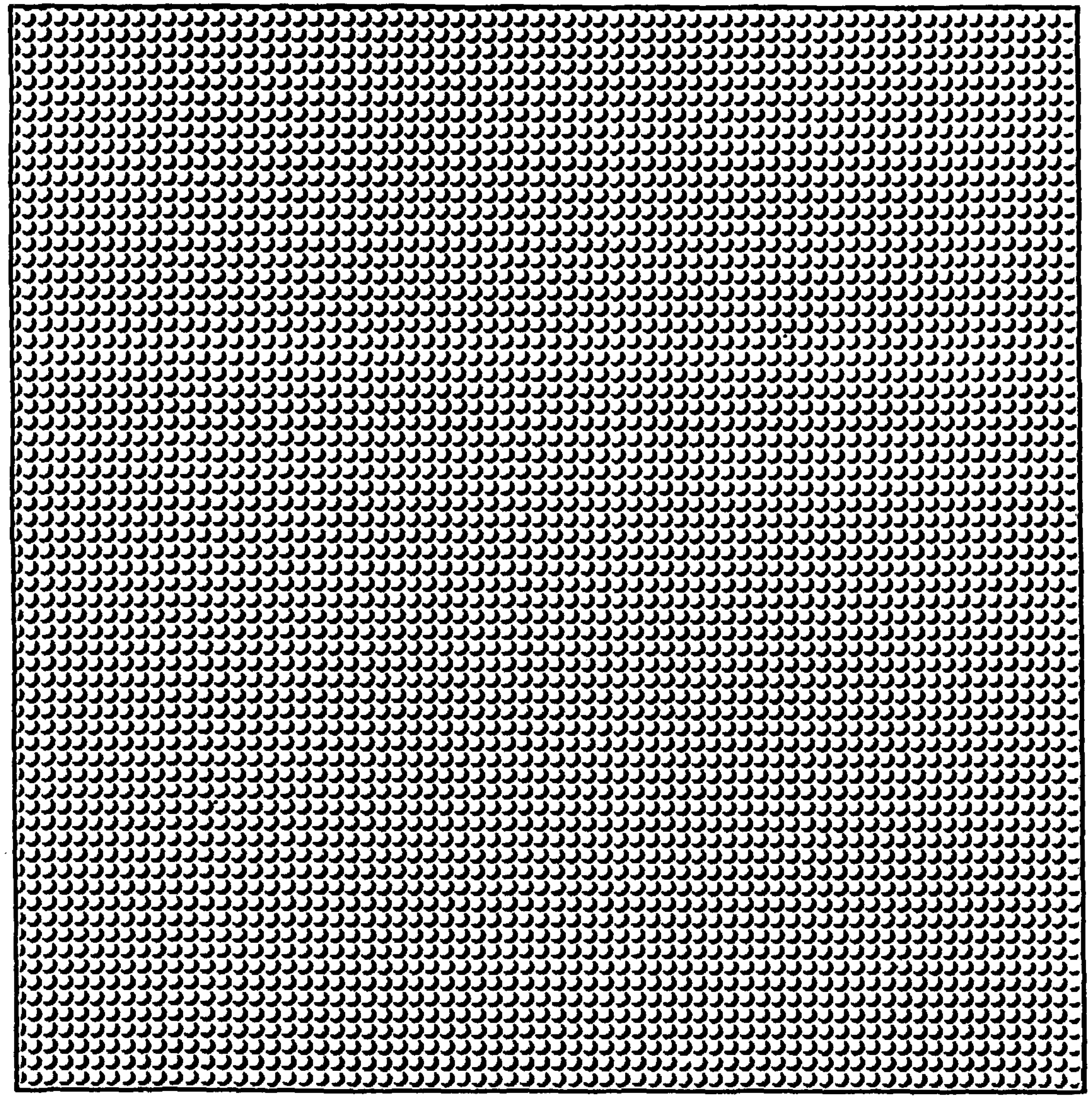

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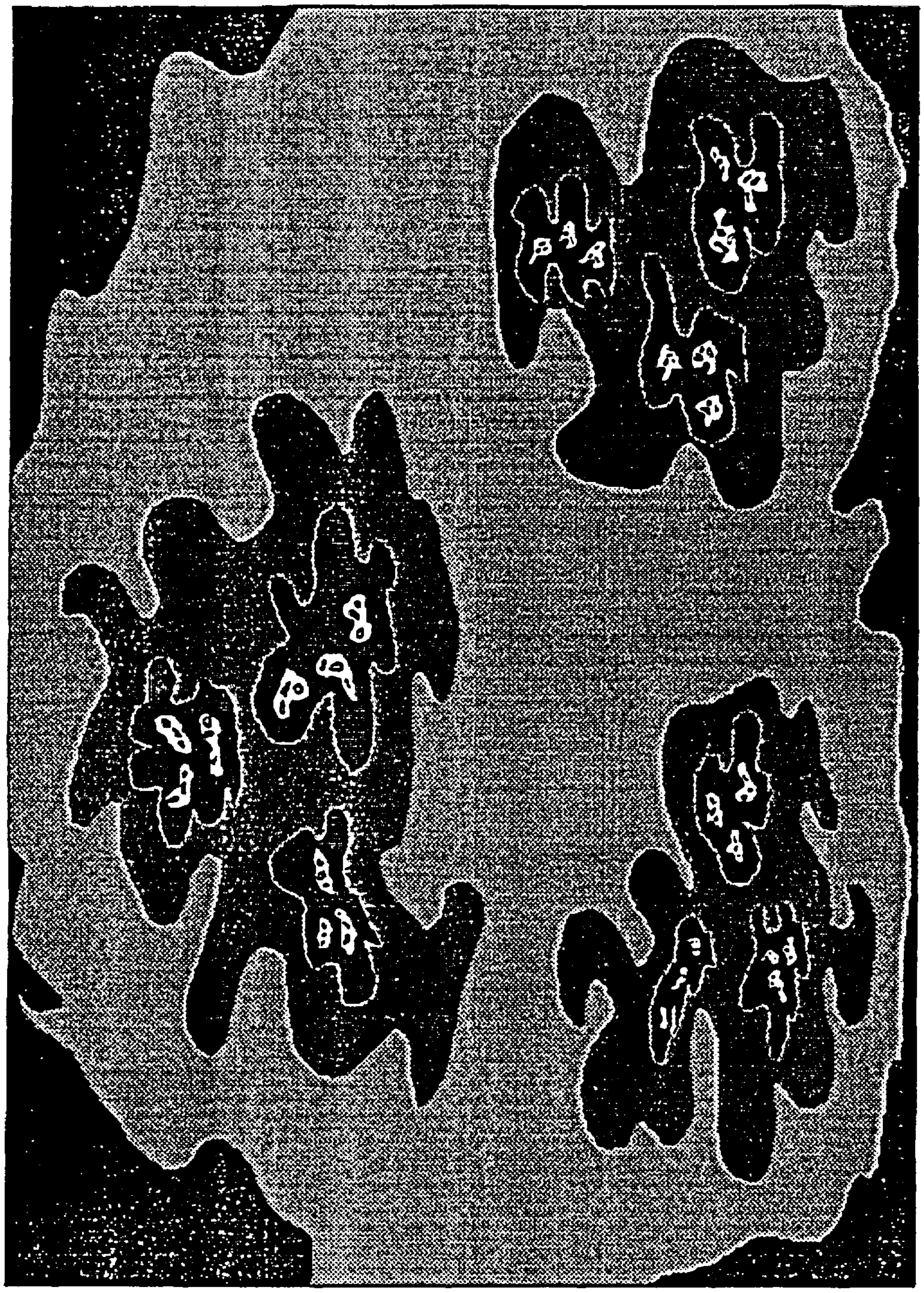


DISCUSSION TOPICS

- INTRO TO FRACTAL SCALING
- SCALE-DEPENDANT DISPERSIVITY (1-D)
- DISPERSION IN SYNTHETIC MEDIA (2-D)
- FRACTAL SOIL-WATER RETENTION
- FUTURE DIRECTIONS

KEY MODEL ELEMENTS

1. LENGTH OF PARTICLE TRACE
   GROWS FASTER THAN STRAIGHT
   LINE LENGTH.

2. TANGENTIAL VELOCITY WITHIN
   INDIVIDUAL STREAMTUBE IS CONSTANT.

3. CONSTANT FRACTAL DIMENSION.

DISCUSSION TOPICS

- INTRO TO FRACTAL SCALING
- SCALE-DEPENDANT DISPERSIVITY (1-D)
- **DISPERSION IN SYNTHETIC MEDIA (2-D)**
- FRACTAL SOIL-WATER RETENTION
- FUTURE DIRECTIONS

ANALYTIC RESULTS

SINGLE STREAMTUBE

$$\alpha_M = \alpha_L \ \varepsilon^{1-D} \ X^{D-1}$$

STREAMTUBE DISTRIBUTION

$$\alpha_M = C_1 \ X^{2D-1}$$

TRANSPORT IN 2-D FRACTAL MEDIA

- OBJECTIVE

  INVESTIGATE TRANSPORT BEHAVIOR IN SELF-SIMILAR MEDIA

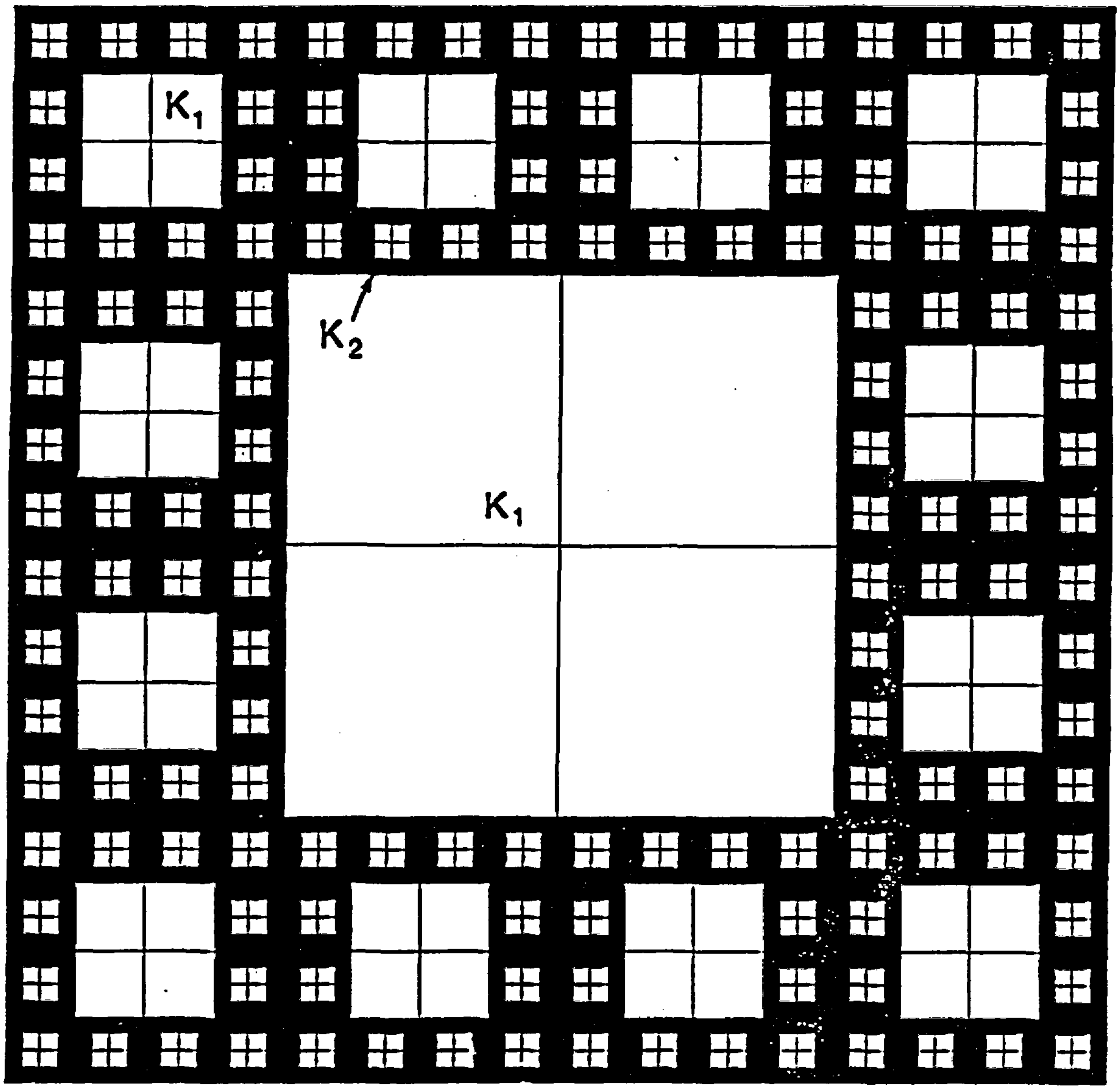
- 2-D FRACTAL HETEROGENEOUS MEDIA

- STEADY-STATE VELOCITY FIELD

  SOLUTION USING MGRID (COLE AND FOOTE,1987)

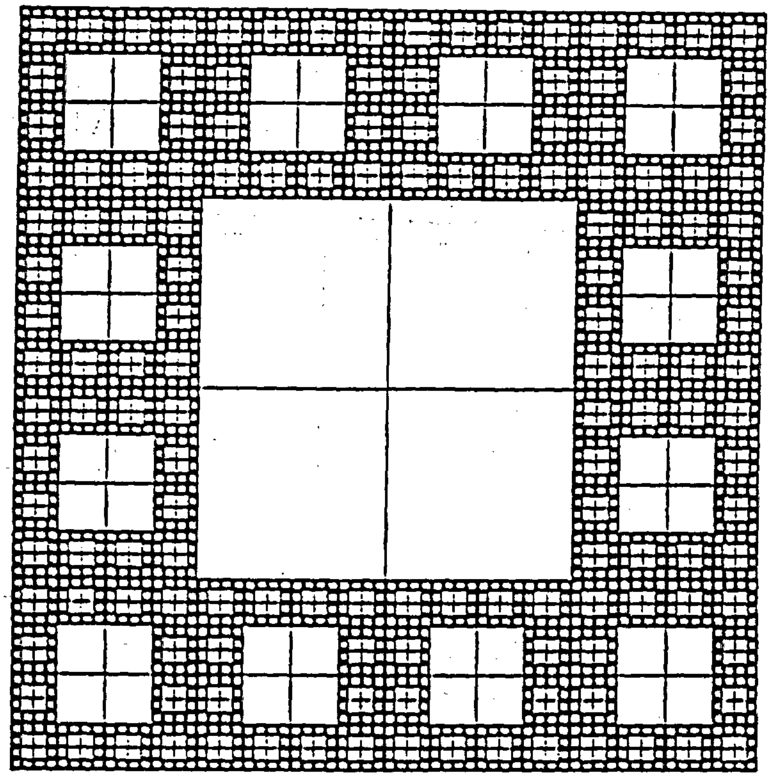
- PARTICLE TRACKER USED TO COLLECT TRANSPORT STATISTICS

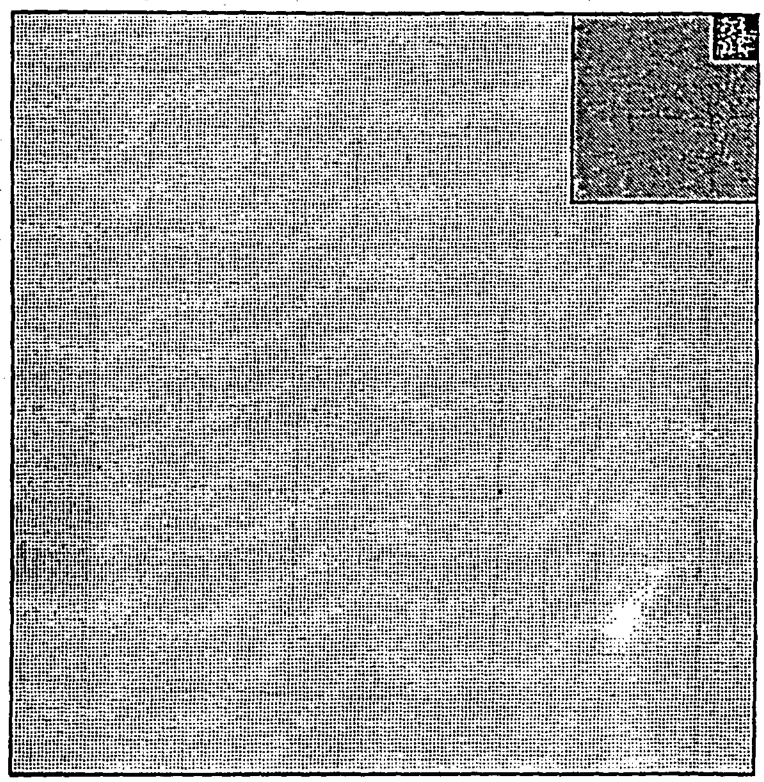
TRANSPORT IN SERPINSKI CARPETS



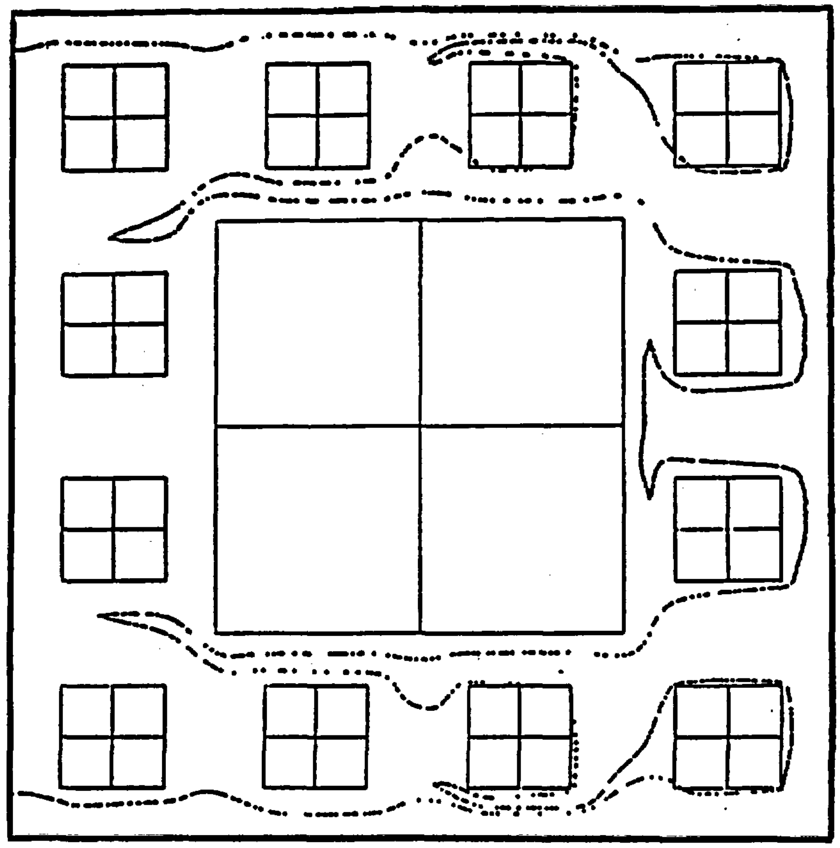
Where: $N_T(>R_i) \tilde{\propto} R_i^{-D}$

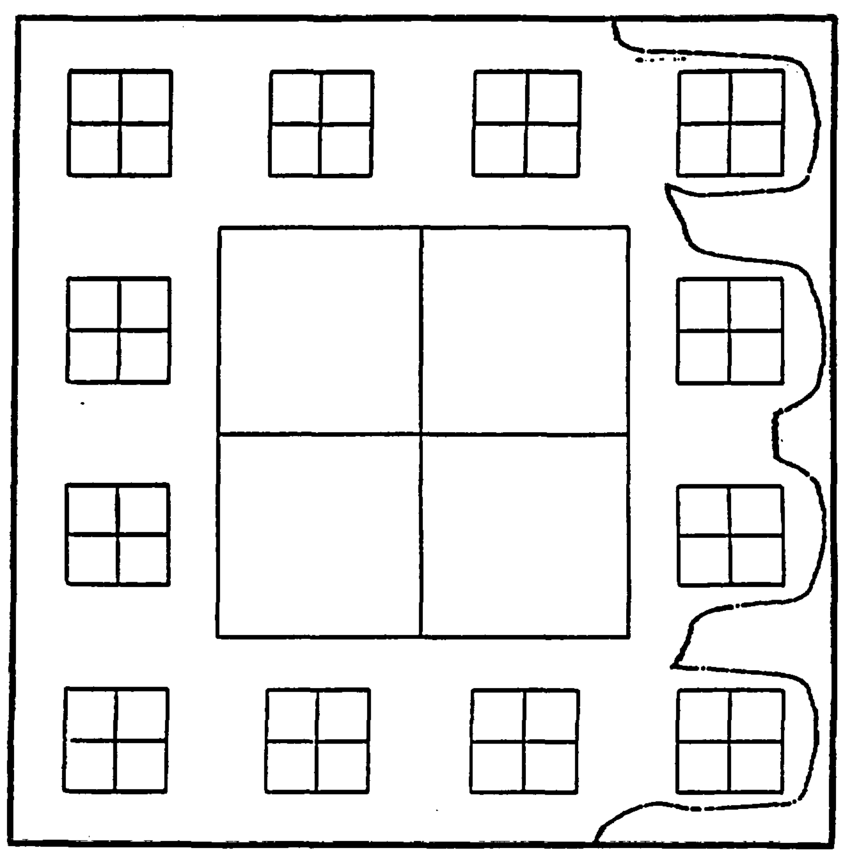
and: $D = \dfrac{\log(b^2-\ell)}{\log(b)}$

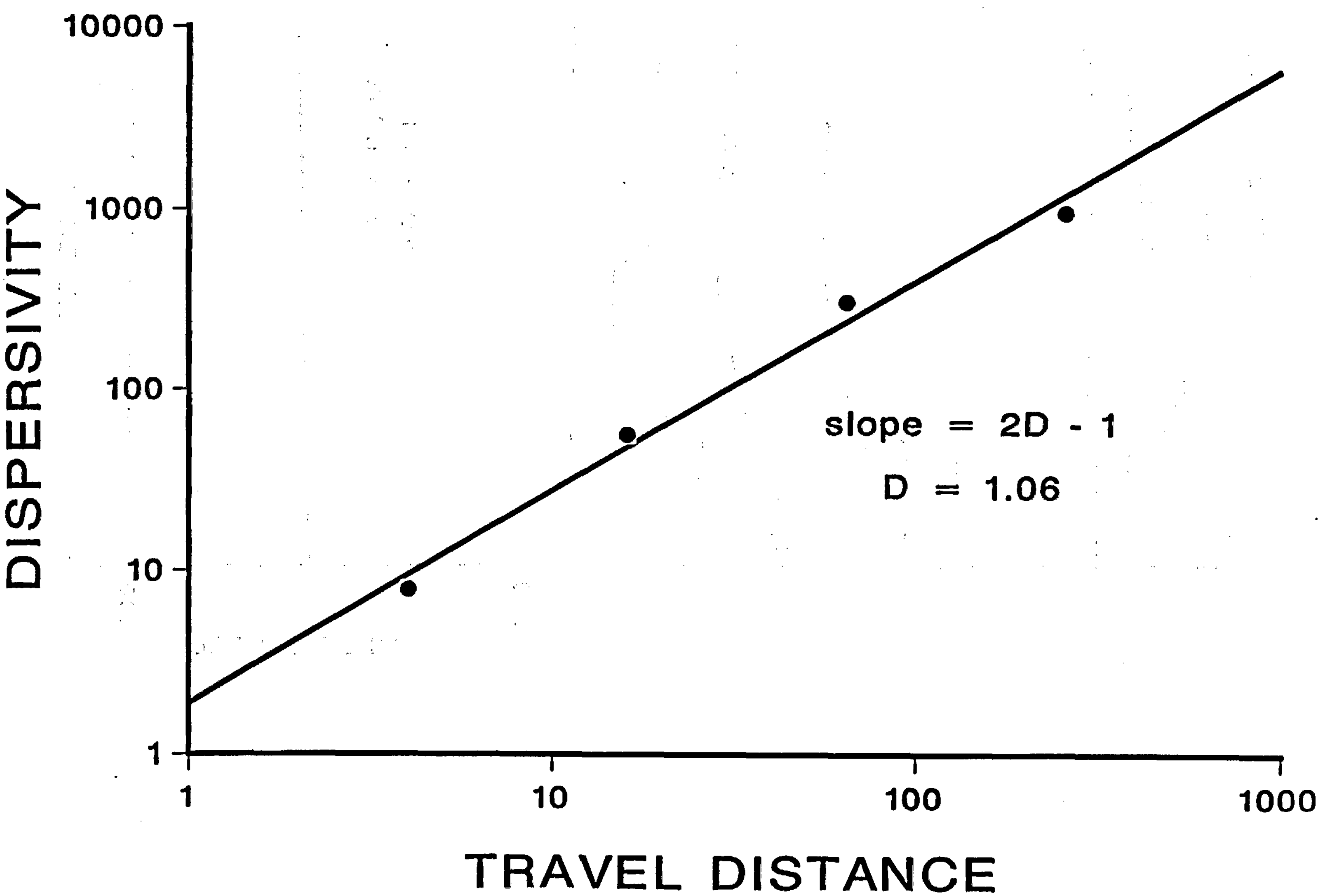




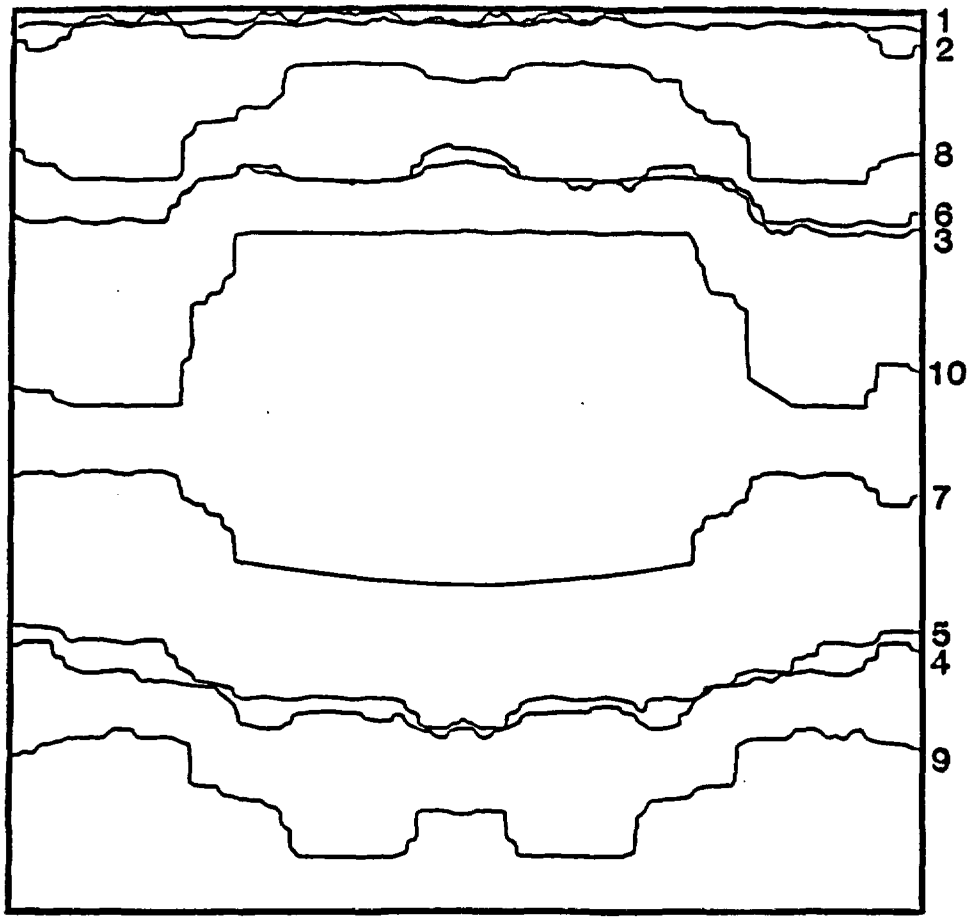
4 length unit scale of observation

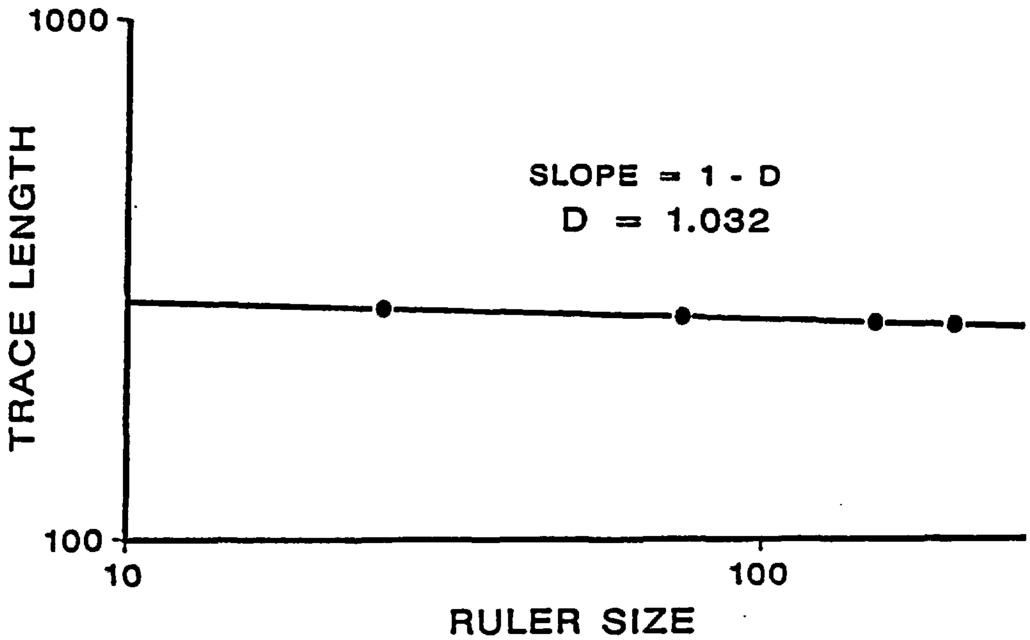





DISPERSIVITY
TRAVEL DISTANCE
10000
1000
100
10
1
1
10
100
1000
slope = 2D - 1
D = 1.06

PARTICLE TRACES





DISCUSSION TOPICS

- INTRO TO FRACTAL SCALING
- SCALE-DEPENDANT DISPERSIVITY (1-D)
- DISPERSION IN SYNTHETIC MEDIA (2-D)
- FRACTAL SOIL-WATER RETENTION
- FUTURE DIRECTIONS

A RELOOK AT ARYA AND PARIS (1981) WATER RETENTION ESTIMATION MODEL

Simple Estimation Model Based
Solely on Particle Size Distribution

REVIEW OF TECHNIQUE

CAPILLARY TUBE MODEL

TUBE DIAMETER PROPORTIONAL TO GRAIN DIAMETER

WATER CONTENT PROPORTIONED TO GRAIN SIZE DISTRIBUTION

ARBITRARY PORE AND GRAIN SIZE DIVISIONS

ARBITRARY FITTING PARAMETER (alpha)

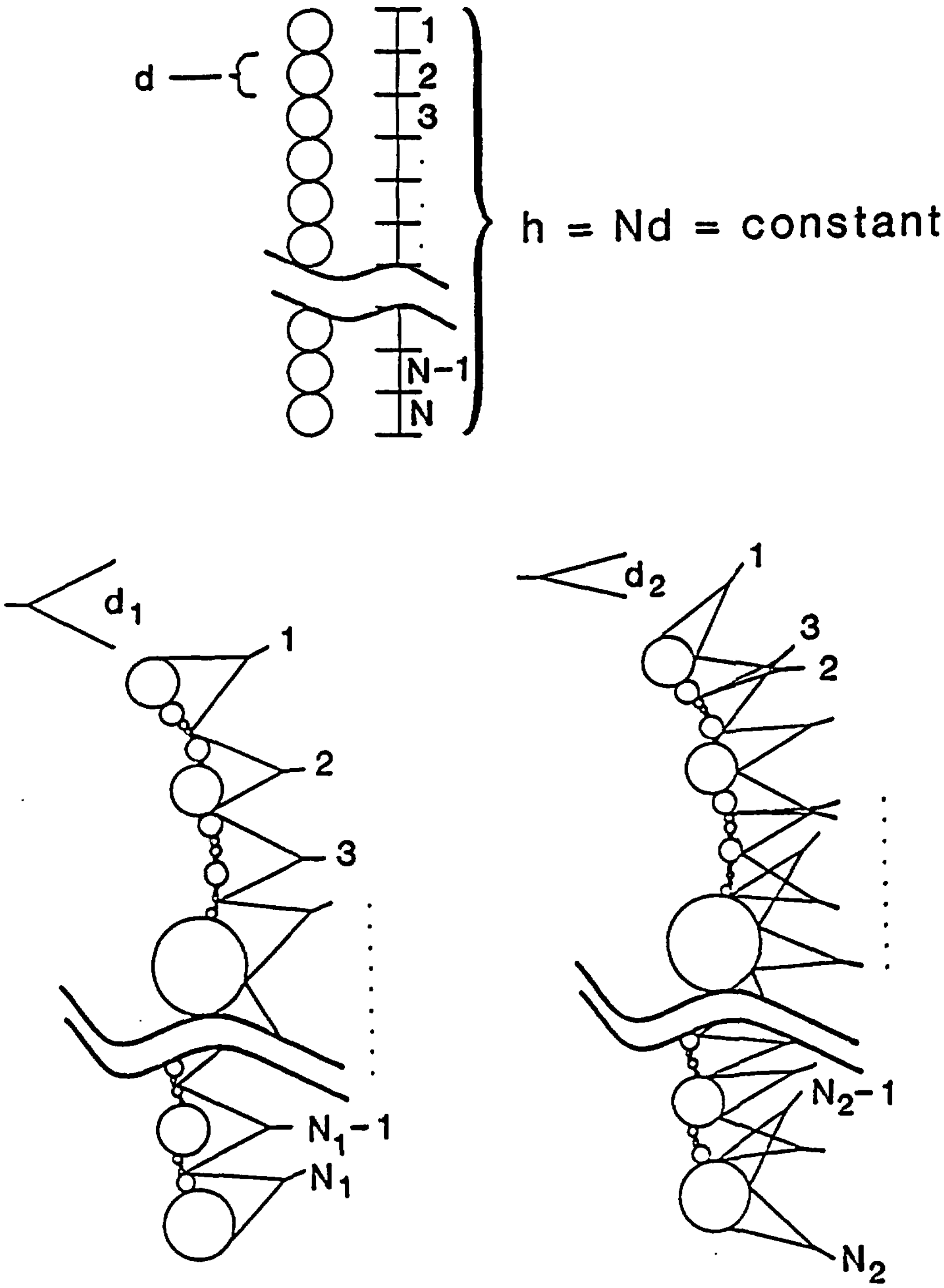
ARYA AND PARIS DEVELOPED

$$\Psi_i \propto R_i^{-1}\left[\frac{2}{3}\, eN_i^{1-\alpha}\right]^{-\frac{1}{2}}$$

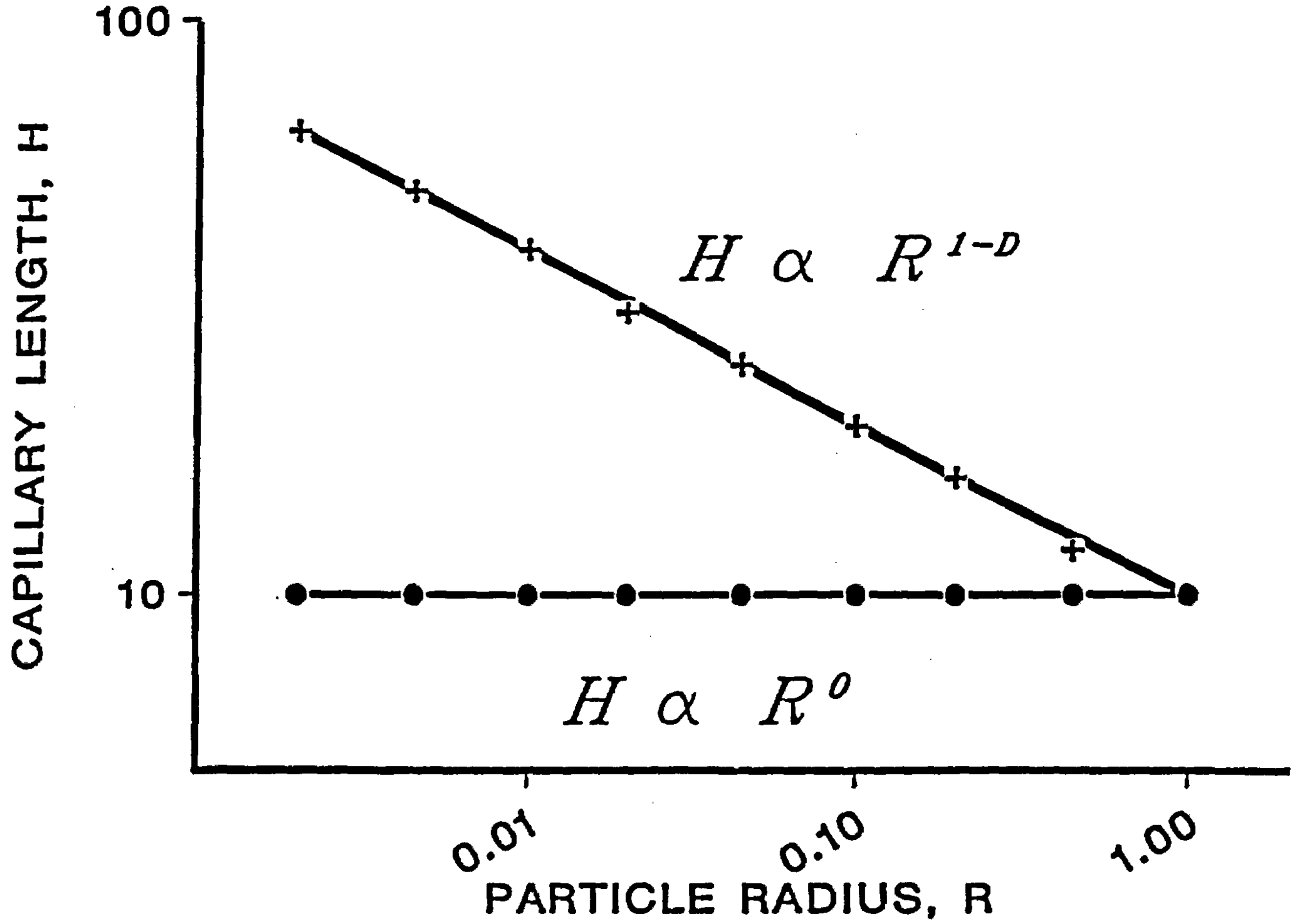
- α CAN BE SHOWN TO BE EQUIVALENT TO FRACTAL DIMENSION OF PORE TRACE.

- THE DIMENSION OF THE PORE TRACE IS RELATED TO THE FRACTAL DIMENSION OF THE PARTICLE SIZE DISTRIBUTION VIA "SLIT ISLAND" THEOREM. (Mandelbrot, 1984)

CAPILLARY TUBE MODELS



$h_1 = N_1 d_1$ $\qquad$ $h_2 = N_2 d_2$

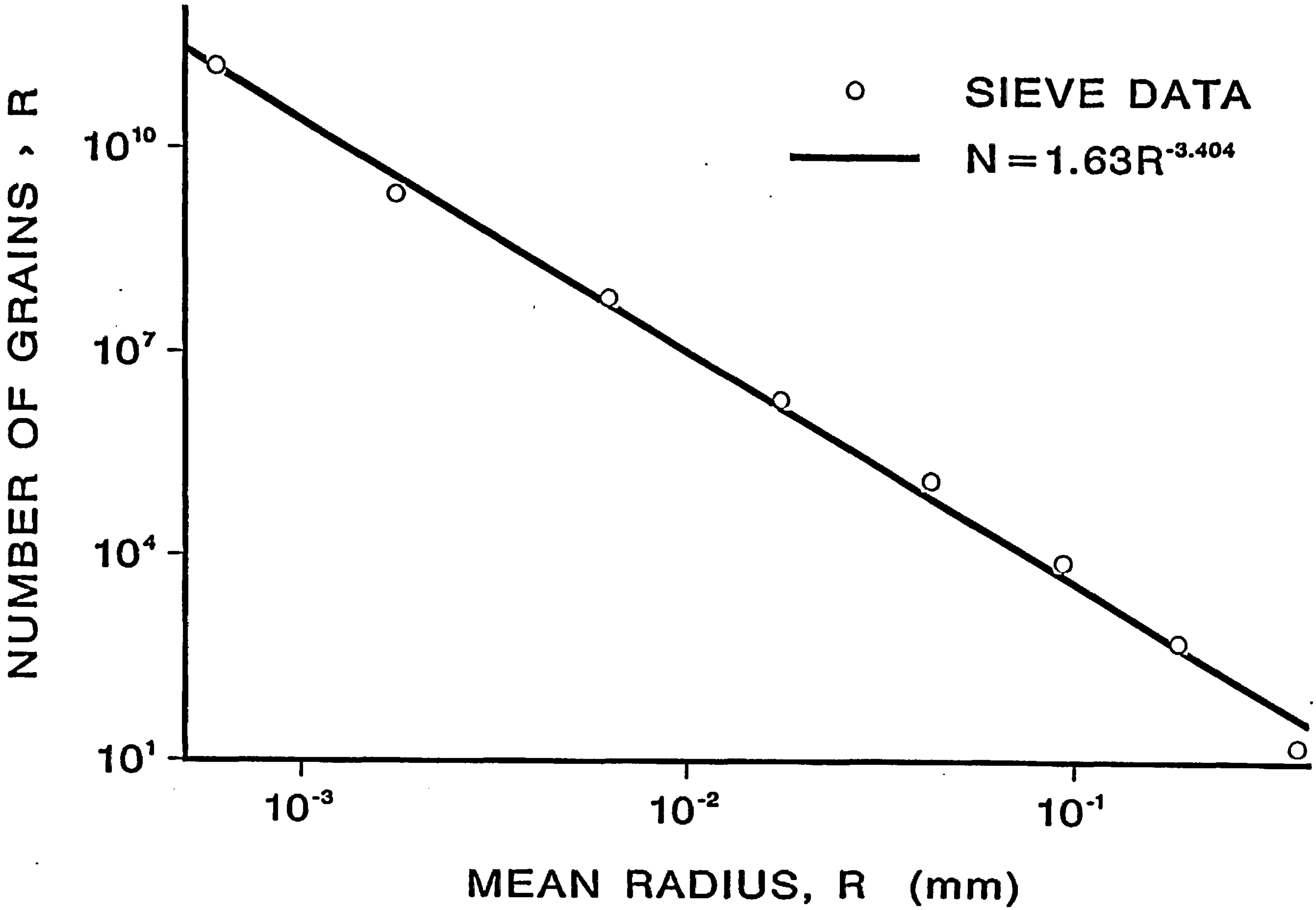


- EUCLIDIAN MODEL

  LENGTH INVARIANT WITH SCALE

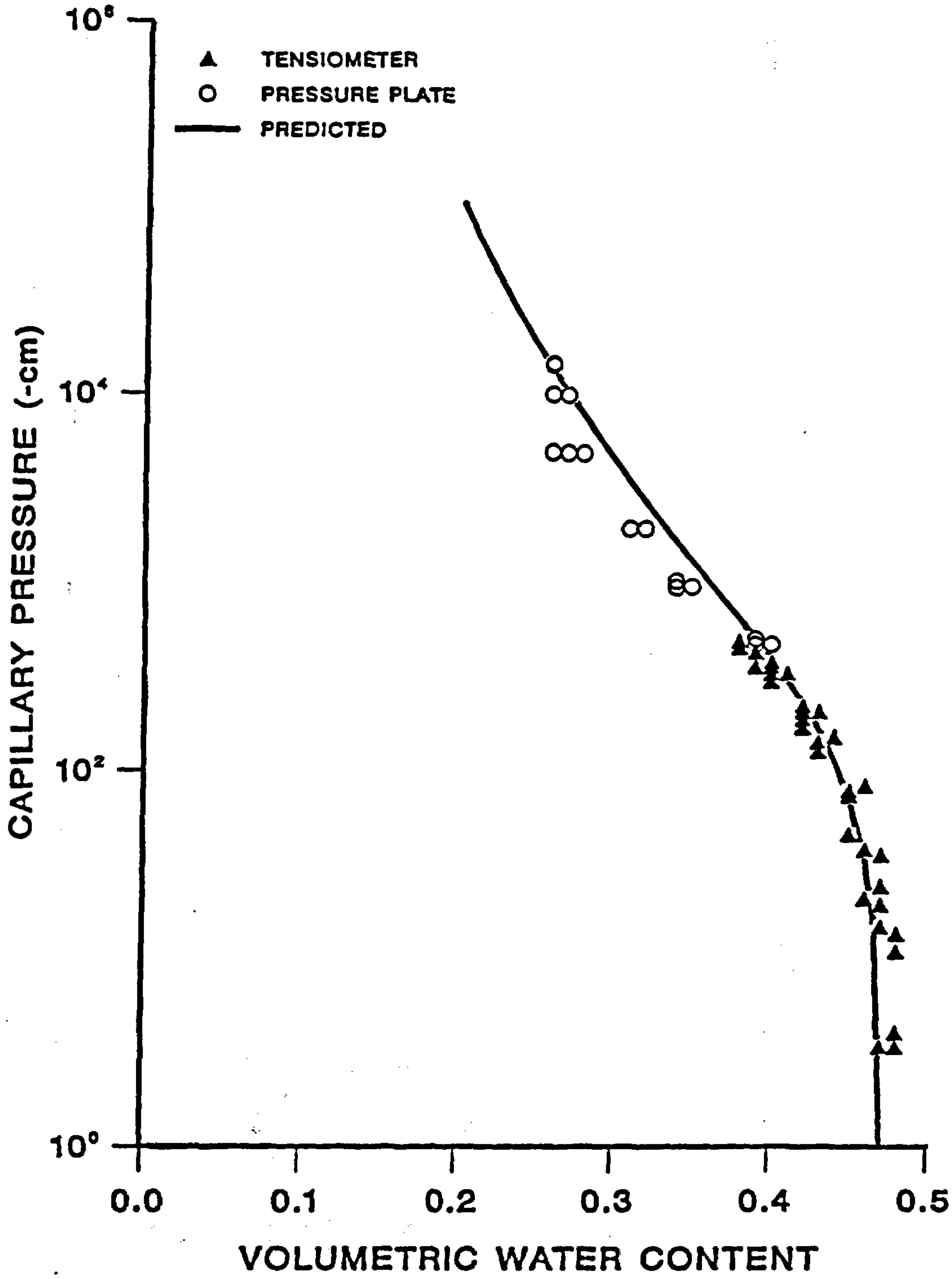
- FRACTAL MODEL

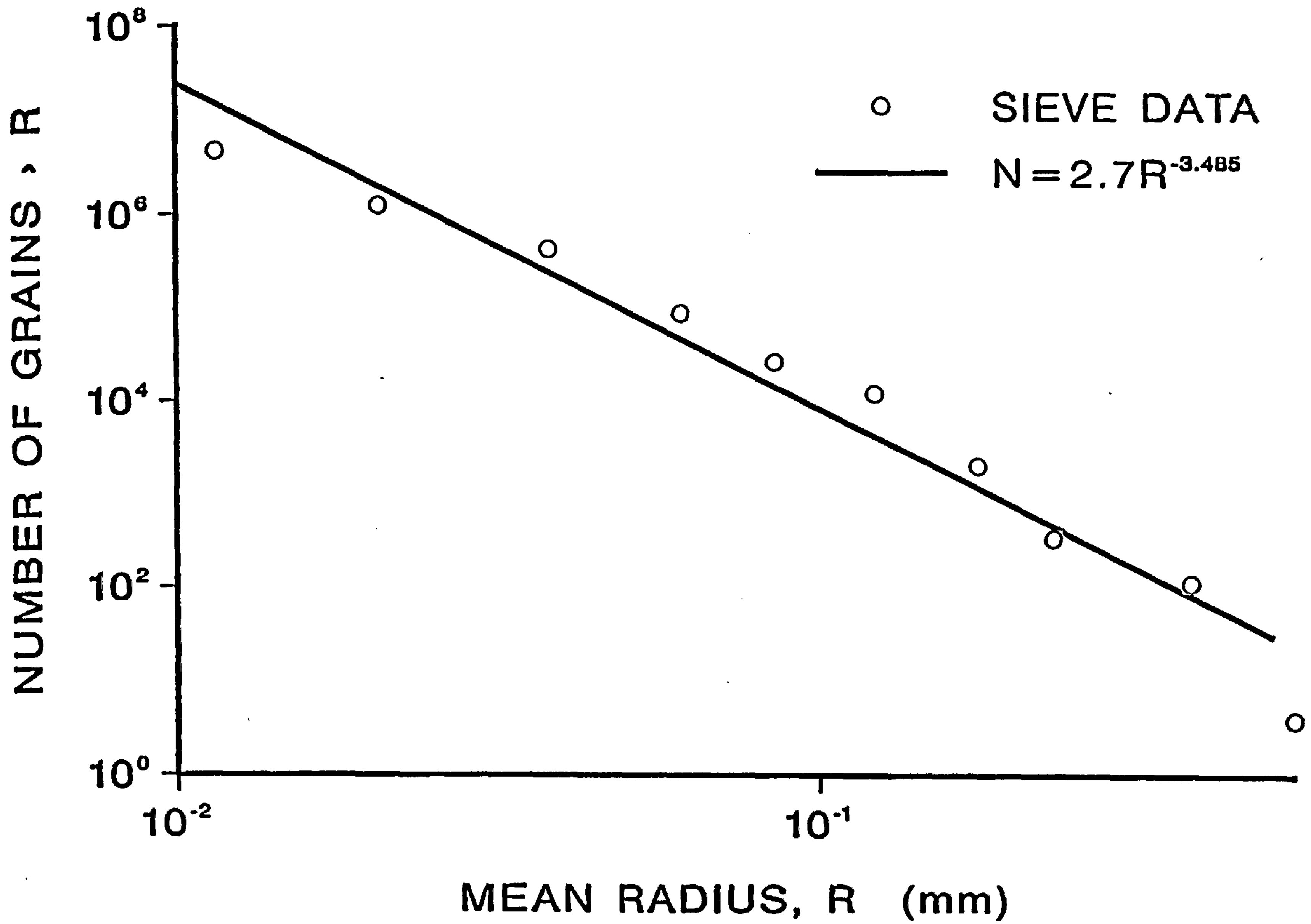
  LENGTH INVERSELY PROPORTIONAL TO SCALE



SIEVE DATA
N=1.63R-3.404
NUMBER OF GRAINS , R
10^10
10^7
10^4
10^1
10^-3
10^-2
10^-1
MEAN RADIUS, R (mm)

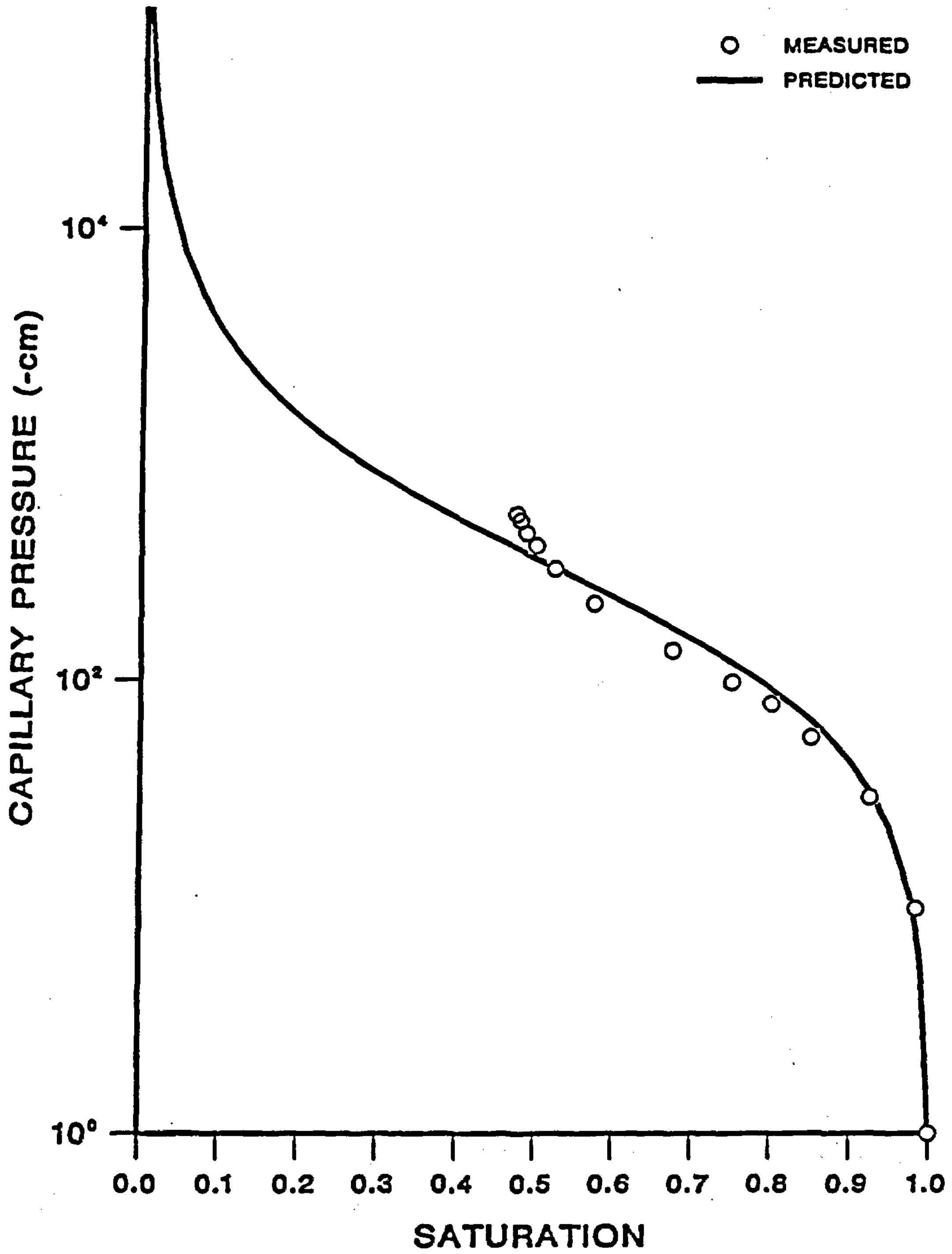
ARYA AND PARIS SOIL B

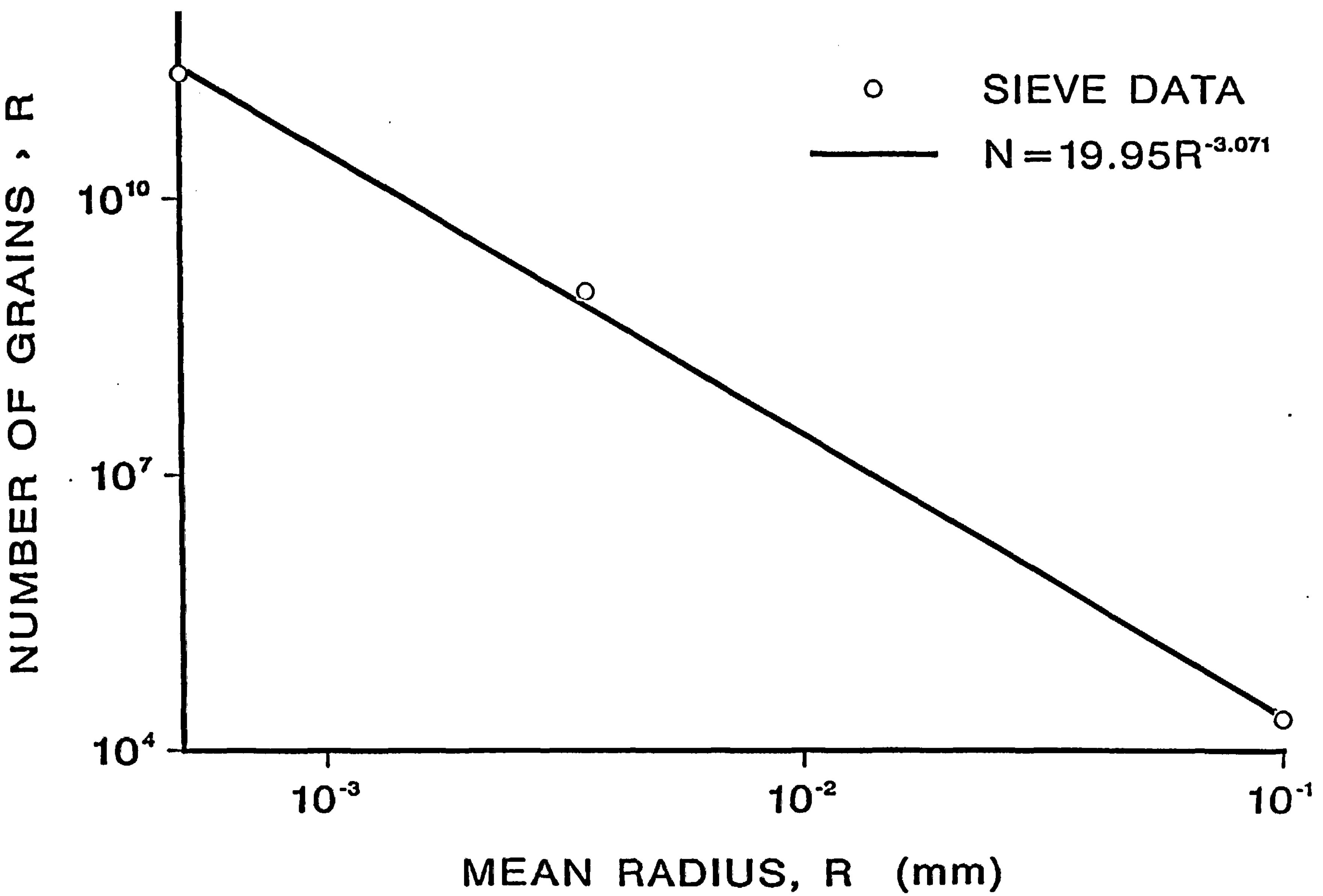




SIEVE DATA
N=2.7R-3.485
NUMBER OF GRAINS , R
MEAN RADIUS, R (mm)
10^8
10^6
10^4
10^2
10^0
10^-2
10^-1

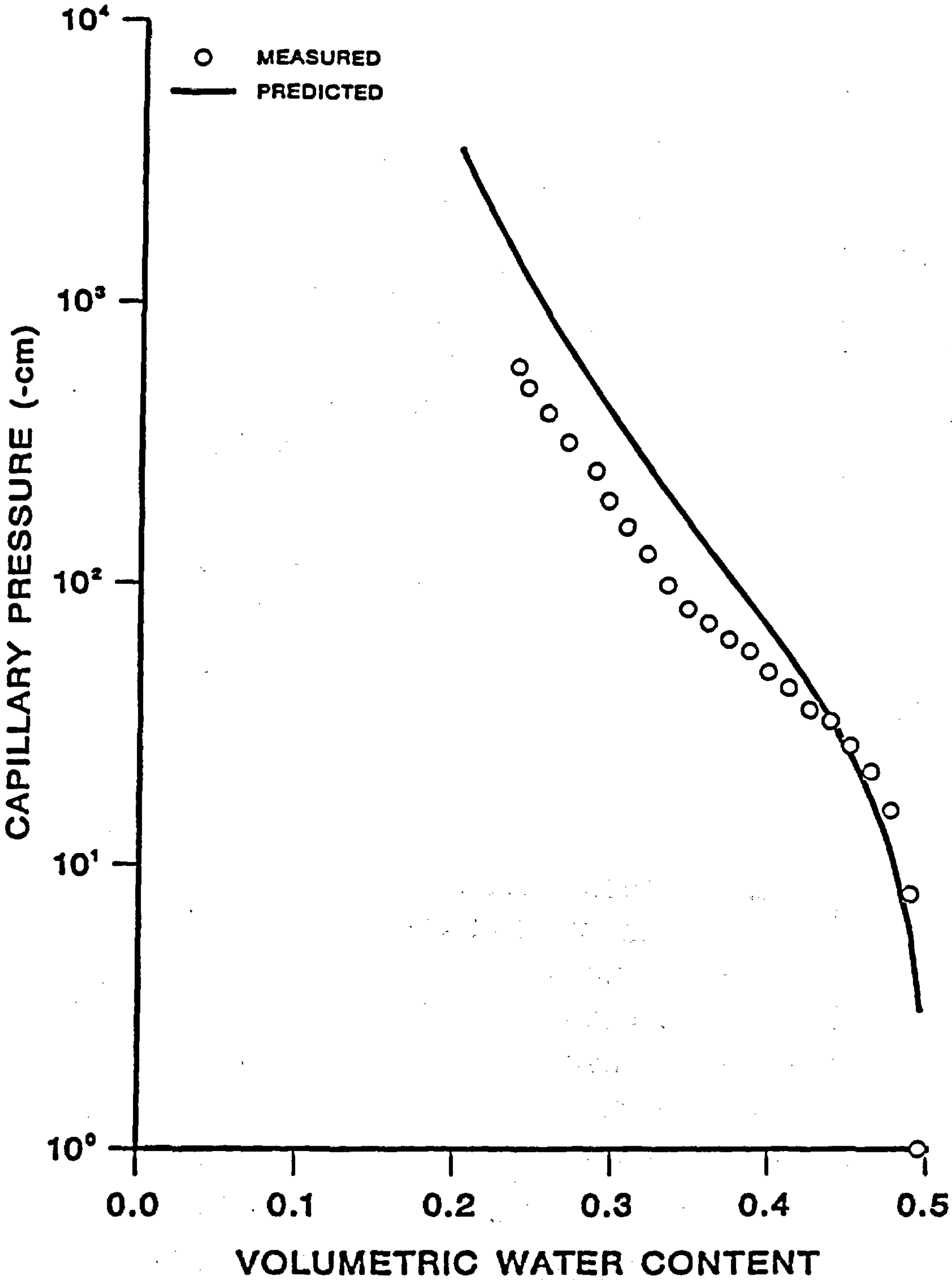
COLUMBIA SILT (2001)



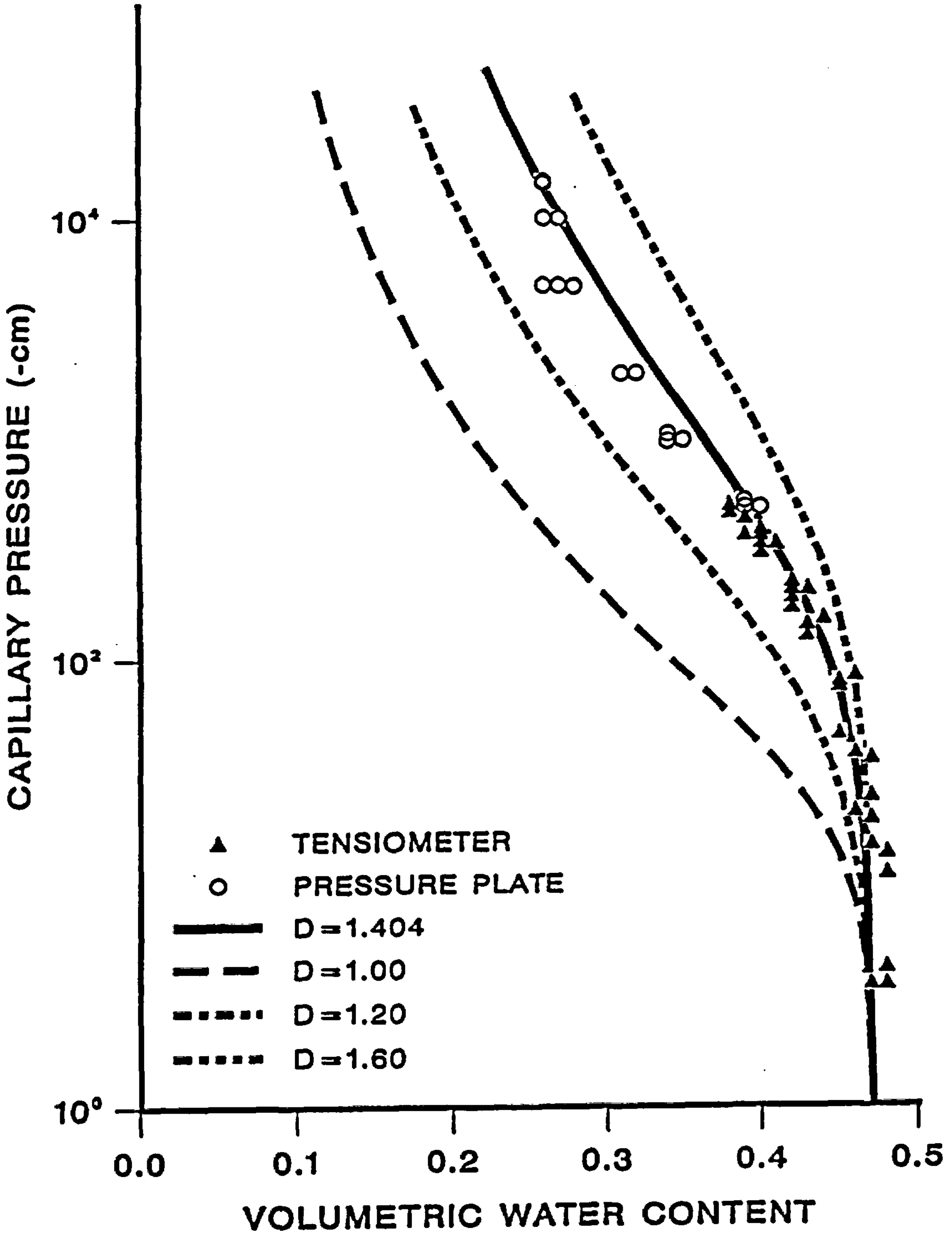


SIEVE DATA
$N = 19.95R^{-3.071}$
NUMBER OF GRAINS , R
200
10^{10}
10^{7}
10^{4}
10^{-3}
10^{-2}
10^{-1}
MEAN RADIUS, R (mm)

YOLO LT. CLAY (3102)



SENSITIVITY TO FRACTAL D



SUMMARY OF FRACTAL DIMENSIONS

Soil Type	Fractal Dimension
Sand	
Sable De Riviere	0.70
Oakley Sand	1.138
Sandy Loam	
A/P Soil F	1.011
Gilat Sandy Loam	1.160
Clay Loam	
Yolo Light Clay	1.071
Silty Clay Loam	
A/P Soil B	1.404
Loam	
A/P Soil D	1.264
River Estate Loam	1.163
Silty Loam	
River Estate Loam	1.419
Silt	
Columbia Silt	1.485

CONCLUSIONS

- FRACTAL SCALING APPEARS TO FIT MANY NATURAL SYSTEMS

- PROVIDES EVOLVING SCALE OF HETEROGENEITY (SPOSITO et al,1986) AND EVOLVING REV

- FRACTAL SCALING ALLOWS FOR SCALE-DEPENDANT PROPERTIES: CONDUCTIVITY, FRACTURES, DISPERSIVITY

- APPLICATIONS TO FLOW AND TRANSPORT ARE BEGINNING TO APPEAR IN A VARIETY OF LITERATURE

DISCUSSION TOPICS

- INTRO TO FRACTAL SCALING
- SCALE-DEPENDANT DISPERSIVITY (1-D)
- DISPERSION IN SYNTHETIC MEDIA (2-D)
- FRACTAL SOIL-WATER RETENTION
- FUTURE DIRECTIONS

FUTURE DIRECTIONS

- DEVELOPMENT OF EXPRESSIONS
  FOR CORRECT H–B AVERAGES

- APPLICATION TO FRACTURE
  NETWORKS AND PERCOLATION THEORY

- FFT GENERATED K FIELDS

- $\psi-\Theta$ AND $K-\psi$ PREDICTION
  IN SYNTHETIC AND REAL SOILS

PREDICTING THE MOBILITIES OF WATER TRACERS IN UNSATURATED YUCCA MOUNTAIN TUFF: WHAT DO WE NEED TO KNOW?

DONALD LANGMUIR
COLORADO SCHOOL OF MINES
GOLDEN, COLORADO

I. WHY DO WE NEED TRACERS?
1. Hydrologic testing in the unsaturated zone
2. Tracing and identifying potential contamination related to construction activities

II. BASIS FOR SELECTING CONSERVATIVE TRACERS
1. Criteria for selection
   -add 'inert to geochemical or biological reactions or transformations'
2. Some example breakthrough curves of 'conserved' and 'less conserved species'
   a. I, Br and Li in Caisson B (crushed tuff) Nyhan et al. 1986. Li loss by adsorption.
   b. Cl, dextrose, fluorescein & I-131 (media?) Davis et al, 1985, Cl a problem because of high background. I loss due to volatilization as $I_2(g)$.
   c. Br and some halogenated hydrocarbons (quartz sand). Loss of BCF, F-11 and F-113 due to adsorption, probably also due to biological processes in longer tests.

III.TENTATIVE LIST OF WATER TRACERS
1. Note need for cheap tracers in large volume tests, such as tracing waters used in Exploratory Shaft construction
2. Unfortunate that the use of radioactive tracers is not allowed, in that they could be valuable, and relatively harmless in small hydrologic tests.
3. Stable isotope spikes could be very useful tracers. Add to the list O-18 and deuterium-enriched water
4. Among the anions listed for large volume tests, borate is known to be adsorbed on some minerals, such as illite, and chlorite clays, and Fe and Al oxyhydroxides (Rhoades et al., 1970, Soil Sci. Soc Am. Proc. 34, 938). Iodide tends to be oxidized and volatilized as I_2 gas, and nitrate may be retarded and consumed by biological activity.

IV. MEASUREMENT AND MODELING OF TRACER ADSORPTION BEHAVIOR
1. Rock sample preparation and characterization for laboratory batch or column tests
   a. Is water flow dominantly via fractures or matrix? How does one sample a fracture and study its adsorption behavior?
   b. If you must grind up a low permeability welded tuff in

order to measure adsorption onto it, what do your adsorption results have to do with in-situ behavior?
c. Rock composition, mineralogy and texture should be studied. What are the minerals and their areas in contact with moving water in matrix or fractures? Methods of study include thin section analysis with particle/crystal size measurement, SEM, XRD, and bulk chemical analysis, with assignment of compositions to individual minerals.
d. How does crushing, sizing and washing change the properties of the original tuff relative to in-situ? Are rock mineral abundances different in different particle sizes of the crushed material, for example? Unless you have answers to such questions, the results of lab experiments using the crushed material cannot be used to predict undisturbed tuff behavior with any confidence.

V. COMPLICATIONS IN INTERPRETING EXPERIMENTAL BATCH AND COLUMN STUDY RESULTS

1. The rate of equilibration of adsorption may be limited by the diffusion rate of sorbate species, particularly when adsorption is within rock matrix. Illustration shows times to 50% adsorption as a function of grain size for some stream sediment materials (Malcolm and Kennedy, 1970, J. Water Pollution Control Fed., May, p. 153). Complete ion exchange equilibrium took about 1-2 days for distances of 0.2 to 0.95 cm. At high column flow rates the slow rate of diffusion into immobile or side-pore water may lead to earlier breakthrough times of solutes (Nkedi-Kizza et al, 1983, Water Resources Res. 19(3), 698). Diffusion into immobile water may also lead to apparent loss of tracers in column studies (Polzer et al., 1987, NUREG/CR-4875).
2. Anion exclusion may result in anion arrival times ahead of bulk water. The effect is most pronounced in tuffs which contain smectite clays and zeolites. Rundberg et al., 1987, LANL Milestone R313) studied anion exclusion in crushed Yucca Mt. tuffs enriched in zeolites or smectite. As shown in the figure, retardation coefficient (R_d) values were generally less than unity for all ions studied except fluoride. The authors point out that anion exclusion can be expected to increase as tuff moisture content decreases, and a higher percentage of residual water is intracrystalline, within the clays and zeolites.
3. Water added to tuff, particular crushed tuff, will react with the minerals present, and tend to dissolve them during batch or column tests. The effect can be pronounced as shown by the plot of tuff dissolution after Reddy and Werner (1987, USGS Open File Report 87-550). The result will be a rapid change in the surface properties of tuff minerals, in part by dissolution, which may be incongruent, and also be readsorption of species such as Al, Fe and Si. Because adsorption is a surface process, such effects can drastically change the adsorption properties of the rock

being tested, and must be studied.

VI. THE ADSORPTION MODEL YOU CHOOSE, DRIVES YOUR EXPERIMENTAL DESIGN, AND THE GENERAL APPLICABILITY OF YOUR CONCLUSIONS

1. If we are satisfied with a distribution coefficient or K_d approach, experimental measurement is very simple, but the porous media remains a black box.
2. If, on the other hand, we wish a more scientific understanding of what is going on in the box, and a more reliable model for predicting adsorption, we need to better understand controls on the adsorption process. The Figure lists some of the important parameters and properties that control adsorption, which must be incorporated in a rigorous adsorption model.
3. In a very general way, the more sorbed a species tends to be, the more independent variables must be taken into account to accurately model and predict its adsorption. As the Figure shows, the number of independent variables increases from 1 in K_d to more than 10 in the surface ionization and complexation (SIC) model.
4. The Table lists parameters needed to model adsorption of a particular tracer anion (or other ion) using the SIC model. Some need be measured only once for a particular rock or mineral (site density, surface area, intrinsic constants for H^+ and OH^- and major ions, and inner layer capacitance). Such models have been applied extensively to modeling adsorption by single minerals, but not by rocks.
5. How do we apply adsorption models to adsorption by rocks? Assuming a K_d (or D) approach is valid, Palmer et al. (J. Inorg. Nucl. Chem 43(12), 3317), suggest a simple additive approach. They show the approach to work for Sr^{2+} adsorption on a binary mixture of illite and montmorillonite, but not for Sr^{2+} adsorption by an alumina/illite mixture. The lack of simple additivity in the second case and elsewhere seems to result from adsorption site blockage by flocculation of sorbing mineral grains and/or preferential dissolution and readsorption of species from one sorbent solid by another. (See also Honeyman, D. B, 1984, PhD Thesis, Stanford Univ.)
6. Although the more complex adsorption models require a more complete understanding of the adsorption process, they are to an extent still just fitting functions. Their validity is only proven if we can predict adsorption behavior for a wide range of conditions of, for example, pH, mineral mixtures, water/rock ratios, and solution compositions. We may never be able to reconstruct the behavior of the black box totally from an understanding of all of its components. Best approach is perhaps to work the problem from both ends at the same time. Perform simple adsorption experiments with single minerals from a rock, to identify major sorbing minerals and dominant processes,

while at the same time studying the rocks' adsorption behavior. It is probably true that in most rocks, only a few minerals dominate the rocks' adsorption properties, and the other minerals represent a practically inert physical matrix which can be ignored.

VII. EXAMPLE TRACER EVALUATION STUDY: BORATE

1. We lack enough inexpensive anionic tracers at Yucca Mt. We are therefore studying the adsorption behavior of borate as a possible tracer. Borate is known to adsorb on clays such as illite and chlorite, and onto some Al and Fe oxy-hydroxides. However, it has been shown an excellent tracer of ground water in some instances, such as at Otis Air Force Base in MA. The relative lack of the sorbing minerals just listed, in Yucca Mt. tuffs suggests that borate might be a useful tracer at Yucca Mt.
2. Goldberg and Glaubig (1986, Soil Sci. Soc. Am. J. 50) have shown they could accurately model B adsorption by soils using a constant capacitance model (a model which, like the SIC model, considers complex-formation of sorbate ions with the mineral surface, but which is otherwise simpler). They have successfully modeled the adsorption process, treating the whole soil as a mixture of a single sorbing clay and inert material.
3. McPhail et al. (1972,) noted, however that silicon and borate compete for the same adsorption sites on Al and Fe oxides. Therefore, the silica content of waters in batch and column tests needs to be considered in any borate adsorption studies.
4. The Figure shows what happens when we put crushed Yucca Mt. tuff in a batch experiment with and without added borate. The borate apparently inhibits readsorption of the silica as the rock dissolves. A more important question that applies to the use of borate as a tracer in tuff, is does the borate concentration remain constant as the tuff dissolves? The last figure shows that it does, perhaps at least in part because readsorption of silica inhibits borate adsorption.

Geochemical Mass Transfer and Mass Transport in Hydrologically Unsaturated Rock

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Abstract. Mass transport by fluid advection and diffusion of aqueous or gas species in hydrologically unsaturated rock is constrained by geochemical reactions among solid, liquid and gas phases. Reactions provide sources and sinks of material, and can affect physical parameters such as porosity, permeability, viscosity, temperature, and two-phase flow quality. Rates of transport of individual species are coupled to the kinetics of interphase and intraphase chemical reactions.

Rates of geochemical processes vary greatly. Rapid reactions such as adsorption at solid surfaces and the hydrolysis of CO_2 ($CO_2 + H_2O \Leftrightarrow H_2CO_3$) can generally be assumed to be at equilibrium in geochemical systems. Many processes such as dissolution, nucleation and growth of silicate minerals, glass devitrification, and diffusion in solid phases are slow, and disequilibrium states persist over geologic time. The concepts of partial and local equilibrium are widely applied in reaction path modeling of the evolution of geochemical systems (e.g. Helgeson, 1968; Helgeson, Garrels and MacKenzie, 1969; Helgeson, 1979).

Of chemical processes occurring in series, the inherently slower process tends to control the overall rate. Mineral dissolution and diffusion of reactant species in an aqueous phase to and from the dissolving interface occur in series, and are coupled by conservation of mass at the reacting interface. The relative significance of diffusion and surface reaction rate in controlling the coupled rate of interfacial mass transfer depends on the diffusion and rate constants as a function of temperature, the distance over which diffusion occurs, and in transient systems, the degree of disequilibrium at the mineral-solution interface. In general, diffusion tends to be the rate-controlling mechanism at high temperature and for large diffusion distances, and the degree of diffusion control tends to increase as local equilibrium is approached at the reacting surface (Murphy, Oelkers, and Lichtner, 1989).

The evolution of water-rock systems in partial equilibrium can be modeled as a function of time and reactive surface area using kinetic equations and data for the rate-limiting mineral dissolution reactions (Helgeson and Murphy, 1983). A substantial data base exits of kinetic parameters for mineral dissolution (Helgeson, Murphy, and Aagaard, 1984; Lasaga, 1984; Wieland, Wehrli, and Stumm, 1988; Murphy and Helgeson, 1989). Kinetic reaction path computations for nonisothermal systems permit simulations of the evolution of groundwater flowing in a thermal gradient in a geologic medium, and the sequence and distribution of secondary minerals produced. Successive zones of dissolution and precipitation of given minerals (e.g. quartz) are predicted to occur in such systems (Murphy, 1988).

Coupled mass transfer between aqueous and solid phases and mass transport by fluid flow can be modeled with Eulerian and Lagrangian mathematical formulations. The Lagrangian formulation uses a frame of reference that is fixed relative to a packet of moving fluid. In the steady state of constant reactive surface area, porosity, permeability, and mineral reaction zone boundaries, the temporal and spatial sequence of mineral dissolution and precipitation can be represented with a single, fluid-centered, reaction path simulation, referred to as a stationary state model. Multiple reaction path formulations apply to systems that are characterized by a series of stationary states (Lichtner, Helgeson, and Murphy, 1987; Lichtner, 1988).

Reaction with a gas phase can strongly affect aqueous solution chemistry such as oxidation potential, pH, and ionic strength. Variations in these parameters can lead to mineral dissolution and precipitation. For instance, volatilization of CO_2 from a bicarbonate groundwater leads to increases in pH, which can lead to precipitation of calcite or dissolution of phases such as clinoptilolite (Arthur and Murphy, 1988). Pressurization with CO_2 can have the reverse effect.

Accurate modeling of mass transport in unsaturated media must take into account the coupled effects of two-phase fluid flow and gas-water-rock geochemistry.

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CHEMICAL SAMPLING AND MASS TRANSFER

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Department of Hydrology and Water Resources

The hydrochemistry and isotope geochemistry of the Apache Leap Tuff Site is being investigated in a series of studies which range in scope from microscale fracture geochemistry to area-wide geochemical mass transfer modeling. The focus is to identify processes and develop sampling techniques which will be transportable to other tuff sites. This presentation examines the following research projects currently underway or recently completed:

- Authigenic Minerals and Stable Isotopes
- Phenocryst Weathering and the Isotope Signature
- Mass Transfer: Rainwater to Spring Water
- Surface Chemistry
- Natural Tracers (Sulfate, Boron Isotopes, etc.)
- Lab Scale Chemical Data
- Lab Scale Tracer Tests and Measurement Methods Development

The variation in $\delta\ ^{18}O$ and $\delta\ ^{13}C$ in authigenic minerals removed from fractures, and the $\delta\ ^{18}O$ in opal removed from the matrix, in the Apache Leap Tuff, were determined by D.S. Weber and have been summarized in Weber and Evans (1988). Secondary quartz and calcite are present as fracture filling material and the $\delta\ ^{18}O$ values indicate precipitation at low temperature probably as meteoric water migrated through the tuff. Fluid movement through the section has left an isotopic imprint both in the matrix and in the fracture system. This process is most likely continuing at present.

A similar study by Rogoff (1989) identified alteraction of phenocrysts at distances perpendicular to major fractures and determined that the weathering has been substantial enough to change the $\delta\ ^{18}O$ and δ D values in the biotite, plagioclase and the bulk rock. The results are interesting in that the isotopic exchange is not consistent with distance and in some instances there appears to be a reversal with more significant exchange at greater distance from the fracture.

The Apache Leap Field Site is near the city of Superior and is surrounded by 4 smelters ranging in distances from 5-90 kilometers. Historical discharges of sulfur gas and other furnace byproducts have given the area a potentially large dose of natural tracers. Sulfur concentrations are quite high both in soil as well as on rock surfaces. Detail studies of fracture surfaces will provide additional estimates of the rate of fluid movement through the unsaturated fracture system at the site.

Samples of the spring water which discharges from the tuff at a location near the field site have been collected and analyzed. Additionally rate and dissolution chemistry of tuff samples have been studied in the lab under controlled conditions of pH, temperature and water-rock ratio. The analyses of spring water samples and the results of the dissolution studies indicate the tuff is rapidly weathering, generating a water dominated by Na, Ca, SO_4, HCO_3 and dissolved silica. Mass transfer modeling indicates that the breakdown of hornblende, feldspar, and chlorite is occurring and these minerals are weathering primarily to smectite, oxyhydroxides, cristobalite and secondary quartz. These reactions will account for the major mass transfer in the system. A clear understanding of the baseline chemistry is required to design the needed future tracer tests and interpret the most likely flow path.

Small blocks of tuff (20 cm x 20 cm x 50 cm) have been removed from the site for laboratory study. Tracer tests have been conducted in the blocks which contain major fractures to determine principal flow paths and develop methods and procedures for measurements. Coated wire specific ion electrodes were used to measure the movement of a calcium tracer by collecting samples at specific sampling points drilled into the block. Tracer movement was most rapid along preferential flow paths. These data have been reported in Chueng (1989).

Lab scale studies are also continuing in an effort to understand reaction mechanisms, interpret flow processes and develop methods to correlate with field scale experiments. Additional work is underway on both the lab and field scale and recommendations for future work will be presented.

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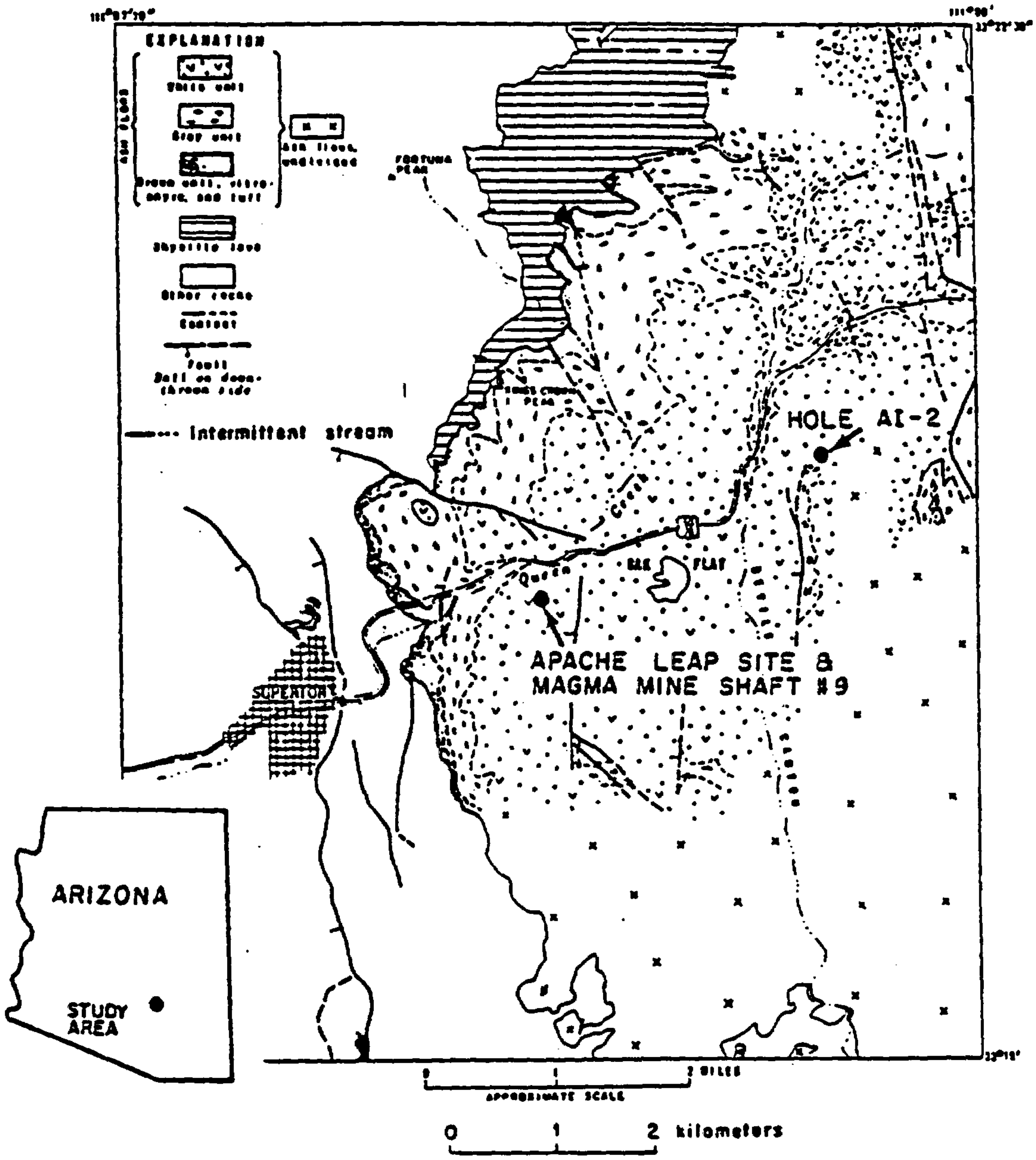
CHEMICAL SAMPLING AND MASS TRANSFER

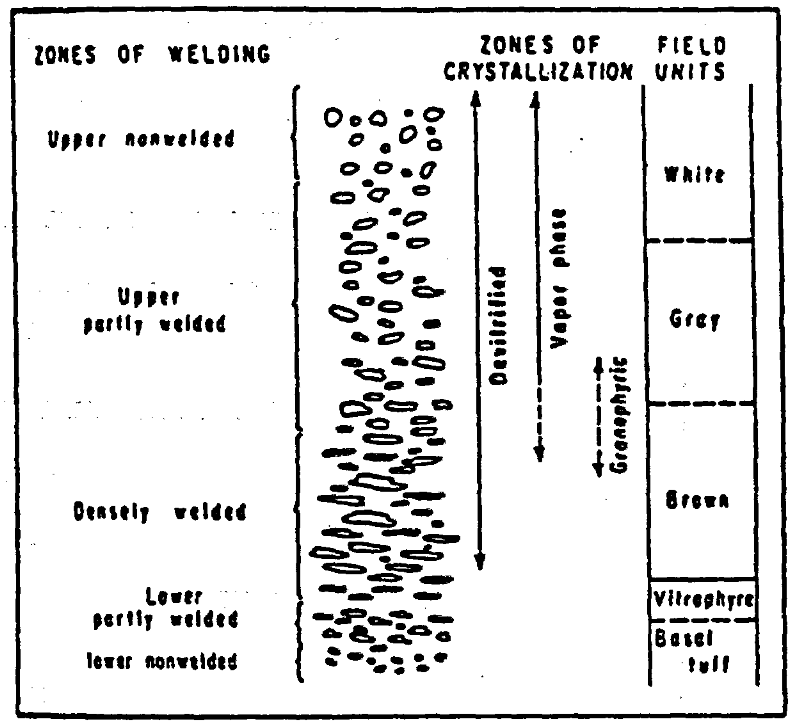
R. L. Bassett

DHWR - University of Arizona

- Geochemical Field Setting
- Authigenic Minerals and Stable Isotopes
- Phenocryst Weathering
- Mass Transfer: Rainwater to Spring Water
- Surface Properties and Transport
- Natural Tracers (Sulfate)
- Lab Scale Chemical Data
- Needed Research



[After Peterson, 1968]



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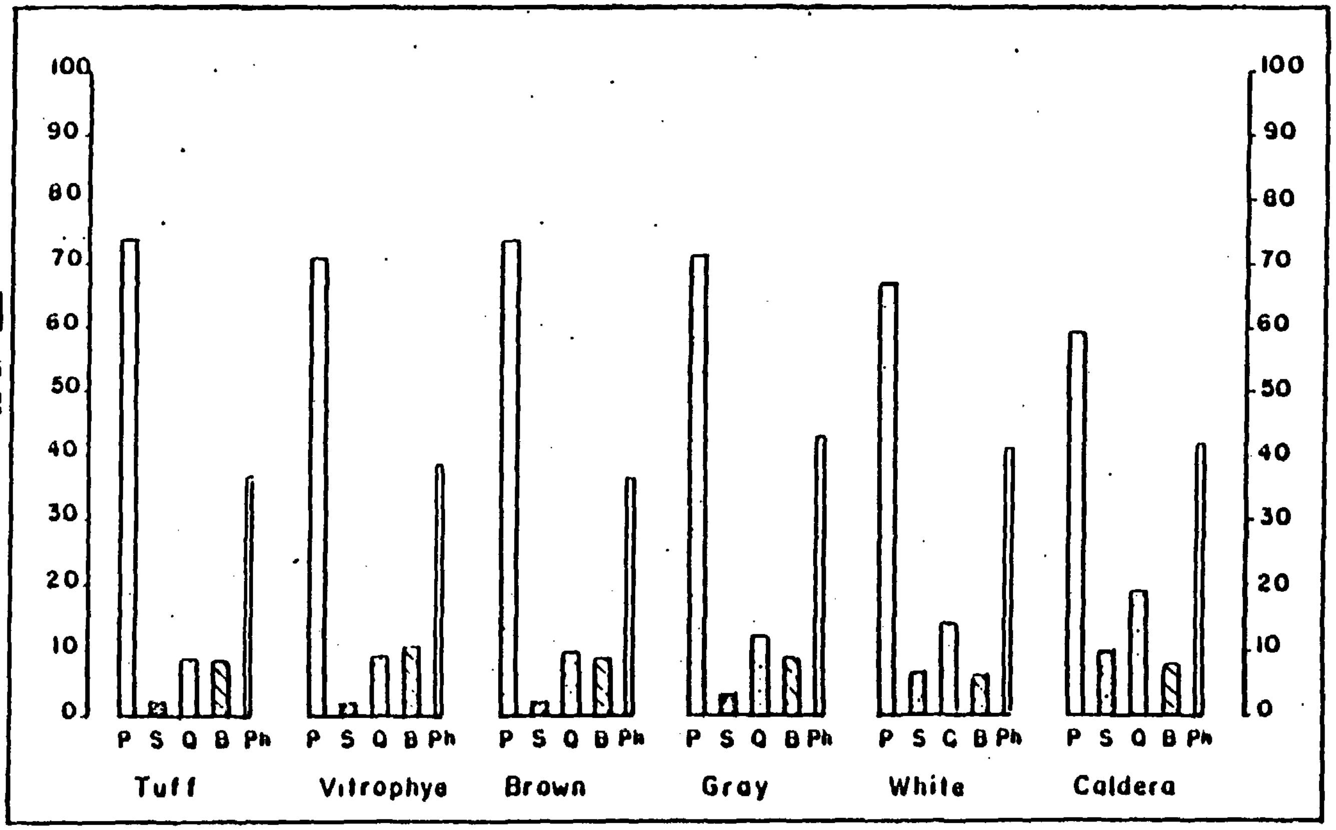
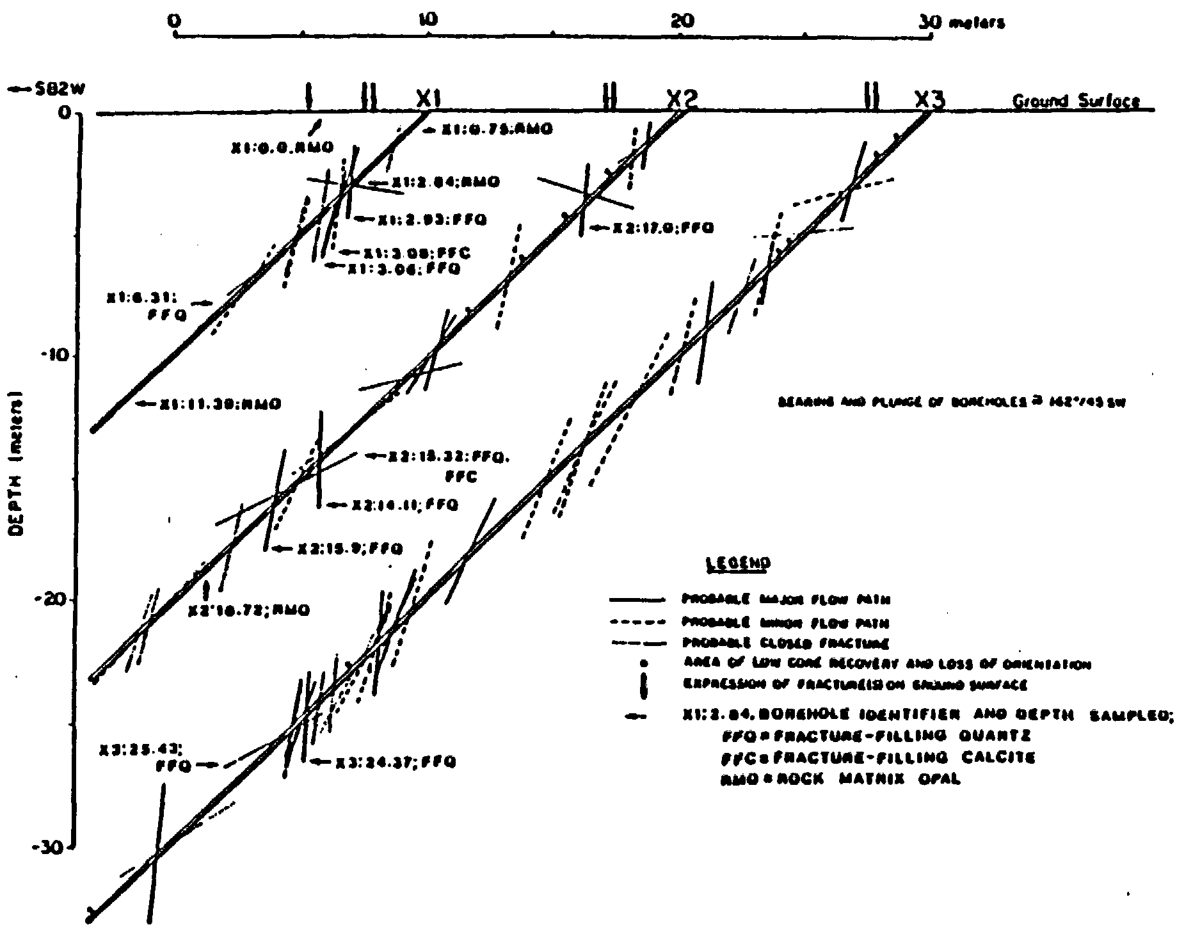


[After Peterson, 1968]

Phenocrysts		41.0		SiO_2	68.70
plagioclase	67.1			Al_2O_3	16.70
sanidine	7.0			Fe_2O_3	2.70
quartz	14.1			FeO	0.10
biotite	6.2			CaO	2.20
magnetite	3.4			MgO	0.38
hornblende	1.8			Na_2O	4.20
	99.6			K_2O	3.60
Groundmass[a]		59.0		H_2O^-	1.40
cristobalite				H_2O^+	NA[a]
K-feldspar				TiO_2	0.40
quartz				CO_2	0.05
plagioclase				P_2O_5	0.15
				MnO	0.08
					100.66

[Weber and Evans, 1988]



[Weber and Evans, 1988]

Quartz (fracture-filling)	$del^{18}O$ (SMOW)
ALS-X1: 2.93	28.51 ± 0.30 (3)
ALS-X1: 3.06	30.66 ± 0.09 (3)
ALS-X2: 3.66	29.59 ± 0.25 (3)
ALS-X1: 6.31	29.55
ALS-X2: 14.11	29.23
ALS-X2: 15.32	28.62 ± 0.00 (2)
ALS-X2: 15.90	29.02
ALS-X3: 24.37	28.69 ± 0.08 (3)
ALS-X3: 25.43	28.11 ± 0.27 (3)

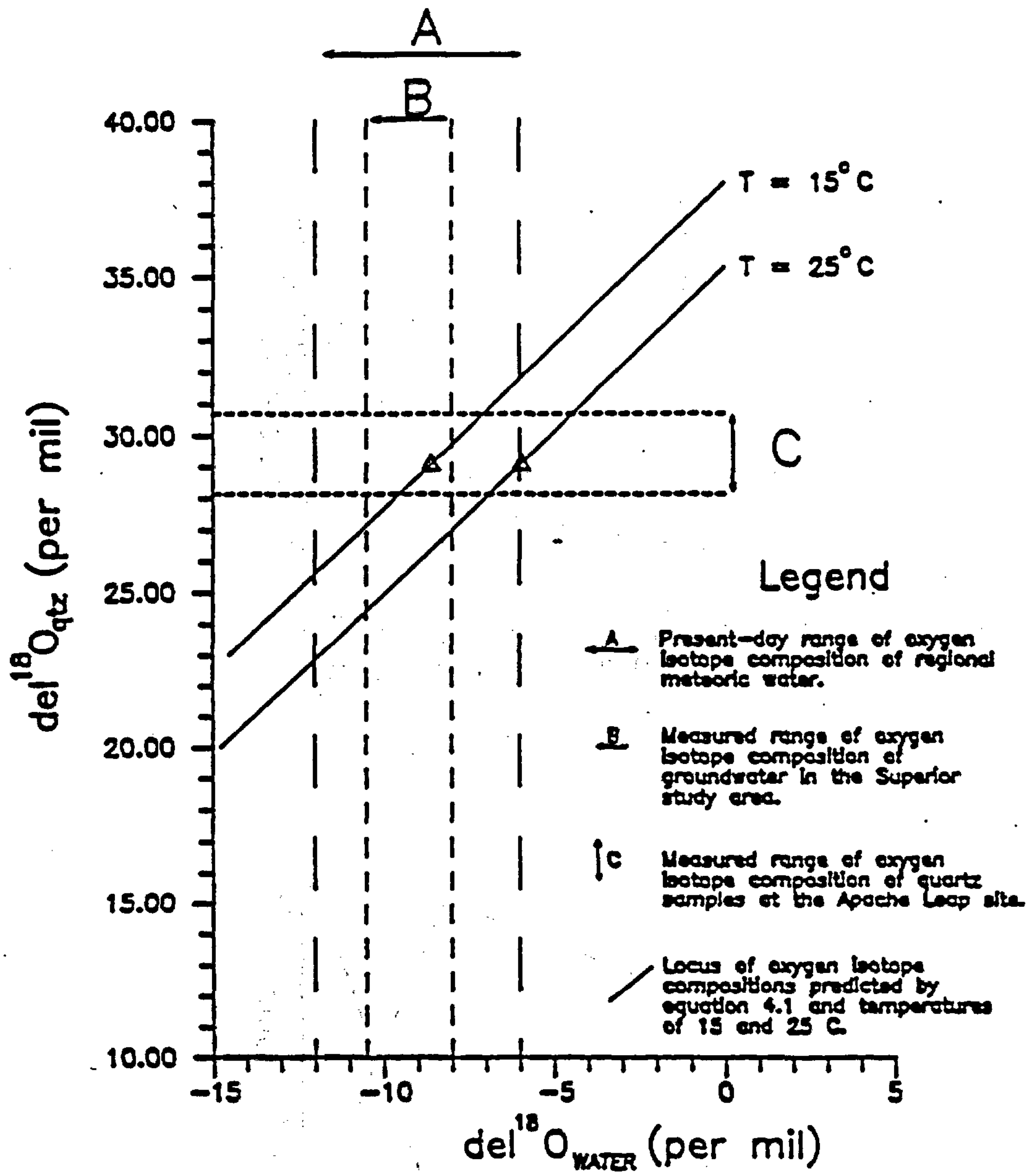
Calcite (fracture-filling)	$del^{18}O$ (SMOW)	$del^{13}C$ (PDB)
ALS-X1: 3.08	23.81 ± 0.20 (2)	-9.31 ± 0.13 (2)
ALS-X2: 15.32	19.47	-9.57
SHAFT9:213.50	17.77	-11.15
SHAFT9:274.50	15.04	-9.73
AS-AI2:334.00	14.20	-9.61
AS-AI2:396.50	14.68	-6.62

Opal (rock matrix)	$del^{18}O$ (SMOW)
ALS-X1: 0.0	18.63
ALS-X1: 0.75	20.54
ALS-X1: 2.84	20.73 ± 0.09 (2)
ALS-X1: 11.39	23.84
ALS-X2-2T: 18.72	25.96
ALS-X2-1T: 18.72	25.53
ALS-X2-NT: 18.72	10.71

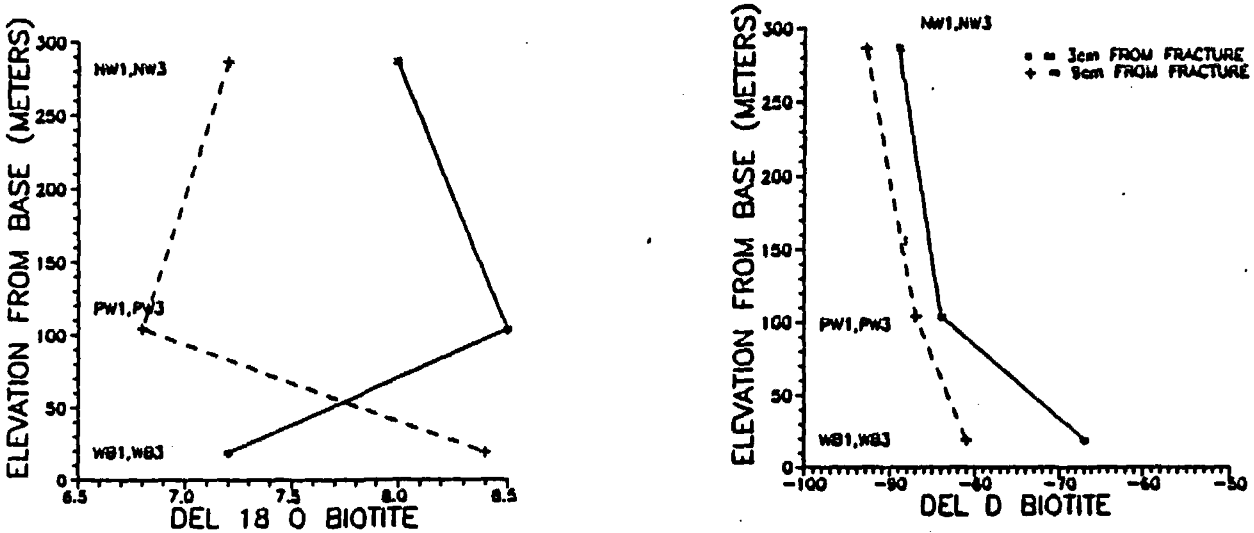
[Weber and Evans, 1988]

Whole Rock (rock matrix)		del^{18}O (SMOW)	
	ALS-X2-WR: 18.72	10.82 ± 0.02 (2)	
Water[c]		del^{18}O (SMOW)	delD (SMOW)
	WM-ALU	-8.29	-62.05
	SPR-WU	-10.09 ± 0.01	-66.49 ± 0.78 (2)
	HOW-BU	-9.93	-68.16
	HOW-LS	-9.93	-67.53

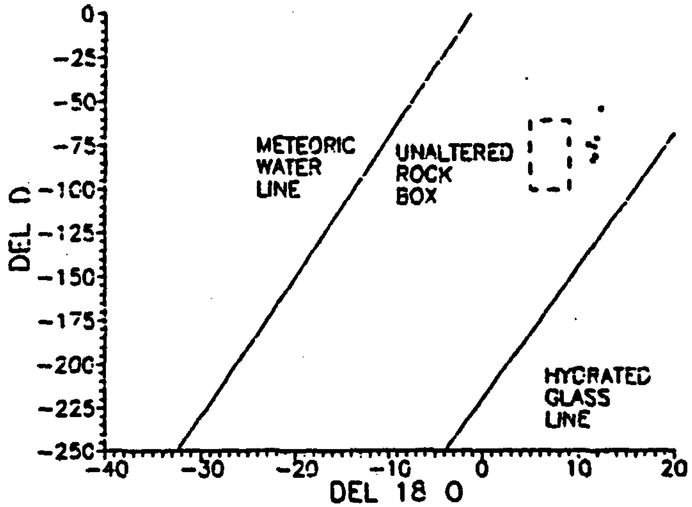
[Weber and Evans, 1988]



[Weber and Evans, 1988]


ELEVATION FROM BASE (METERS)
NW1,NW3
PW1,PW3
WB1,WB3
DEL 18 O BIOTITE
NW1,NW3
PW1,PW3
WB1,WB3
• = 3cm FROM FRACTURE
+ = 9cm FROM FRACTURE
DEL D BIOTITE

[Rogoff, 1989]



0
-25
-50
-75
-100
-125
-150
-175
-200
-225
-250
DEL D
-40
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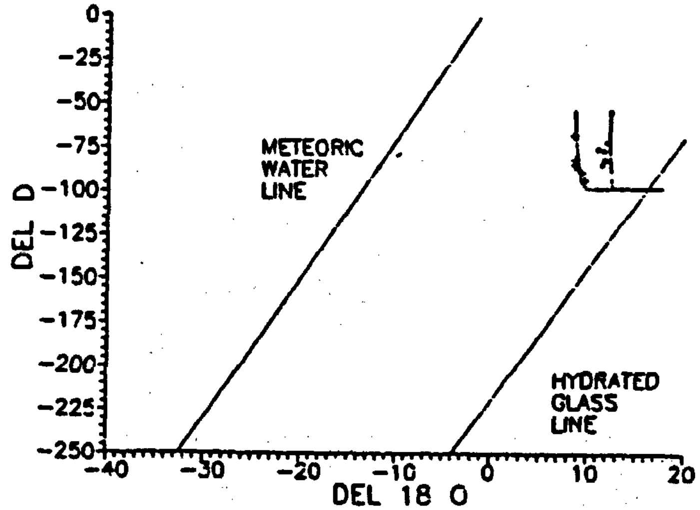
10
20
DEL 18 O
METEORIC WATER LINE
UNALTERED ROCK BOX
HYDRATED GLASS LINE



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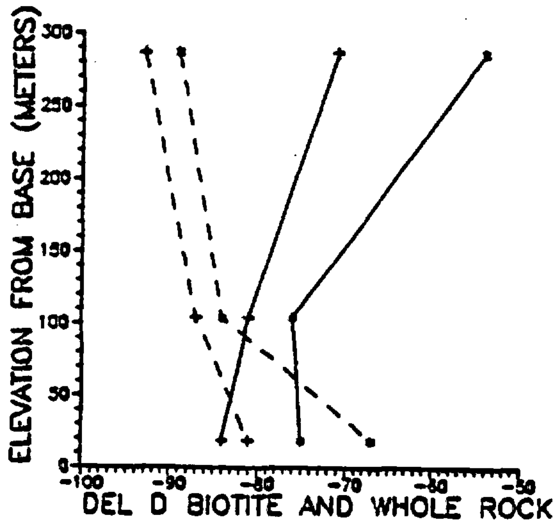
METEORIC WATER LINE
HYDRATED GLASS LINE

[Rogoff, 1989]



ELEVATION FROM BASE (METERS)
300
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-70
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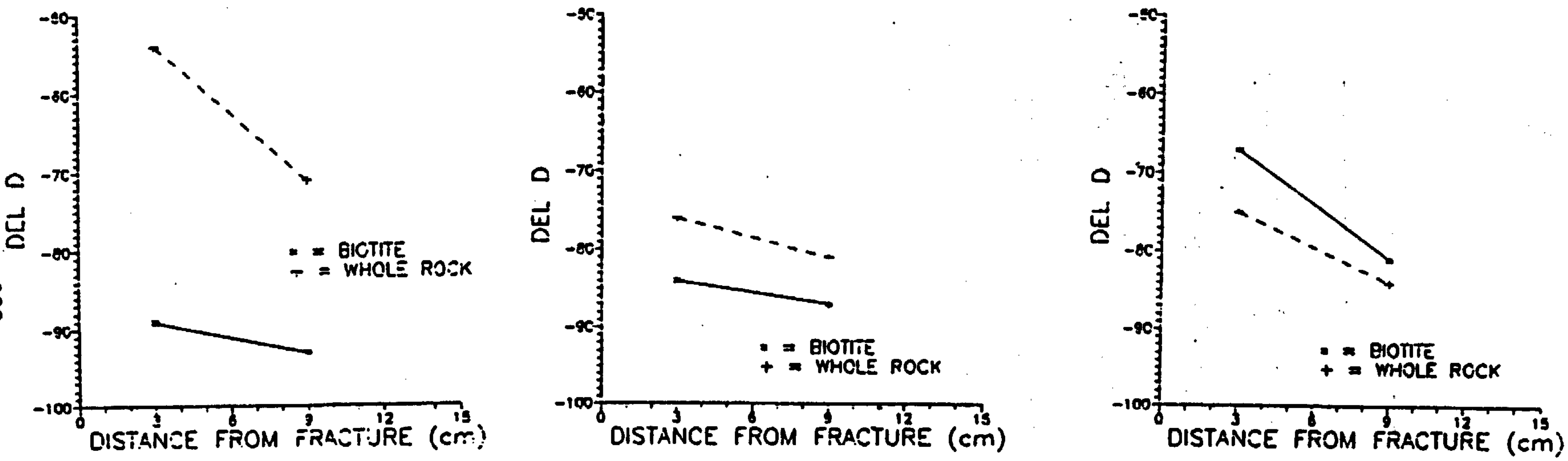
-50
DEL D BIOTITE AND WHOLE ROCK

[Rogoff, 1989]


DEL D
-50
-60
-70
-80
-90
-100
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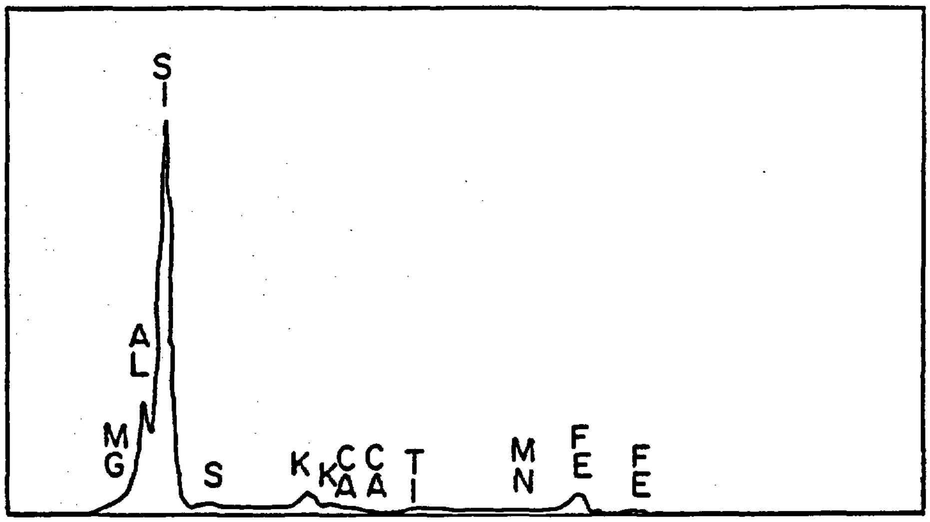
3
6
9
12
15
DISTANCE FROM FRACTURE (cm)
= BIOTITE
+ = WHOLE ROCK

[Rogoff, 1989]

SULFATE CONTENT

	mg/gm
Depression above fracture	44.2
Adjacent to fracture	5.0
Closed depression (small)	9.6
Closed depression (large)	20.0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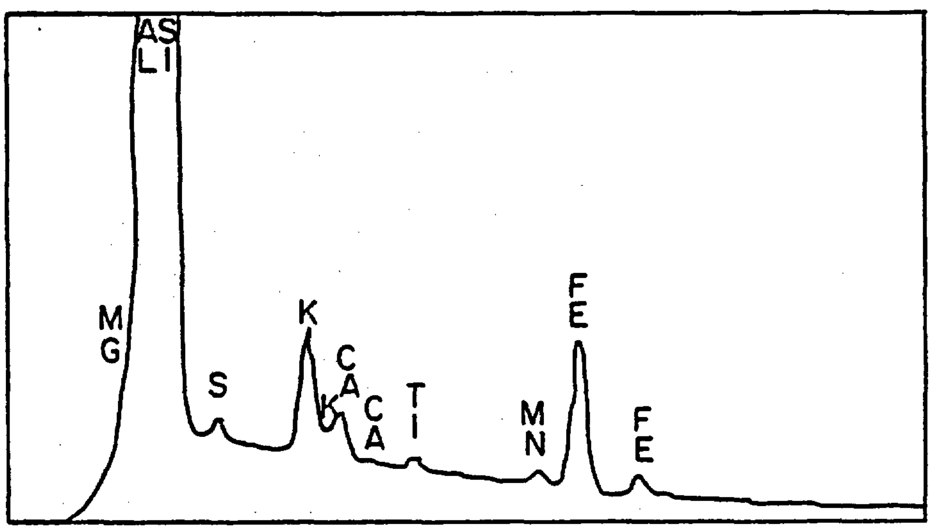
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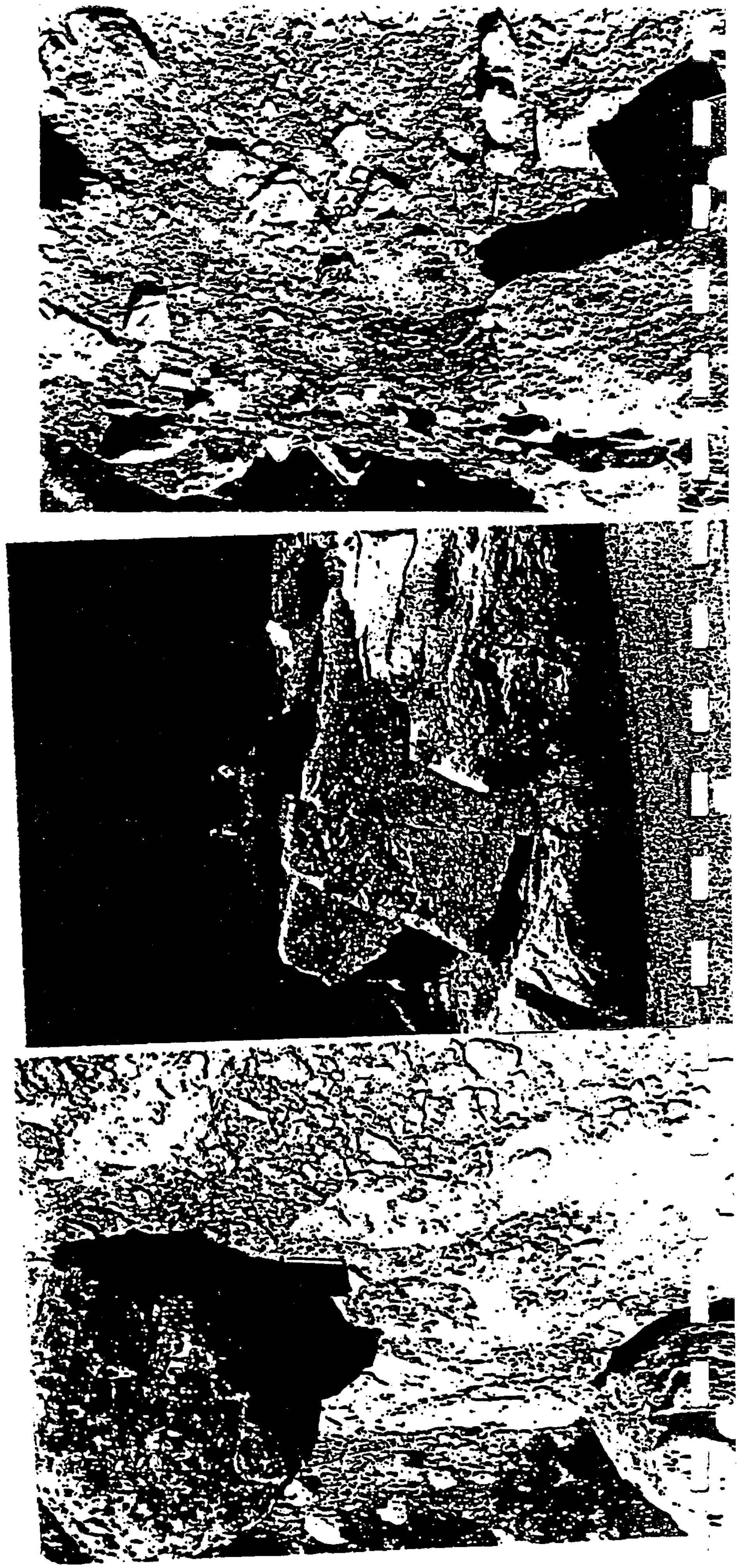

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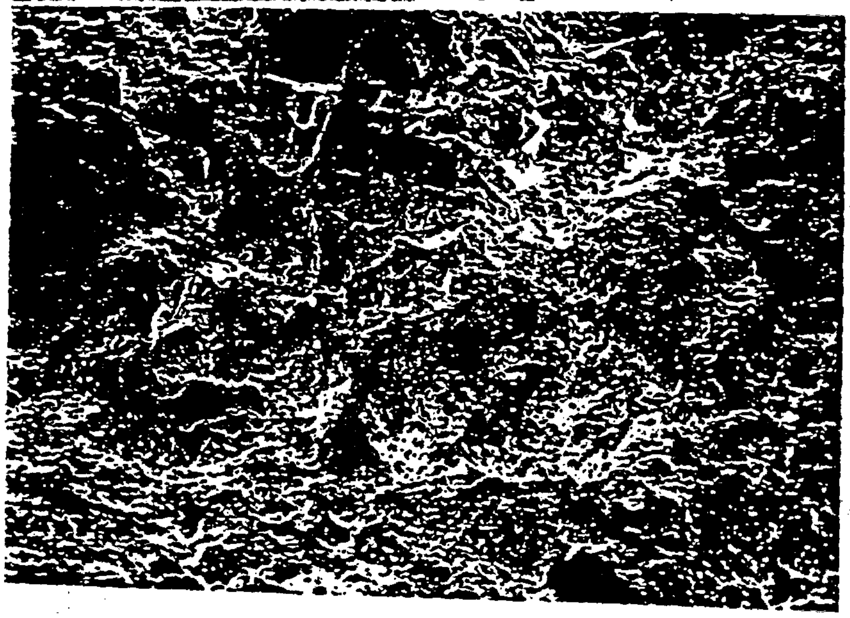
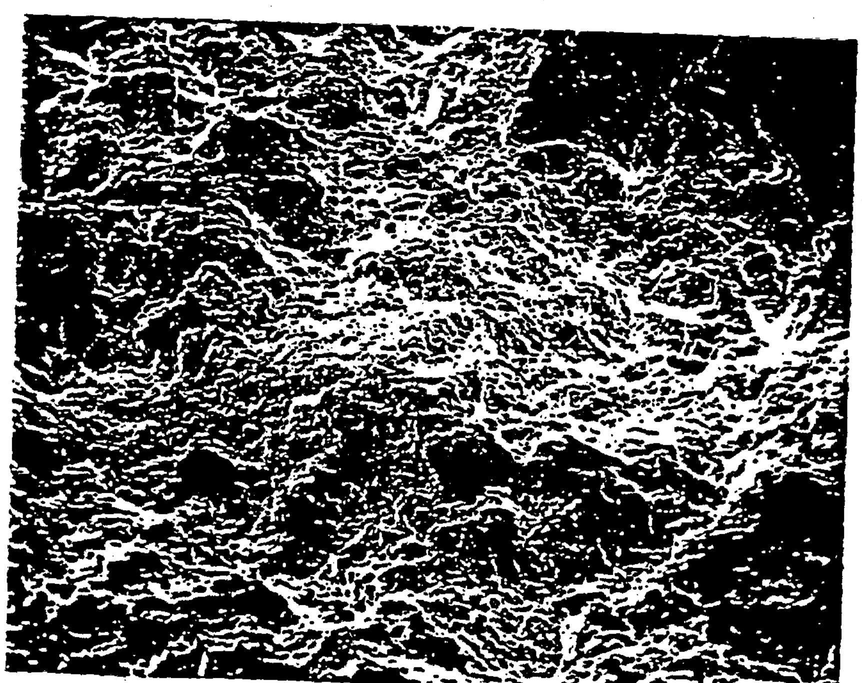
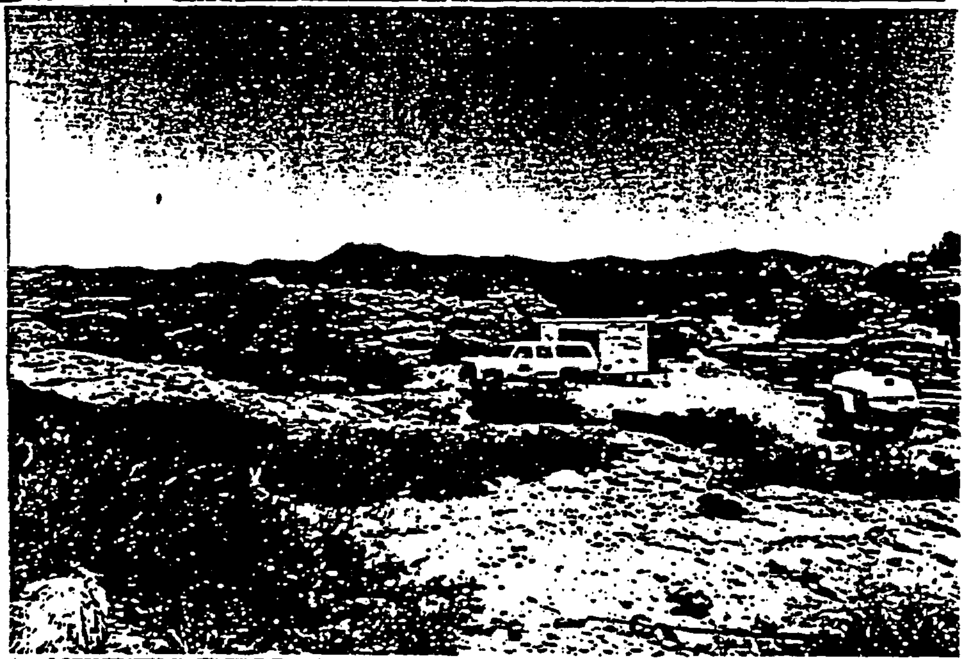


30X (1)



30X (2)



SPRING IN LOWER WHITE UNIT

	6/17/86	9/25/88	11/30/88	Tuff Leachate
Na	13.0	14.0	21.2	4.8
K	3.5	1.4	1.2	—
Mg	4.6	5.4	4.6	2.4
Ca	12.8	19.5	21.4	7.02
Cl	6.0	4.7	3.5	—
SO_4	33.4	33.2	29.0	—
Alk	46.4	36.2	41.7	—
Al	—	.22	.40	.056
Fe	—	.26	.3	<.006
SiO_2	33.8	51.0	50.0	10.9
pH	7.2	5.69	6.32	4.75
T°C	28.5	14.2	12.0	25.0

Plagioclase (An 30) to Montmorillonite

$$1.79\ Na_{0.70}Ca_{0.30}Al_{1.30}Si_{2.70}O_8 + 1.97\ H_2CO_3 + 2.34\ H_2O \longleftrightarrow 1.97\ HCO_3^-$$

$$1.25\ Na^+ + 0.36\ Ca^{++} + 1.16\ H_4SiO_4 + Ca_{0.17}Al_{2.33}Si_{3.67}O_{10}(OH)_2$$

Biotite to Chlorite

$$2\ KMg_3AlSi_3O_{10}(OH)_2 + 4\ H_2CO_3 + 6\ H_2O \longleftrightarrow 3\ H_4SiO_4$$
$$+ Mg^{++} + 2\ K^+ + 4\ HCO_3^- + Mg_5Al_2Si_3O_{10}(OH)_8$$

Homblende ---> Oxyhydroxides

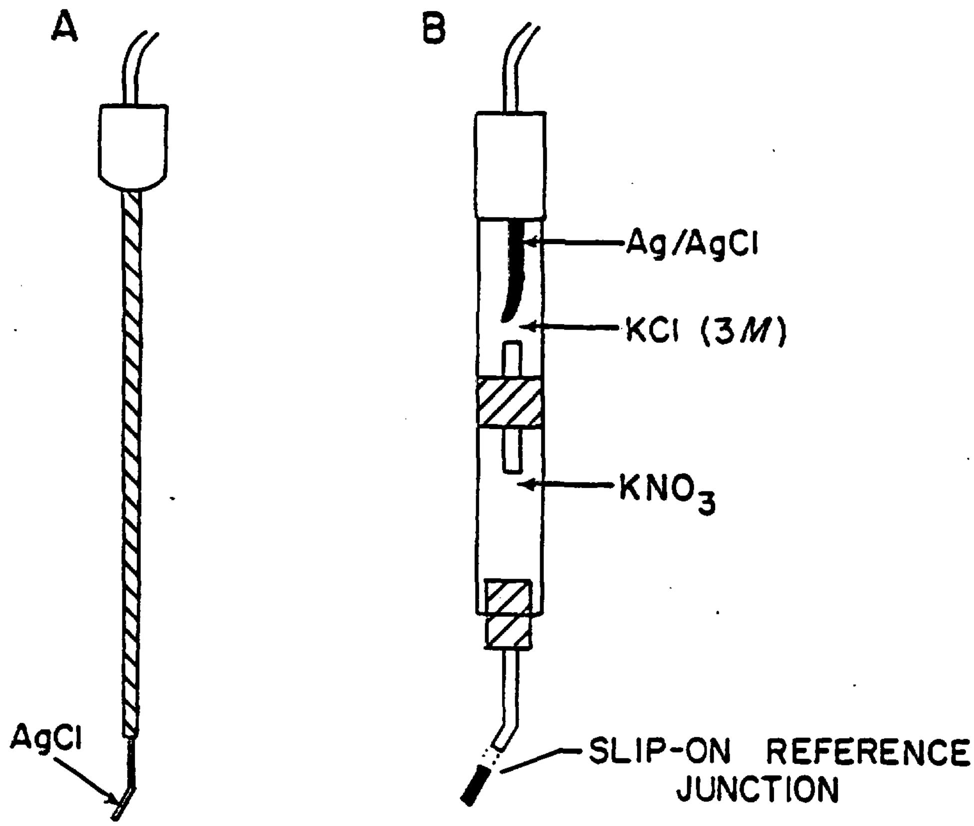
$$(Ca_{1.87}Na_{0.28}K_{0.12})(Ti_{0.16}Mg_{3.32}Fe^{3+}_{0.60}Fe^{2+}_{0.96}Al_{0.14})[Si_6(Si_{1.04}Al_{0.96})O_{.22}]OH_{1.57}$$

$$+ 9.43\ H_2CO_3 + 12.57\ H_2O \longleftrightarrow 1.87\ Ca^{++} + 0.28\ Na^{+} + 0.12\ K^{+}$$
$$+ 3.32\ Mg^{++} + 7.04\ H_4SiO_4 + 1.56\ Fe(OH)_3 + 1.1\ Al(OH)_3$$
$$+ 0.16\ TiO_2$$

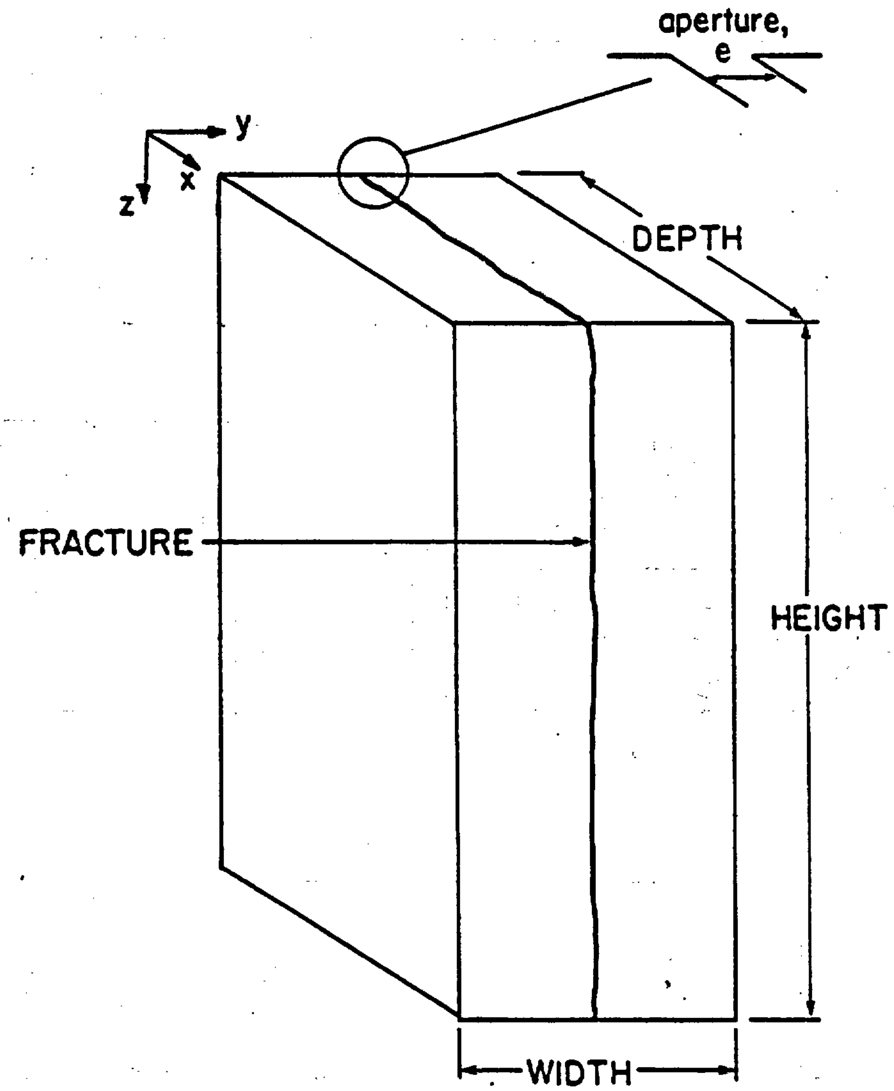
Excess Silica ---> Qtz & Cristobalite

$$H_4SiO_4 \longrightarrow SiO_2 + 2H_2O$$

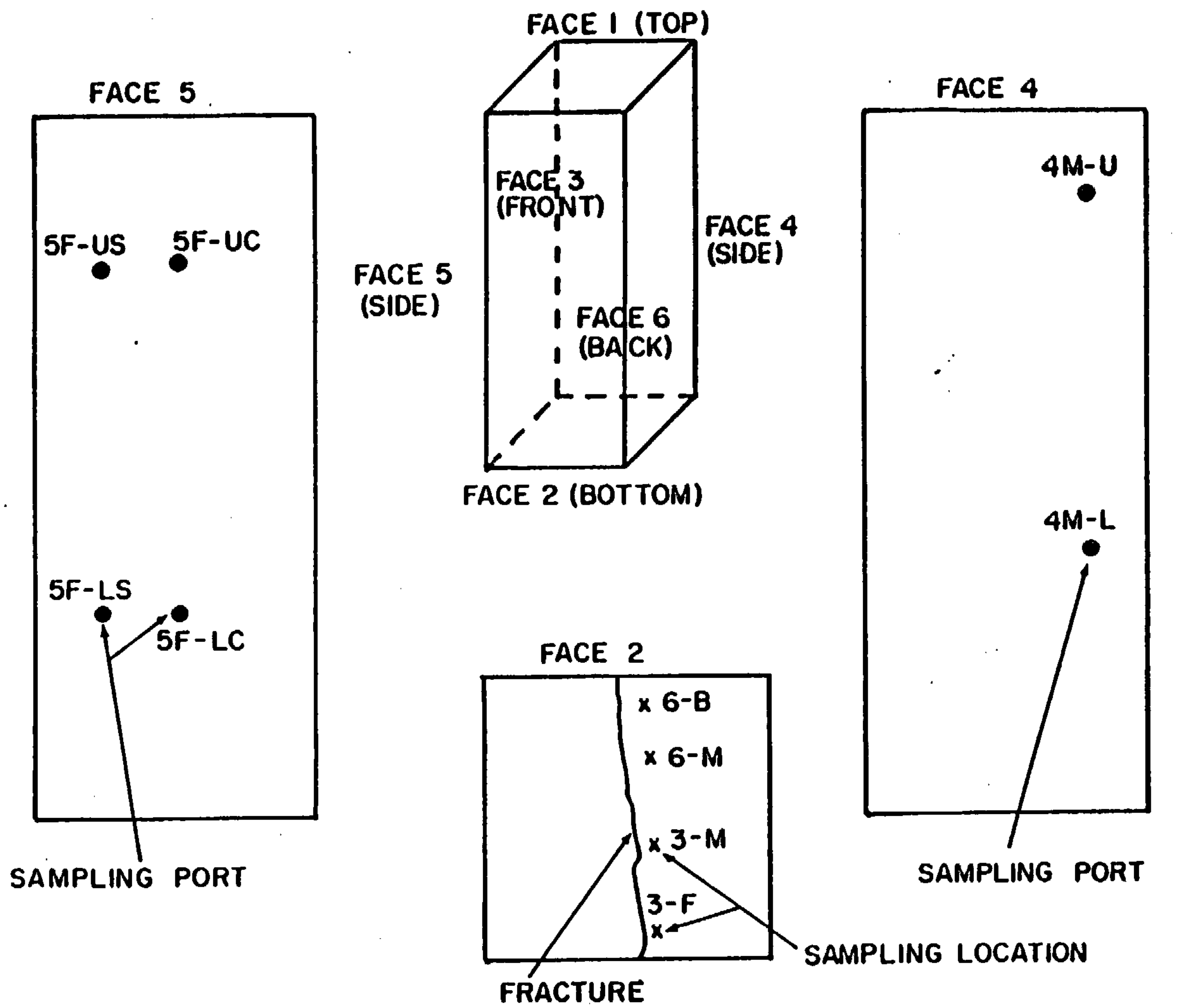
	TUFF			ALTERATION PHASES	
0.215	Plagioclase		0.189	$Al(OH)_3$	
0.195	Biotite	+ Rainwater →	1.43	SiO_2	+Spring Water
0.226	Hornblende		0.263	Chlorite	
0.132	NaCl		0.348	$Fe(OH)_3$	
0.593	H_2CO_3		*or*		
			0.29	Montmorillonite	
			1.13	SiO_2	



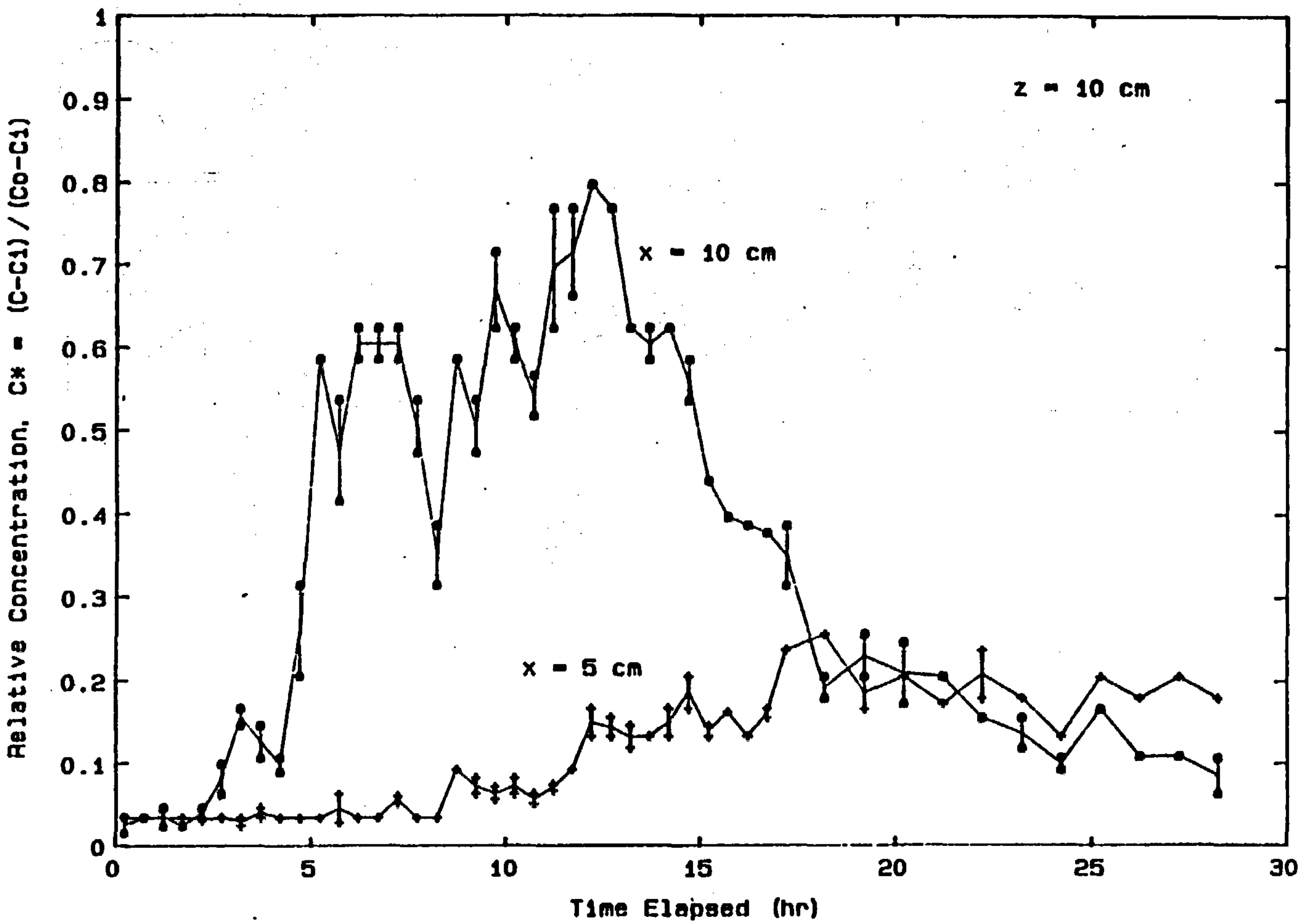
[Chueng, 1989]



[Chueng, 1989]

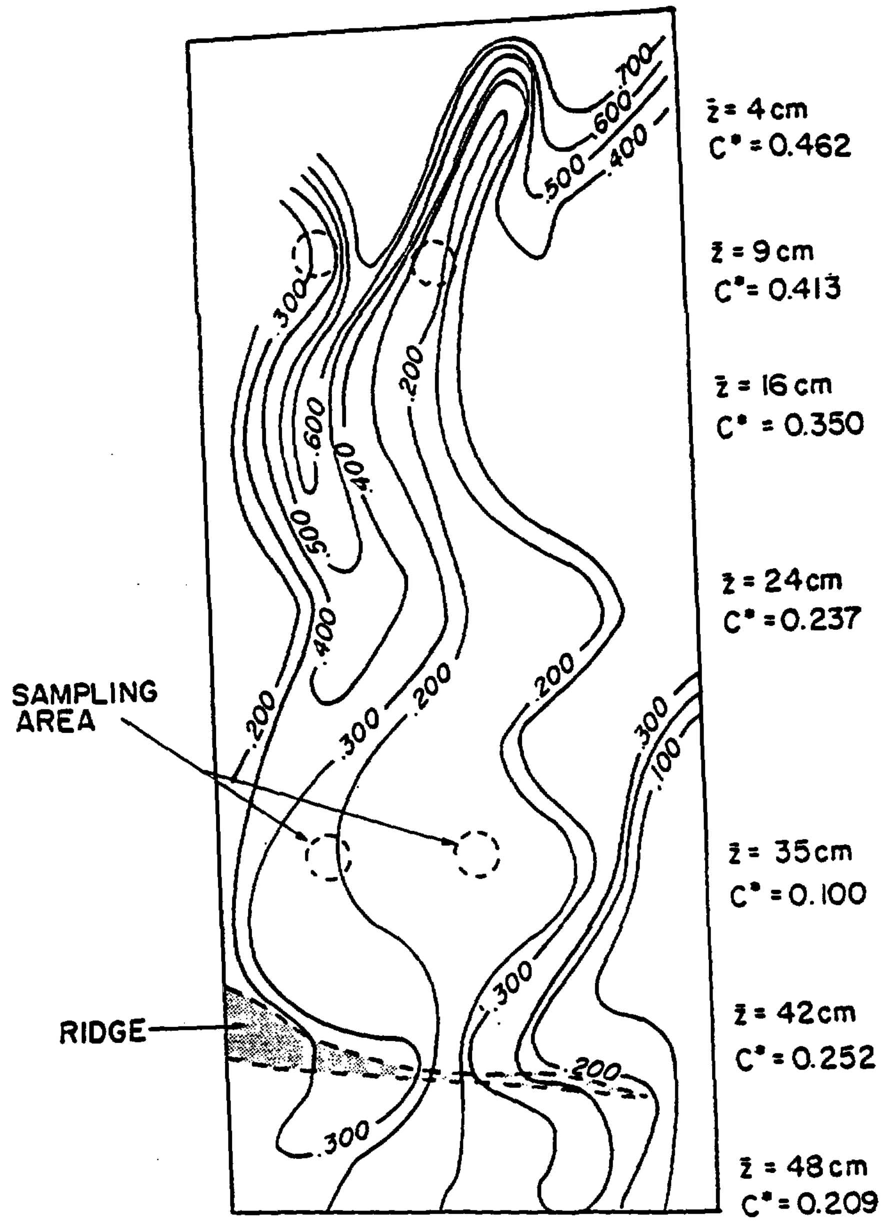

FACE 5
5F-US
5F-UC
5F-LS
5F-LC
SAMPLING PORT
FACE 1 (TOP)
FACE 3 (FRONT)
FACE 4 (SIDE)
FACE 5 (SIDE)
FACE 6 (BACK)
FACE 2 (BOTTOM)
FACE 2
x 6-B
x 6-M
x 3-M
3-F
x
SAMPLING LOCATION
FRACTURE
FACE 4
4M-U
4M-L
SAMPLING PORT

[Chueng, 1989]



Relative Concentration, C* = (C-Ci)/(Co-Ci)
Time Elapsed (hr)
z = 10 cm
x = 10 cm
x = 5 cm
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
5
10
15
20
25
30

[Chueng, 1989]



.700
.600
.500
.400
.300
.200
.100
SAMPLING AREA
RIDGE
$\bar{z}$ = 4 cm
C* = 0.462
$\bar{z}$ = 9 cm
C* = 0.413
$\bar{z}$ = 16 cm
C* = 0.350
$\bar{z}$ = 24 cm
C* = 0.237
$\bar{z}$ = 35 cm
C* = 0.100
$\bar{z}$ = 42 cm
C* = 0.252
$\bar{z}$ = 48 cm
C* = 0.209

[Chueng, 1989]

MAJOR RESEARCH AREAS

- Natural Evolution of Water Chemistry
  - natural tracers (isotopes, chemical species)
  - interpret secondary mineralization
  - lab scale comparison
- Lab: Tuff Surface Chemistry
  - analogy to field conditions
  - dissolution rates
  - adsorption characteristics (tracers/surrogates)
- Lab: Tracer Studies & Sampling Methods
  - spatial variation
  - species selection
  - in-situ and outflow
- Field and Tracer Studies
  - pre-determined flow path
  - water-rock interaction
  - in-situ sampling and analysis

CONCLUSIONS

- Active Mineral Dissolution --> Secondary Minerals
- Stable Isotopes Indicate L.T. Fracture and Matrix Reactions
- Alteration Phases Have High Potential For pH Dependent Sorption
- Natural Tracers May Provide Rates
- Mass Transfer Modeling Supports Water Chemistry -- Suggests Mechanisms
- Lab Data May be Scaled to the Field
- Continued Development of In-Situ Analytical Methods

Monitoring of Gas Movement in a Borehole Completed in the Unsaturated Zone at Yucca Mountain, Nevada

I C Yang, and C A Peters (USGS, Lakewood, CO 80225; D. C. Thorstenson and J C Woodward (USGS, Reston, VA 22092)

Environmental isotopes and trace gases in the unsaturated zone have been analyzed in the borehole of test well USW UZ-1 at Yucca Mountain, for the past 4 years. Samples were analyzed for concentrations of $^{12}CO_2$, $^{14}CO_2$, $^{13}CO_2$, SF_6, CH_4, and HTO, D_2O, $H_2{}^{18}O$ in water vapor. The borehole was drilled using a vacuum reverse-air circulation method to a depth of 387 m in 1983, with SF_6 used as a tracer in the drilling air. The borehole was completed with 15 instrument stations that include gas sampling probes. The stations are isolated from each other by silica flour and cement grout.

At the shallowest station, the CO_2 concentration was about 1 percent by volume. The origin of this CO_2 is unknown; this concentration was substantially greater than the CO_2 concentrations analyzed in soils at other locations of Yucca Mountain. The CO_2 concentrations at the deeper stations had substantial variations with time (ranging from 0.03 to 0.1 percent by volume) during the first 2 years (1984 and 1985). The time variability of the CO_2 concentrations and the presence of residual SF_6 indicate that the borehole should have been pumped longer during or after the stemming of the borehole. Stabilized $^{14}CO_2$ concentrations indicate post-bomb activities at shallow depths; concentrations decreased steadily to about 40 percent modern at the deepest station. There was little systematic depth variation in $\partial^{13}C$ with values generally between -16 and -20 ‰. Tritium concentrations in water vapor from all 15 probes were less than 10 Tritium units (T.U.). Stable-isotope ratios of D/H and $^{18}O/^{16}O$ varied considerably with time, possibly due to condensation distillation inside the probe tube during pumping.

The distribution of CH_4 with depth in the borehole of test well USW UZ-1 may represent a combination of effects of residual air, contamination by stemming materials, and contamination of the probe 15 by drilling fluid. The increased concentrations of CH_4 and CO_2, at station 15 and the shift to "lighter" ^{13}C values, indicate contamination from polymer drilling fluid used in the drilling of geologic test hole USW G-1 located 305 m to the southeast of test well USW UZ-1. About 8.7 million liters of polymer drilling fluid were lost in the drilling of test hole USW G-1; the presence of this drilling fluid was confirmed by chemical analyses of the fluid that collected in the bottom of test well USW UZ-1 during drilling.

Site Selection Criteria and Preliminary Results from the Valles Caldera Natural Analog Study

J. L. Krumhansl
and
H. W. Stockman
Geochemistry Division 6233

The Geochemistry Division, 6233 at Sandia National Laboratory is presently involved in a NRC sponsored natural analog study. This work is directed at providing information on the thermally driven chemical changes expected when high-level nuclear waste is disposed of in tuffaceous rocks. This study was motivated by three factors: (1) a regulatory requirement mandates such activities, (2) the realization that laboratory studies involve only small amounts of rock observed over short time periods, (3) the feeling that a thermal event in a natural setting may illustrate synergisms that fail to occur in a carefully controlled laboratory environment. Toward this end, sites where tuffaceous rocks had been heated were reviewed with the following selection criteria in mind: (1) accessibility, (2) a young age and simple geologic history, (3) a heating cycle that involved many decades at temperatures in a range 150-350°C., and (4) an unsaturated hydrologic regime. The site selected is in the Jemez mountains of northern New Mexico, where the thick Banco Bonito obsidian flow overlies a variety of tuffaceous rocks. Evidence of heating is given by a reddish baked zone extending several tens of feet into the underlying tuff. Geomorphological and mineralogical evidence suggests the tuffs were never saturated with liquid water; however, heating of the tuffs undoubtedly saturated the pores with steam from the dehydration of the volcanic glass.

To date, this study has focused on two research objectives; the extent to which heating caused secondary mineral development in the tuffs, and documenting any evidence of elemental transport. A third longer range objective is to assess whether short term laboratory experiments gave results consistent with lessons learned from the natural analog study.

In spite of the obvious baked zone along the contact, surprisingly little alteration was found in these rocks. In the VC-1 core the only secondary mineral detectable was a trace of montmorillonite. However, the reddish coloration probably reflects formation of very small amounts of hematite as well. The glass shards in the tuffs contain <u>ca.</u> 2% "low temperature" water, in part from perlitization. In samples collected from outcrop, other secondary minerals were identified; calcium sulfate, halite and sodium sulfate. As these salts are highly soluble, they presumably reflect seasonal drying of present-day groundwaters.

The strategy taken to locate evidence for transport was to examine the contact regions for elemental concentration gradients. To date, samples have been examined, from both an outcrop and the VC-1 core. Neither sample set shows evidence for extensive elemental transport. The outcrop samples, however, appear to have been more homogenous before emplacement so the discussion emphasizes these results.

In samples taken from outcrop mobile elements, such as Cs and Rb, showed little variation with distance from the contact. Immobile elements (Th, Ta, Hf, Co, REE) show only very slight compositional trends which probably existed in the tuff prior to heating. It is noteworthy that the Cs/Rb ratio, which is a sensitive indicator of hydrothermal alteration, also does not vary with distance from the contact. In contrast, H_2O and chlorine are depleted adjacent to the contact, and give the only evidence of transport to date. Before ruling out the possibility of finding additional evidence of transport, however, the experimental matrix needs to be expanded to include samples from beyond the red baked zone.

Finally, the results of some preliminary hydrothermal experiments shed light on conditions under which transport and alteration are likely to occur in tuffs. Small amounts of pulverized obsidian were treated with deionized water at 150°C. for eleven months. At the test's conclusions small flakes of clay resembling those found in the VC-1 core were found. The solution in contact with the obsidian was mildly basic, (pH near 9), contained elevated alkali concentrations (Na = 78 ppm, K = 8 ppm), as well as high concentrations of dissolves silica (260 ppm Si) and aluminum (6.5 ppm). In contrast, iron was relatively immobile (0.5 ppm) as would be expected from the elevated pH. Thus, in the future, analytic efforts will give particular emphasis to elements which are likely to be mobile in basic solutions. These experiments also make it clear that only a brief exposure to high-temperature liquid water was required to cause the small amount of alteration seen in the VC-1 core. Hence, most of the time the tuffs were at elevated temperatures, they were probably unsaturated.

Although this report is preliminary, it is evident at even this early date that: (1) picking a natural analog site is, at best, an uncertain undertaking, and (2) heating a large body of unsaturated tuffaceous rocks for a long time did not create conditions condusive to either pervasive alteration or large scale elemental transport.

*This work was supported by Sandia National Laboratories under contract to the U.S. Department of Energy (DE-AC04-76DP00789).

RATIONALE FOR A NATURAL ANALOG STUDY

1) Longer Times

2) Larger Scale

3) Natural Setting

4) Regulatory Requirement

OBJECTIVES OF THE VALLES CALDERA NATURAL ANALOG STUDY

1) Document evidence of transport in unsaturated tuffs

2) Assess extent of mineralogic changes

3) Compare results of short term laboratory hydrothermal experiments with the outcome of the long term natural analog study

PROGRAM DESCRIPTION

FIELD WORK

* Examine tuffaceous units below the Banco Bonito Obsidian Flow

LABORATORY ACTIVITIES

* Assemble a comprehensive database on heated tuff samples from both VC-1 core and outcrop samples
    - mineralogy
    - major elements
    - trace elements

* Hydrothrmal Experiments
    - mineralogy and composition of treated tuff
    - aqueous phase chemistry

* Age and Temperature Determination on Samples
    - ^{39}Ar / ^{40}Ar

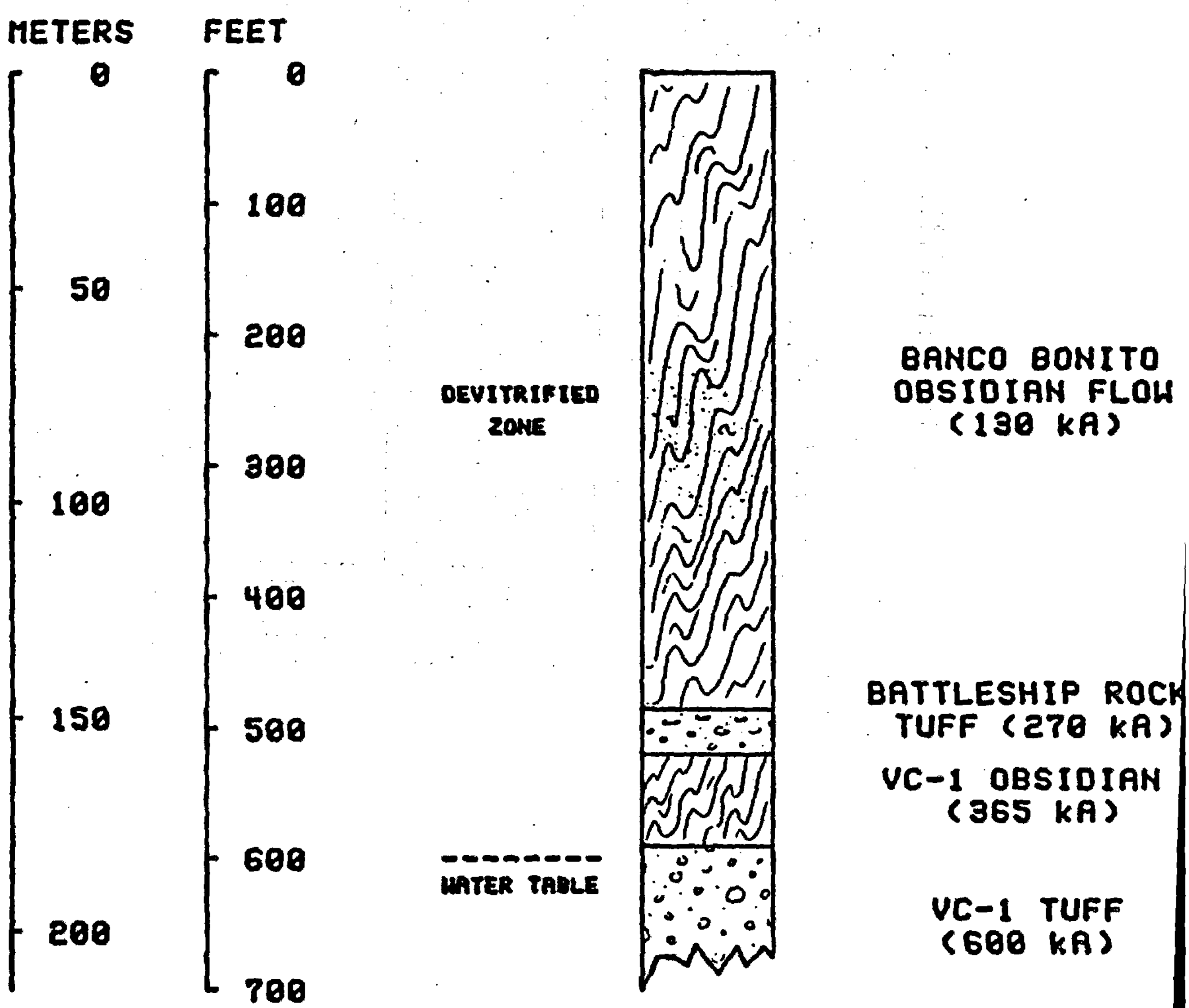
MODELING ACTIVITIES

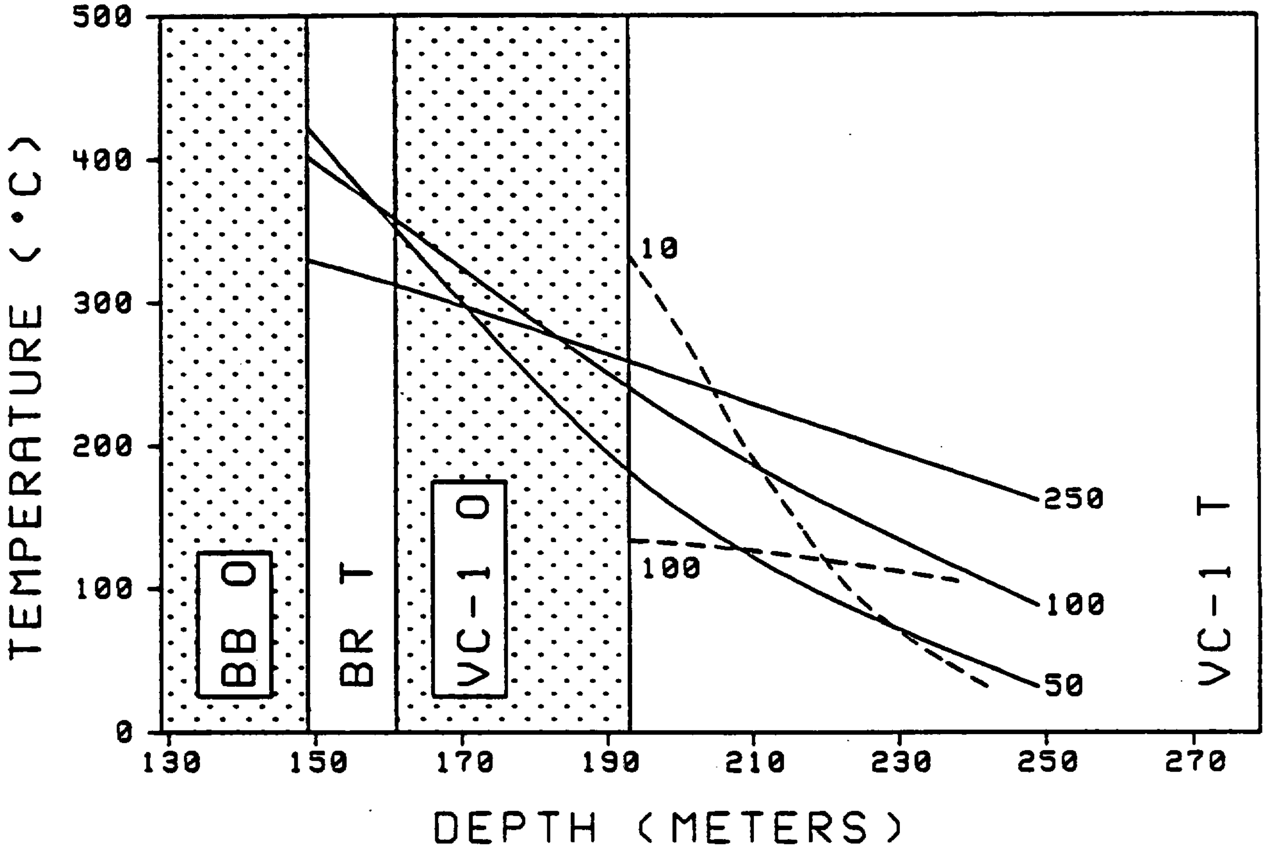
* Thermal Profile Computation

ANALYTIC TOOLS

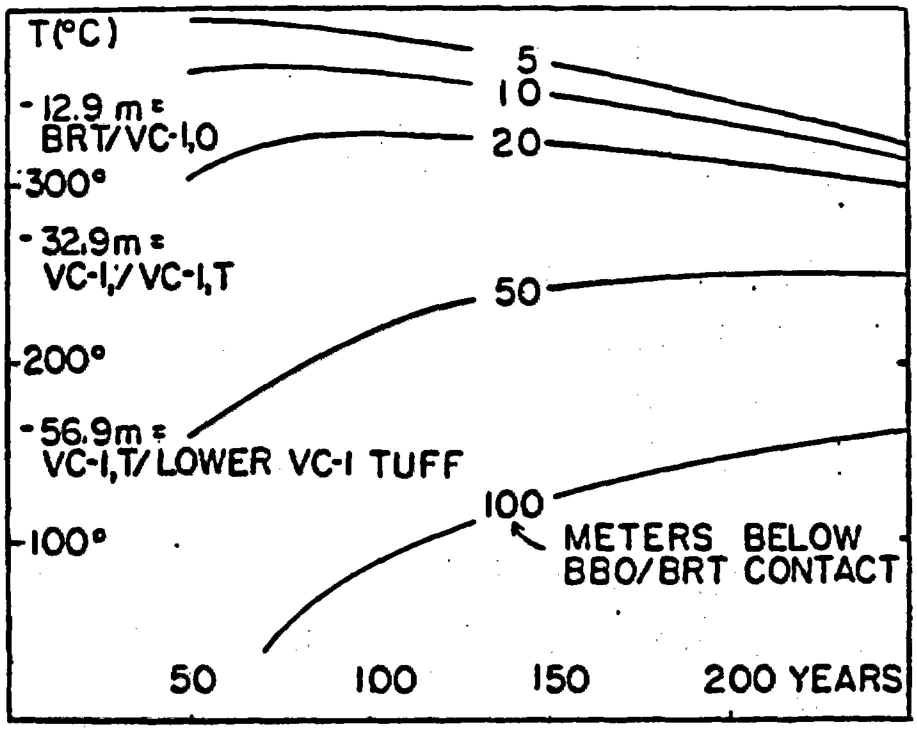
INAA Ion chromatography D.C. Plasma Spectroscopy X-ray Fluorescence	CHEMICAL COMPOSITION
S.E.M. X-ray Diffraction Petrographic Examination	MINERALOGY AND TEXTURE

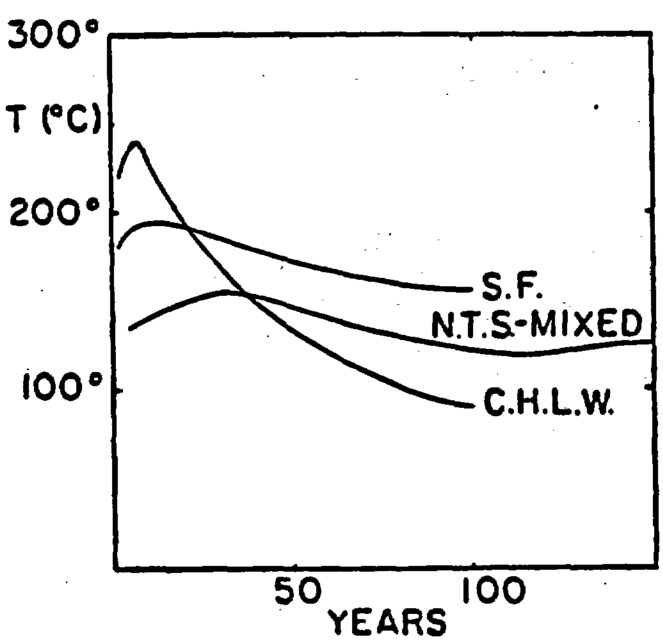
VC-1 STRATIGRAPHY

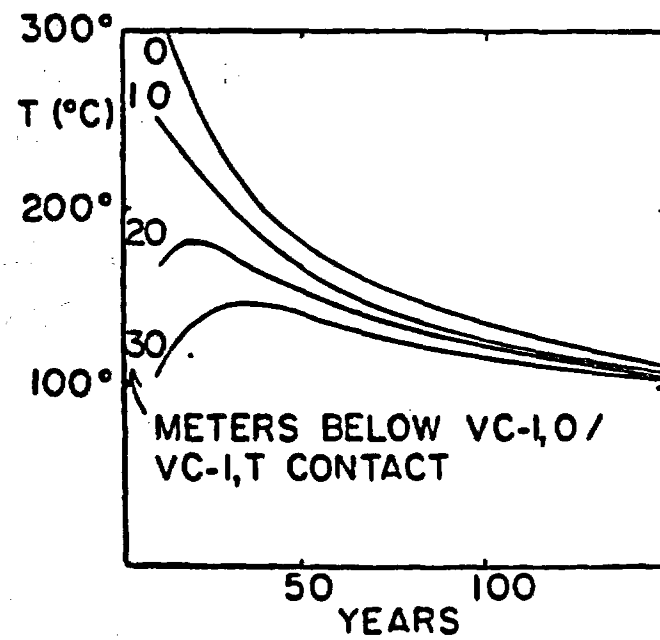




500
400
300
200
100
0
TEMPERATURE (•C)
130
150
170
190
210
230
250
270
DEPTH (METERS)
BB O
BR T
VC-1 O
VC-1 T
10
100
250
100
50


T(°C)
12.9 m = BRT/VC-1,O
300°
32.9m = VC-1,/VC-1,T
200°
56.9m = VC-1,T/LOWER VC-1 TUFF
100°
5
10
20
50
100
METERS BELOW BBO/BRT CONTACT
50
100
150
200 YEARS


300°
T (°C)
200°
100°
S.F.
N.T.S-MIXED
C.H.L.W.
50
100
YEARS


300°
T (°C)
200°
100°
0
10
20
30
METERS BELOW VC-1,O / VC-1,T CONTACT
50
100
YEARS

The Search For Evidence Of Transport

Rock Analyses
- * whole rock
- * clasts
- * matrix

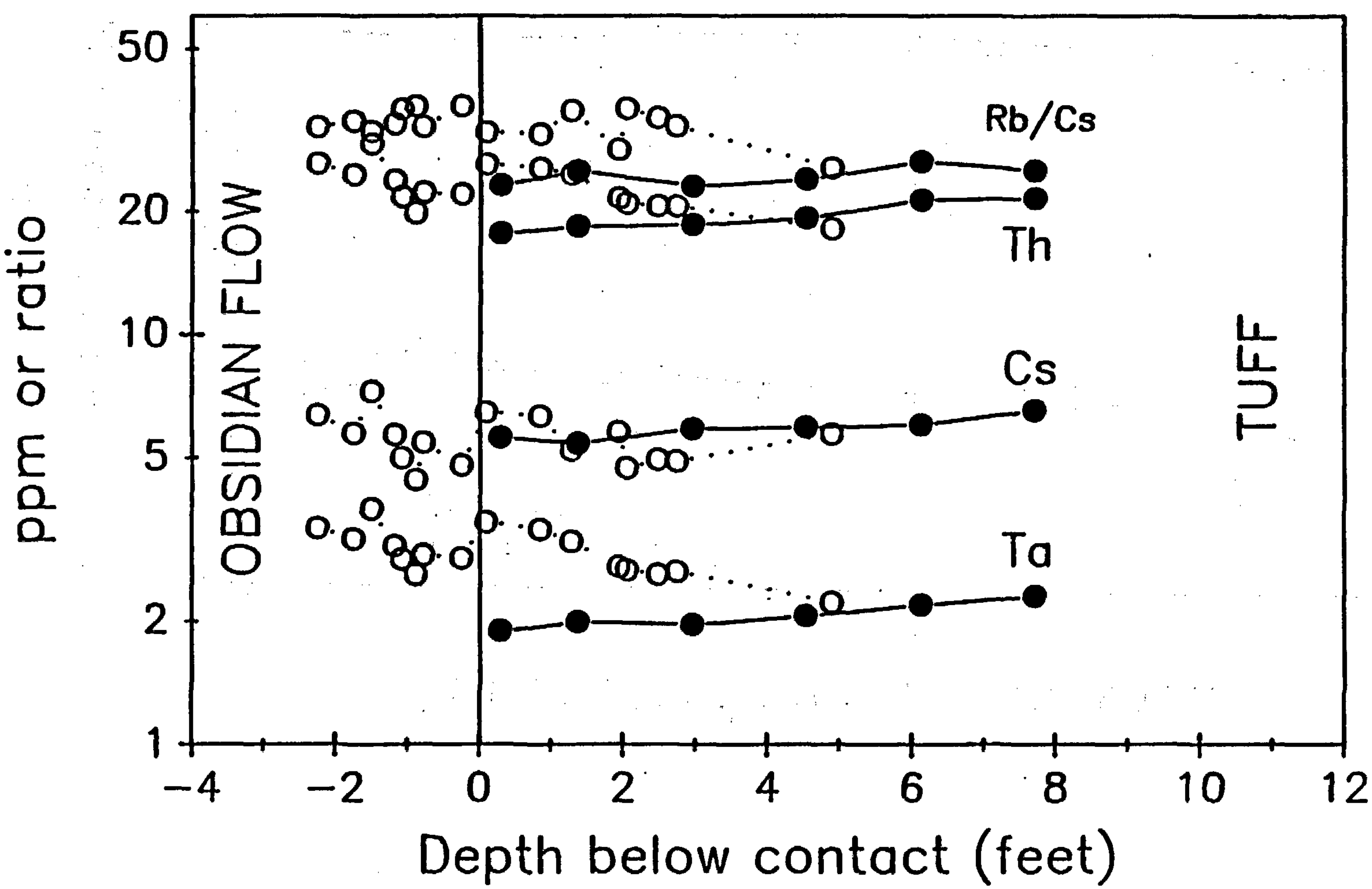
Concentration profiles documented for five feet below the contact at "outcrop 8" and in the VC-1 core

Both suites of rocks examined for Cl, Sc, Cs, Eu, Tb, Yb, Hf, Ta, Th, Rb, Ba, Nd, Lu, and others

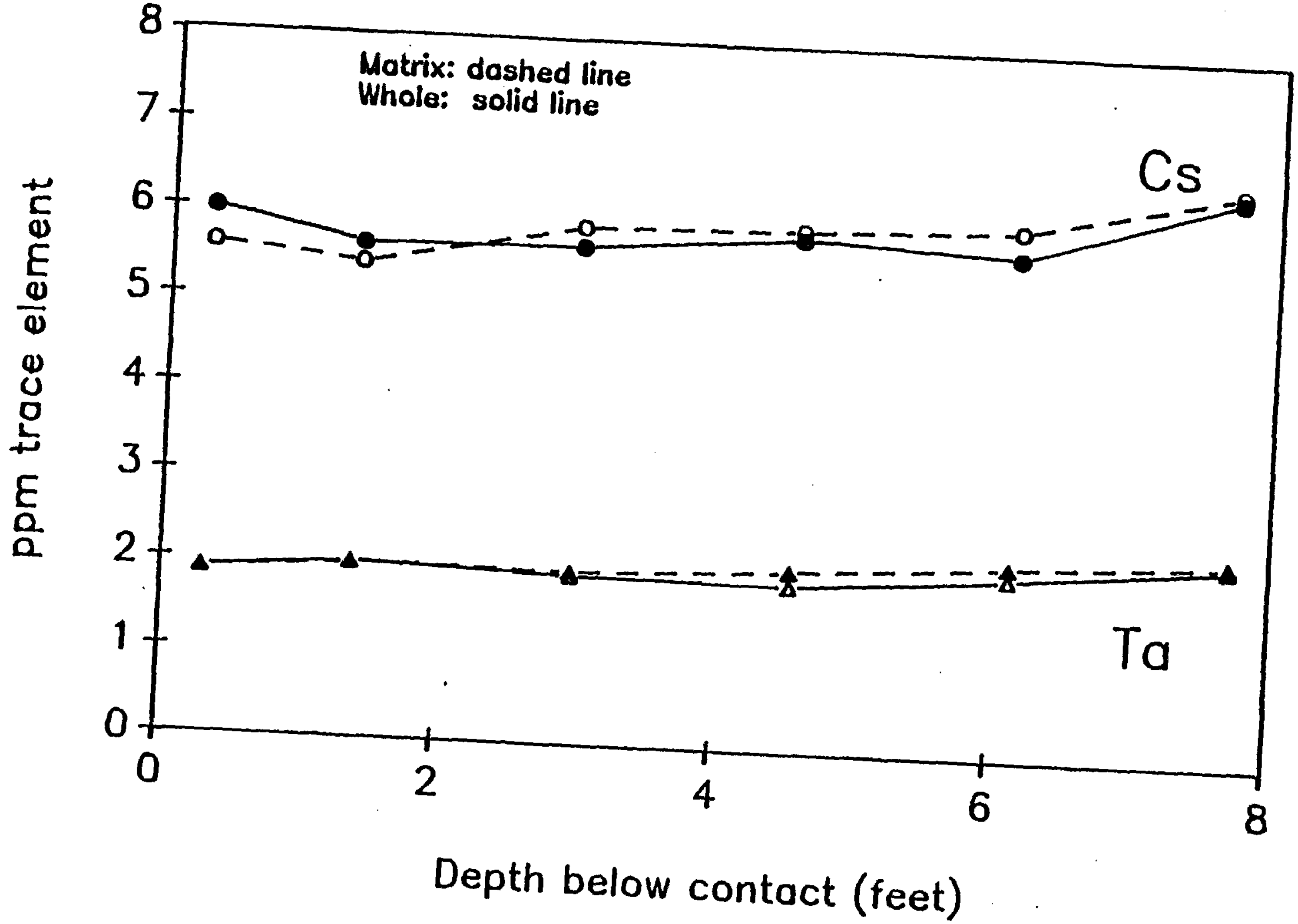
Finding: The thermal event failed to mobilize most components.

* Cl and H_2O are exceptions; H_2O pattern may be obscured by re-adsorption.

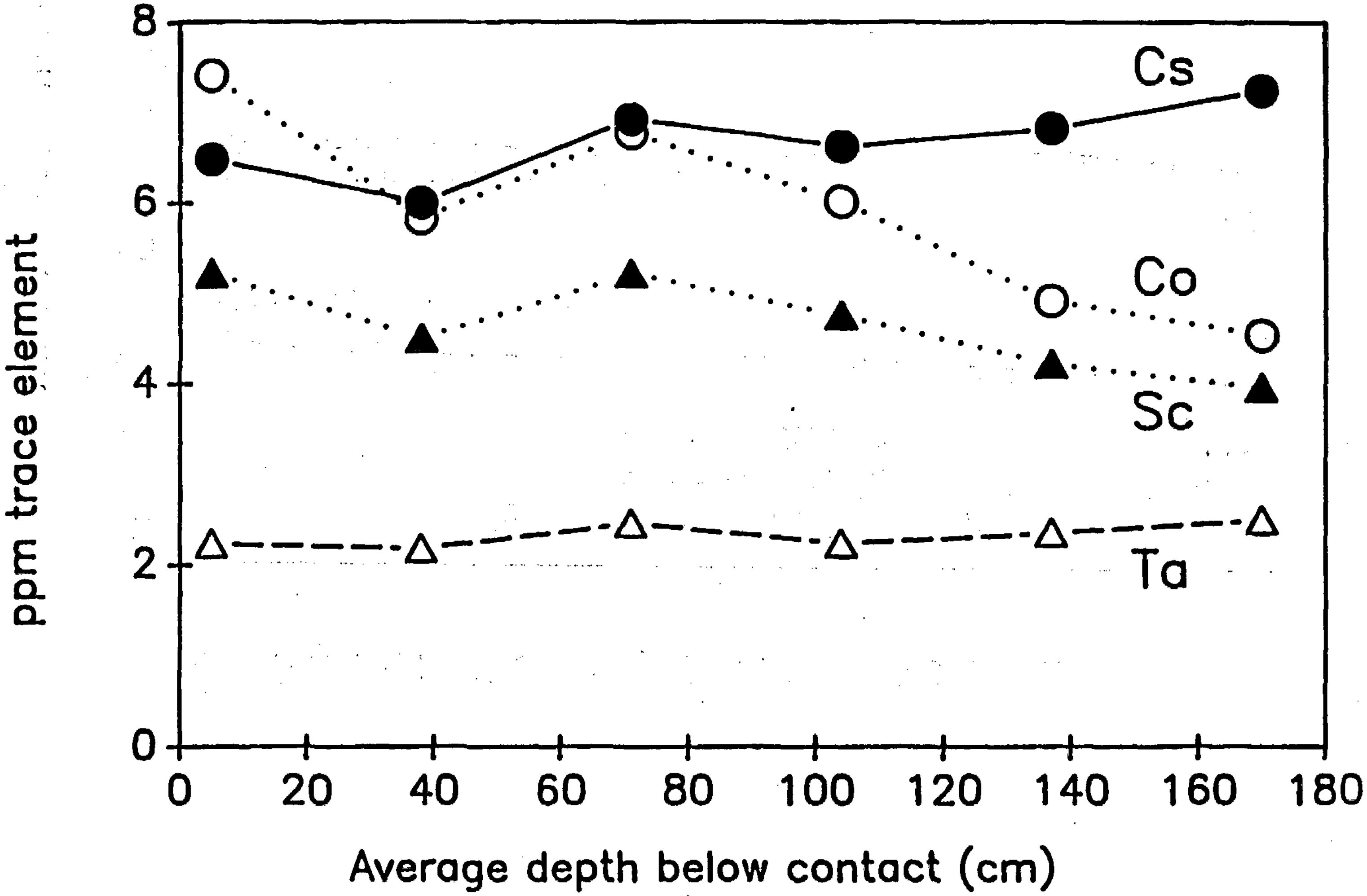
Outcrop (solid) vs. VC−1 core (dotted)



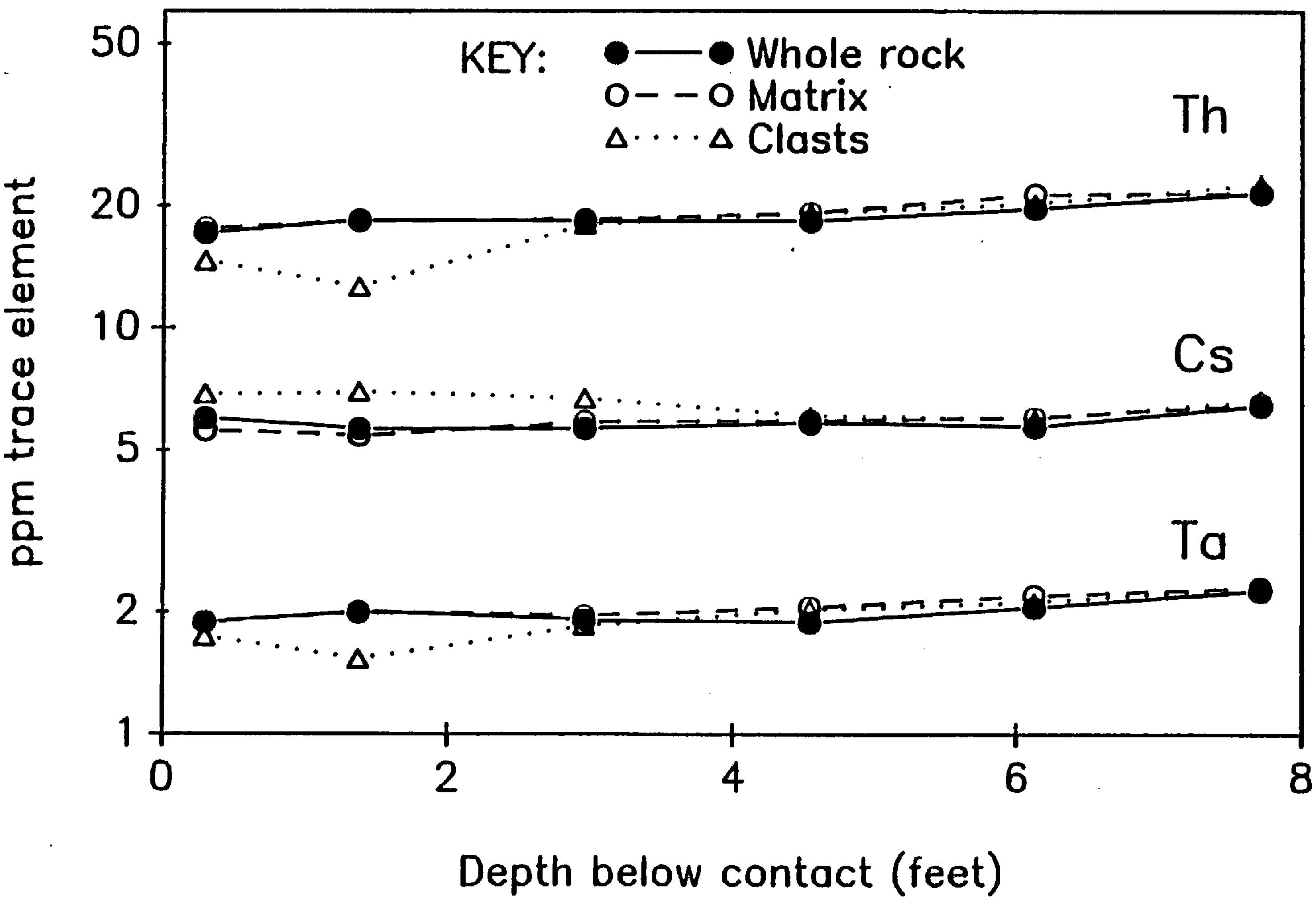
Site 8: Matrix vs. Whole Rock



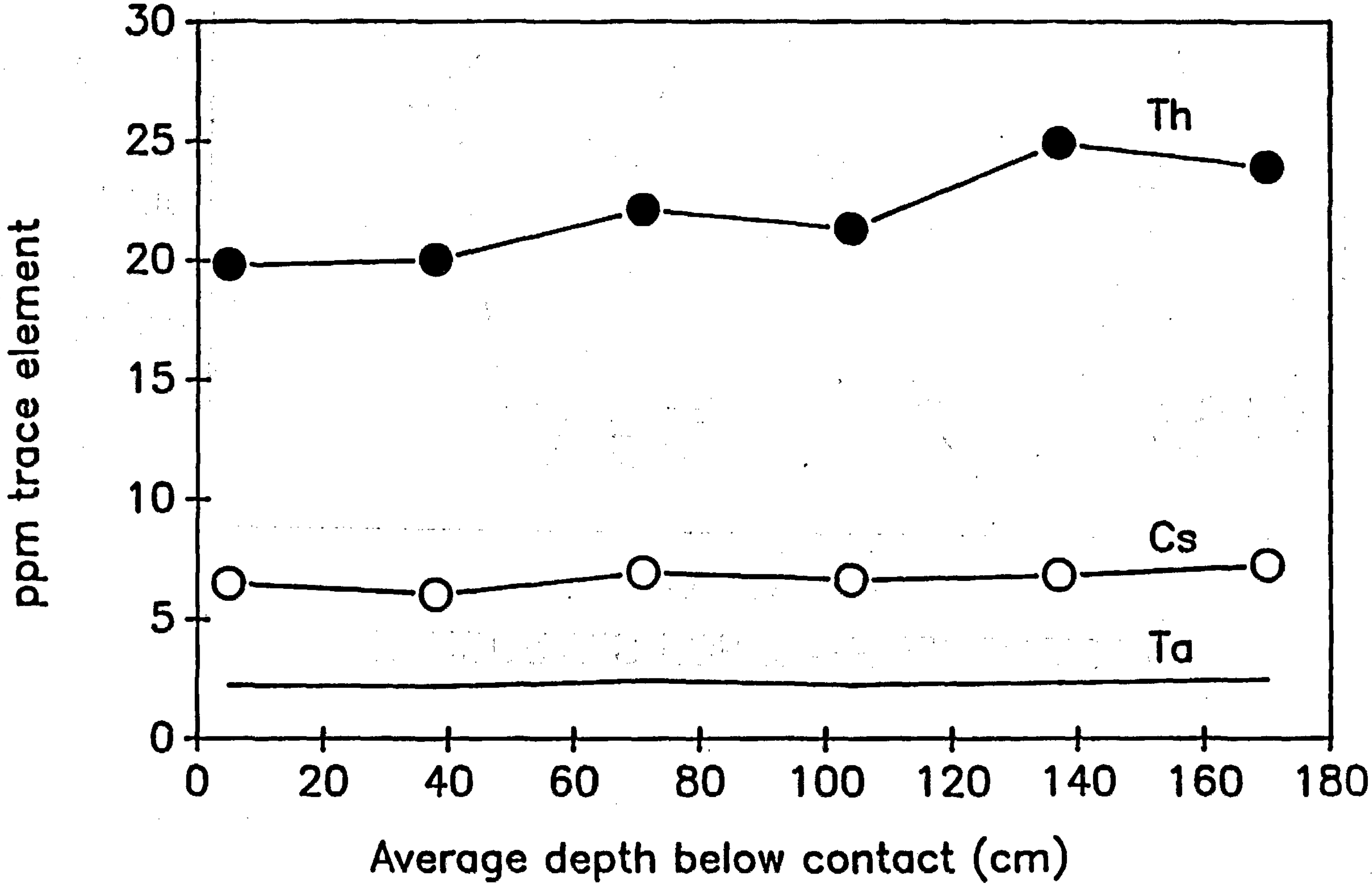
Matrix composition, site 8



Outcrop: matrix, whole rock, and clasts

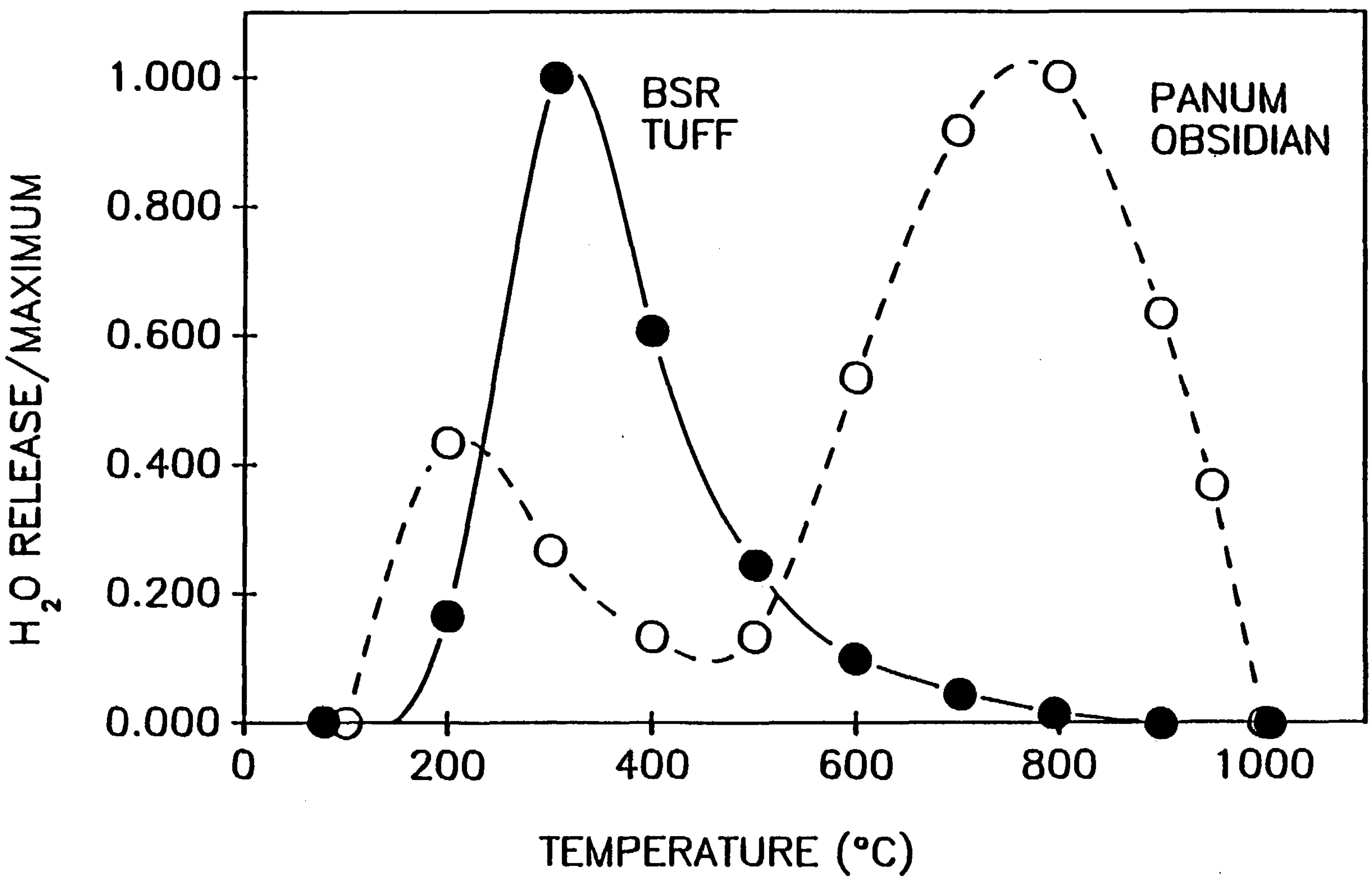


Matrix composition, site 8

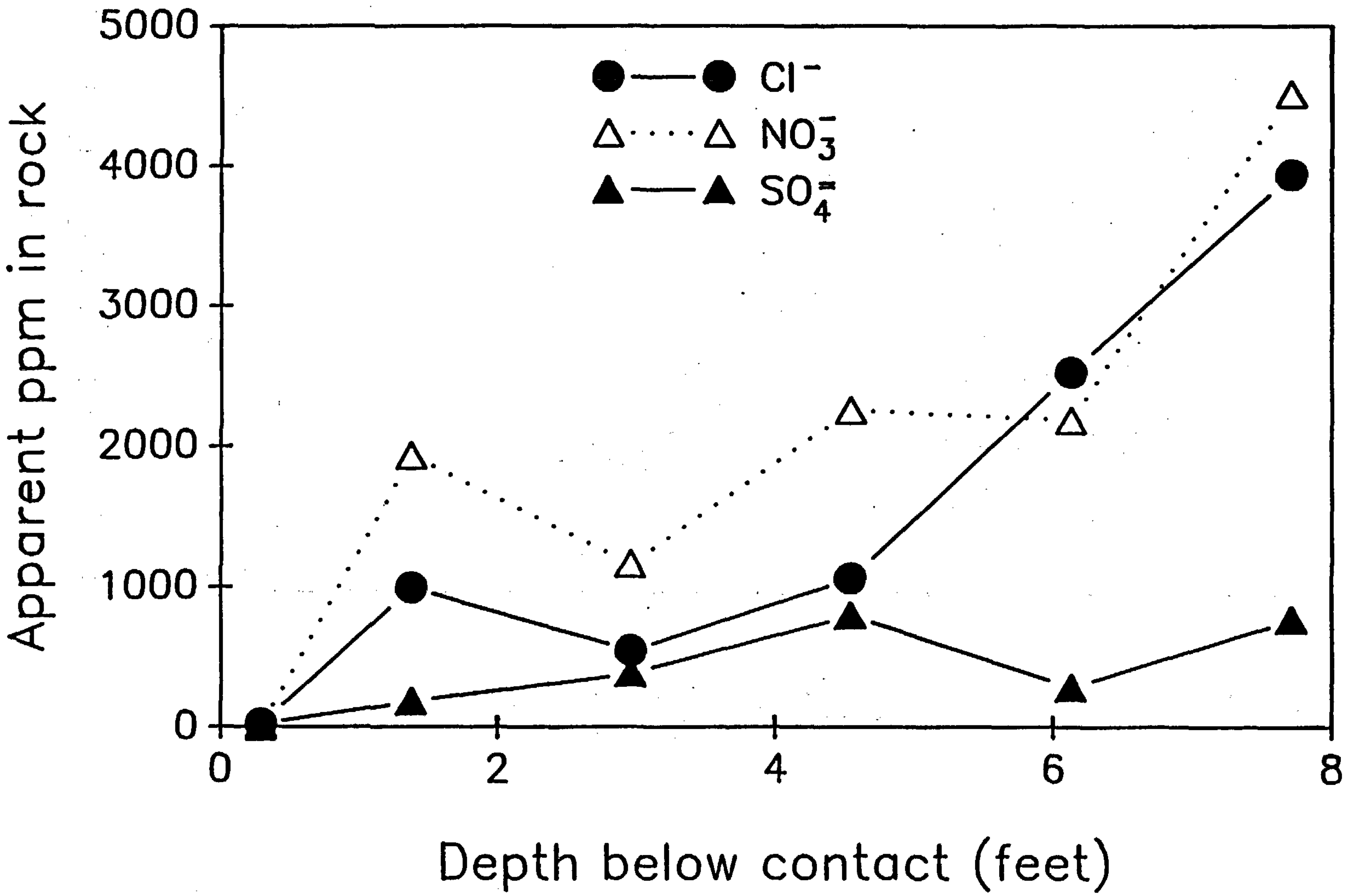


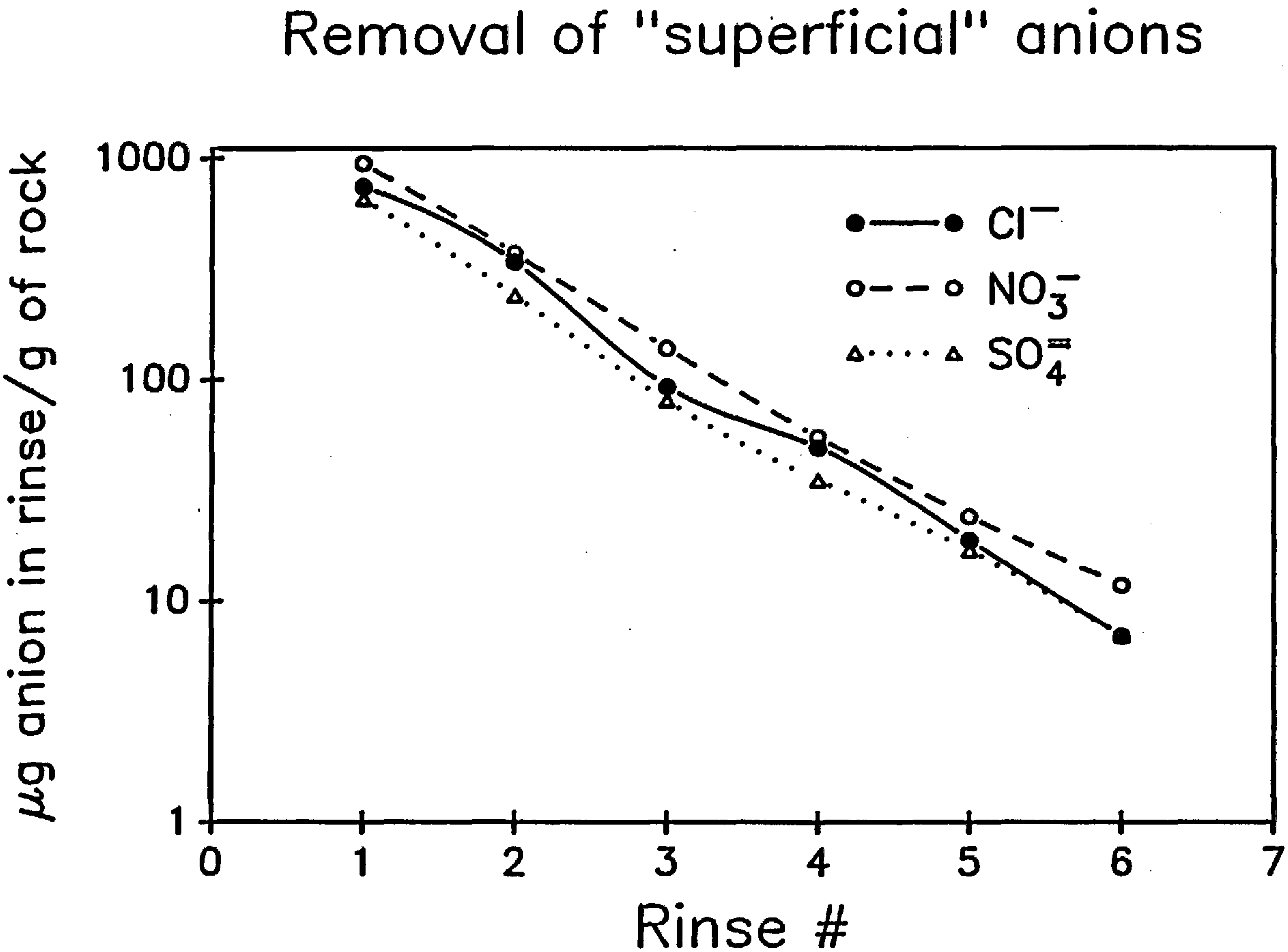
PYROGRAMS FOR TUFF vs. OBSIDIAN

(FILE= H20_BSR)

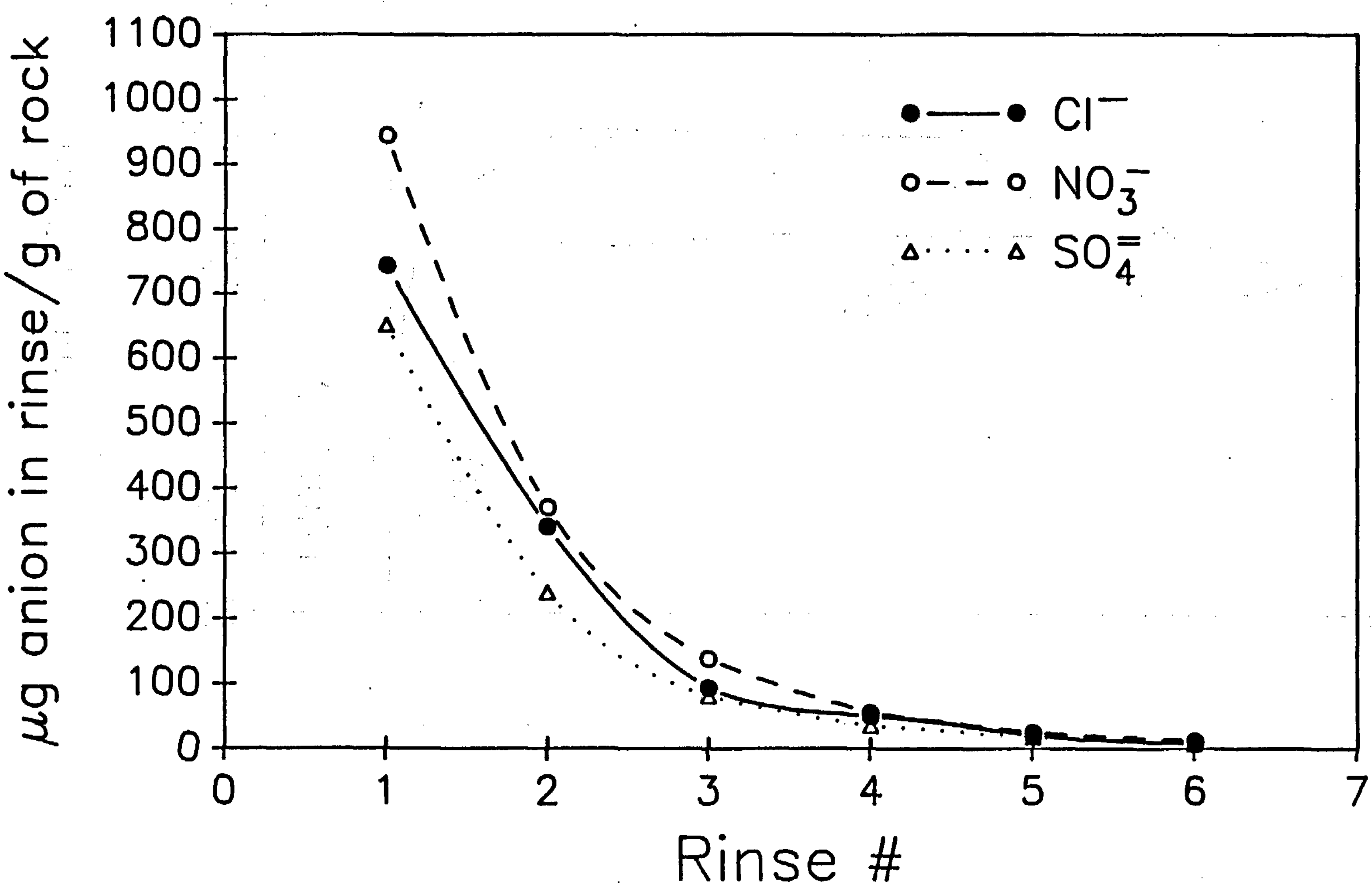


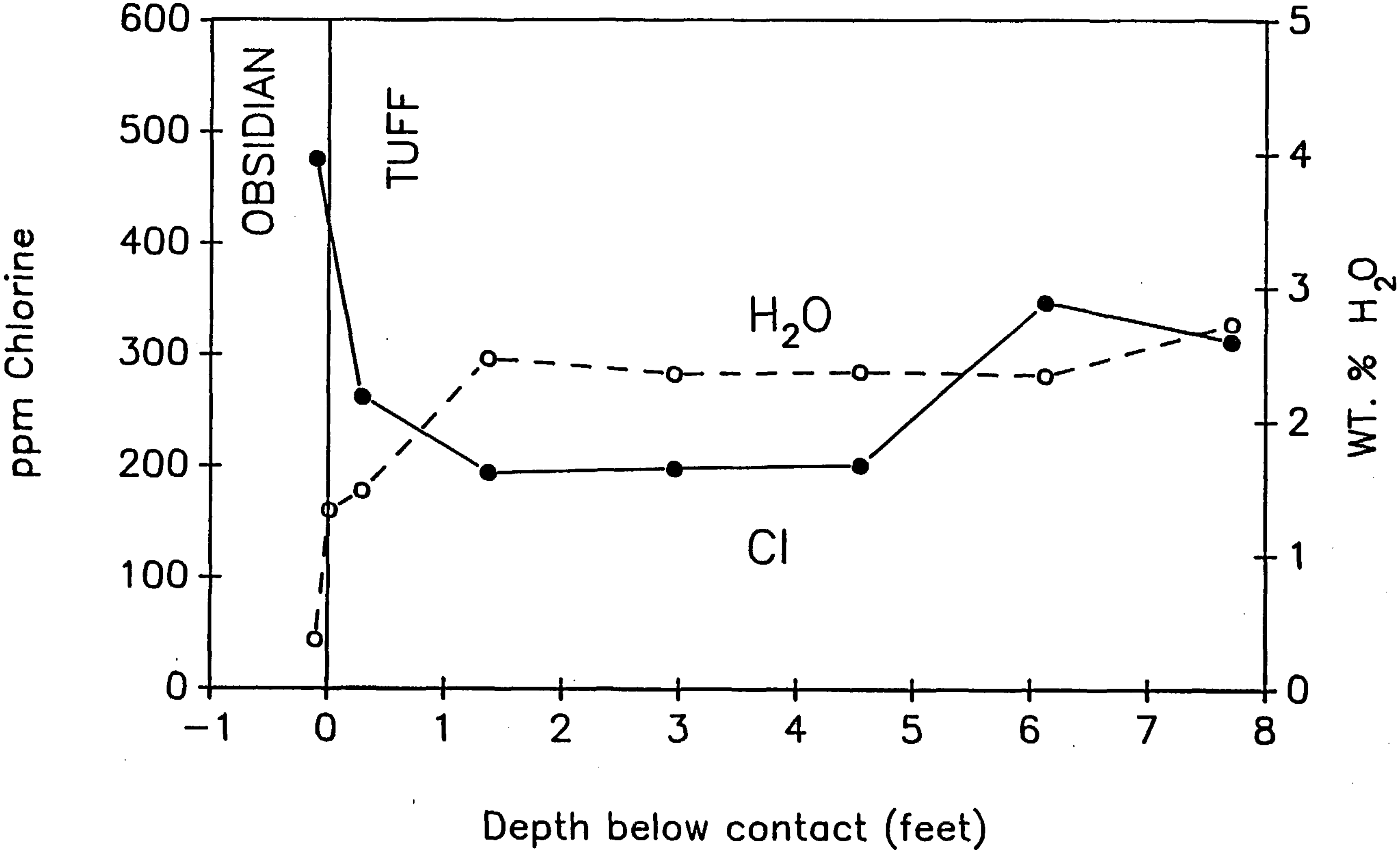
Leachable anions, outcrop 8




Removal of "superficial" anions
μg anion in rinse/g of rock
1000
100
10
1
0
1
2
3
4
5
6
7
Rinse #
Cl^-
NO_3^-
$SO_4^=$

Removal of "superficial" anions




OBSIDIAN
TUFF
H_2O
Cl
ppm Chlorine
WT. % H_2O
Depth below contact (feet)
0
100
200
300
400
500
600
0
1
2
3
4
5
−1
0
1
2
3
4
5
6
7
8

The Search For Mineralogic Alteration Effects

Only very small amounts of clay (montmorillonite?) were found.

Other secondary minerals found are highly soluble and result from drying of present-day "ground" waters.

Outcrop samples were fresher than VC-1 core.

Finding: In general the tuffs are still very fresh.

Preliminary Hydrothermal Experimental Results

* Fresh Panum Crater obsidian with deionized water at 150° and 250°C.

* Alteration products similar to VC-1 clays were seen.

* Fluid chemistry was obtained:

	1 month 250°C	1 month 150°C	11 months 150°C
pH	8.2	8.6	~9
Sc (ppm)	342	163	263
Fe (ppm)	0.23	0.35	0.52
Ca (ppm)	< 0.1	< 0.1	0.5
Mg (ppm)	0.211	0.5	26
Al (ppm)	12.7	17.6	8.4
K (ppm)	7	5	7
Na (ppm)	74	53	78

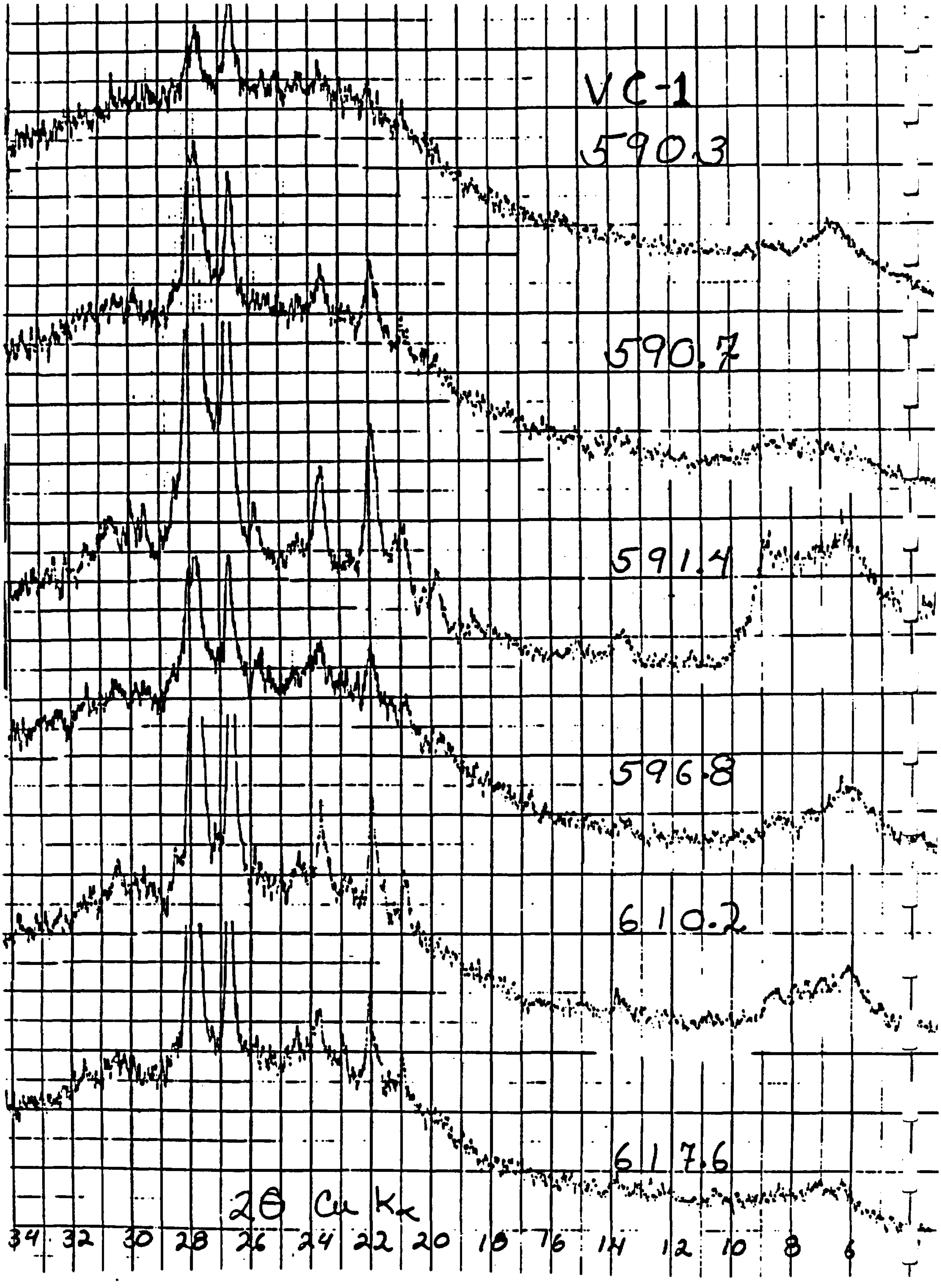
<u>Finding</u>: Elemental transport requires solubility in basic solutions.

<u>Finding</u>: Clays developed in less than a year.

CONCLUSIONS

1) Picking an "ideal" natural analog site is difficult

2) Heating a large body of unsaturated tuff failed to produce conditions conducive to extensive alteration or elemental transport


VC-1
590.3
590.7
591.4
596.8
610.2
617.6
2θ Cu Kα
34 32 30 28 26 24 22 20 18 16 14 12 10 8 6

NRC XRAY

Table 1
X Ray Analyses of Banco Bonito-Battleship Rock Units

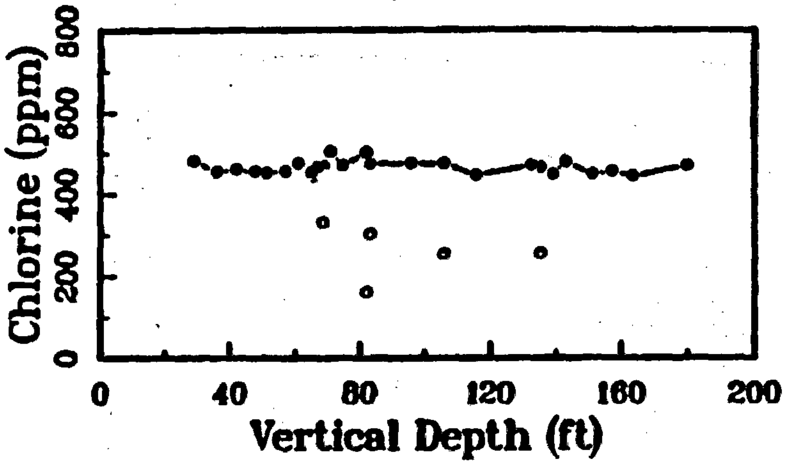
		Glass	Shoulder	Illite		Smectite	
467.8	Obsidian-Bulk	Good	----	8.9	2	n.d.	
479.3	"	Good	10.2	8.4	4	n.d.	
480.8	"	Small	----	n.d.		n.d.	
488.1	"	Huge	10.5	8.9	4	6.1 (U.6) h = 2	
486.13	"	Huge	----	8.9	6	n.d.	
492.47	"	n.d.	----	n.d.		n.d.	
499	"	Small	----	8.4	h = 5	n.d.	

Table 2
X-Ray Analyses Of VC-1 Tuff

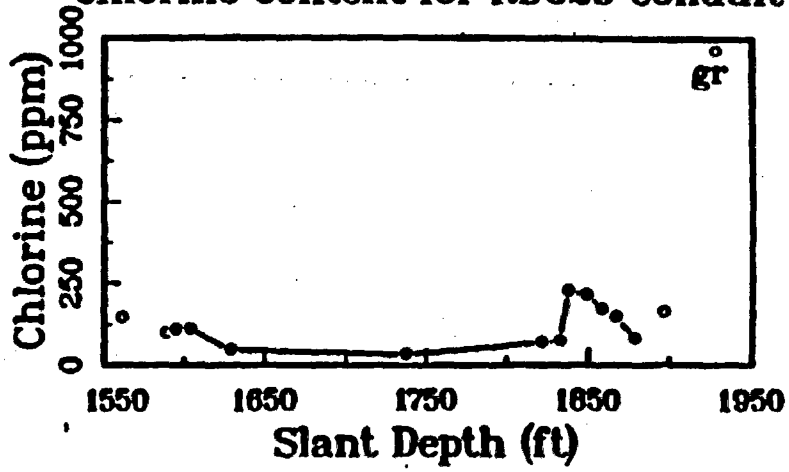
		Glass	Shoulder	Illite		Smectite	
590.3	VC - 1 Obsidian	Good	----	n.d.		5.1	h = 40
590.5 - 591.0	Tuff Bulk	Good	----	n.d.		n.d.	
	#1	----	----	8.9	h = 5	5.1	23
	#2	----	----	n.d.		5??	3
	#3	----	----	8.9	5	5.3	25
	#4	----	----	8.9	8	5.1	22
	#5	----	----	9.0	9	5.2	27
	#6	----	----	n.d.		5.1	13
591.1 - 591.5	Tuff Bulk	Small	2.8 - 3.0	8.9	9	5.1	30
596.7 - 597.1	Tuff Bulk	Good	3.0	n.d.		5.1	25
610.2	Tuff Bulk	Good	3.0	8.8	2	5.2	17
617.5	Tuff Bulk	Small	2.8	n.d.		5.2	9
622.8	Tuff Bulk	Good	3.0.	n.d.		5.2	10
635	Tuff Bulk	Good	----	8.8	3	5.1	9
640	Tuff Bulk	Good	2.8!	n.d.		5.3	10

```
==========      0     Banco Bonito Obsidian Flow              130 Ka
==========
==========
==========
==========
==========      100
==========
==========
==========
==========
==========      200
==========
==========
==========
==========
==========      300
==========
==========
==========
==========
==========      400
==========
==========
==========
========== 488 - Sharp Contact
++++++++++      500   Battleship Rock Ignimbrite              270 Ka
++++++++++ 530
==========            VC-1 Obsidian Flow                      365 Ka
==========
========== 591 - Baked Contact, or is it weathered ????
oooooooooo      600 - Current Water Table
oooooooooo
oooooooooo            Upper VC-1 Tuff                         >500 Ka
oooooooooo
oooooooooo
oooooooooo      700
oooooooooo
oooooooooo
oooooooooo 773
0000000000
0000000000      800
0000000000
0000000000            Lower VC-1 Tuff, Inc. Fluvial Seds ??  age unknown
0000000000
```

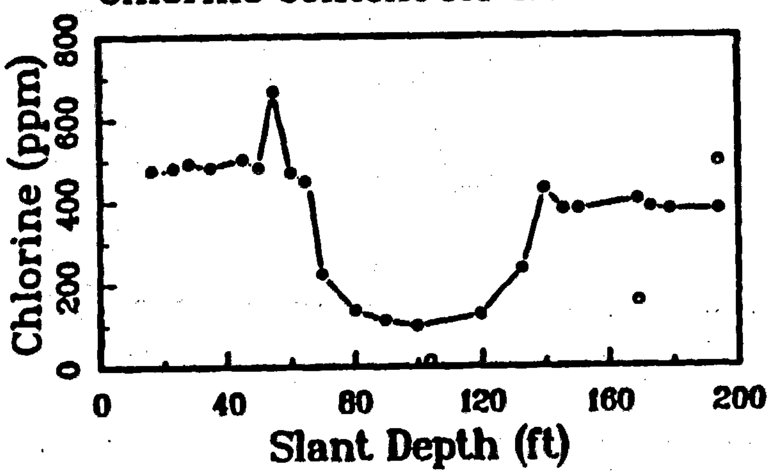
Chlorine Content for RD02a Flow



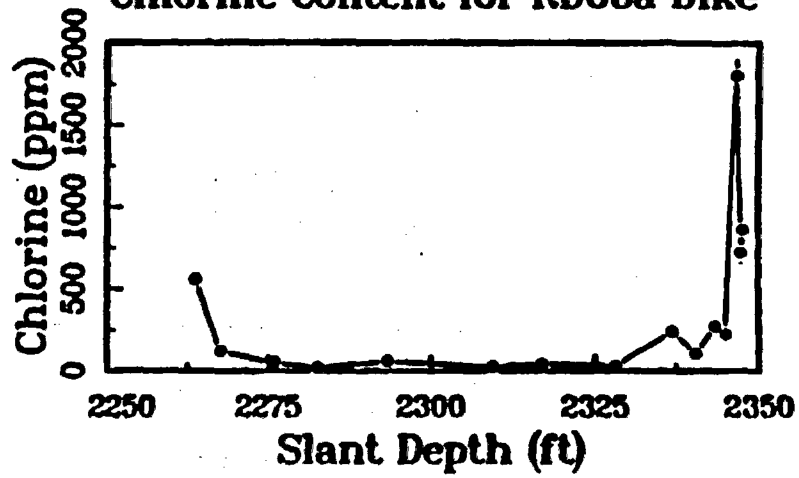
Chlorine Content for RD02b Conduit

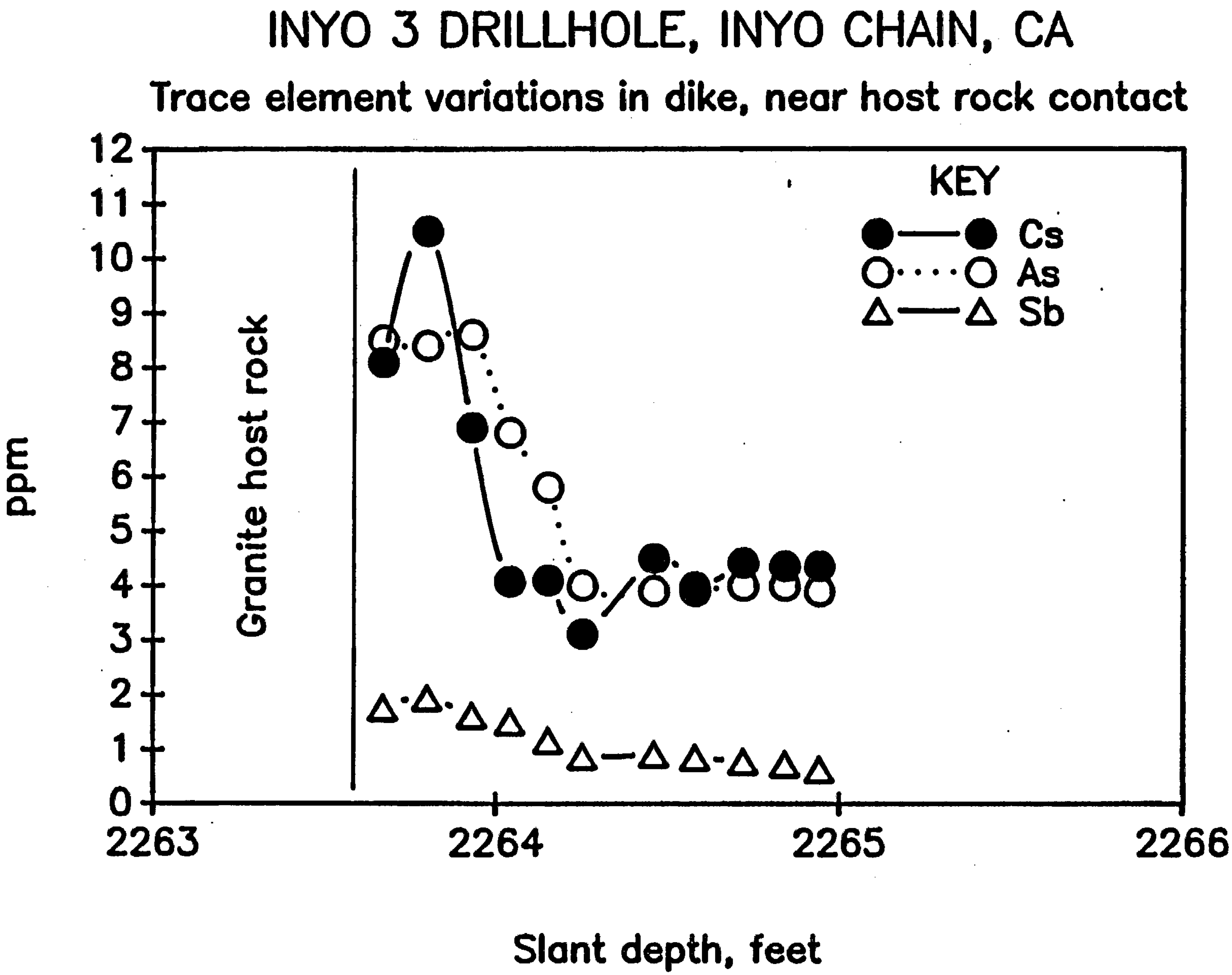


Chlorine Content for RD02b Flow



Chlorine Content for RD03a Dike




INYO 3 DRILLHOLE, INYO CHAIN, CA
Trace element variations in dike, near host rock contact
KEY
Cs
As
Sb
Granite host rock
ppm
Slant depth, feet
0
1
2
3
4
5
6
7
8
9
10
11
12
2263
2264
2265
2266

CURRENT ISSUES IN THE MODELING OF NONISOTHERMAL MULTIPHASE FLOWS IN FRACTURED MEDIA

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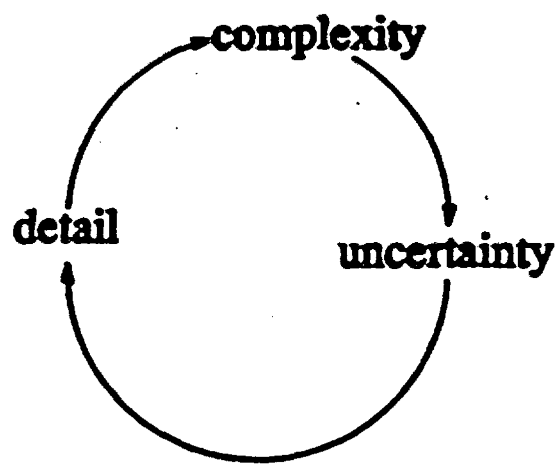
Earth Sciences Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

MODELING GOALS AND NEEDS

GOAL: A credible site model for thermal and hydrologic effects

NEEDS:

- Identify processes
- Quantify them (governing equations)
- Fluid and formation parameters



- Mathematical and numerical methods
- Verification and validation

WHAT HAS BEEN ACCOMPLISHED

- we know what the significant processes are
- we can describe much of them quantitatively
- simulators can handle the difficult numerics of highly non-linear nonisothermal multiphase processes
- several approaches have been developed for dealing with the geometric complexity of flow in fractured-porous media (no "patent" solutions though)
- studies of idealized systems have given initial insight into likely conditions, and have clarified limitations and gaps of present knowledge

  ★ thermohydrologic conditions near waste packages

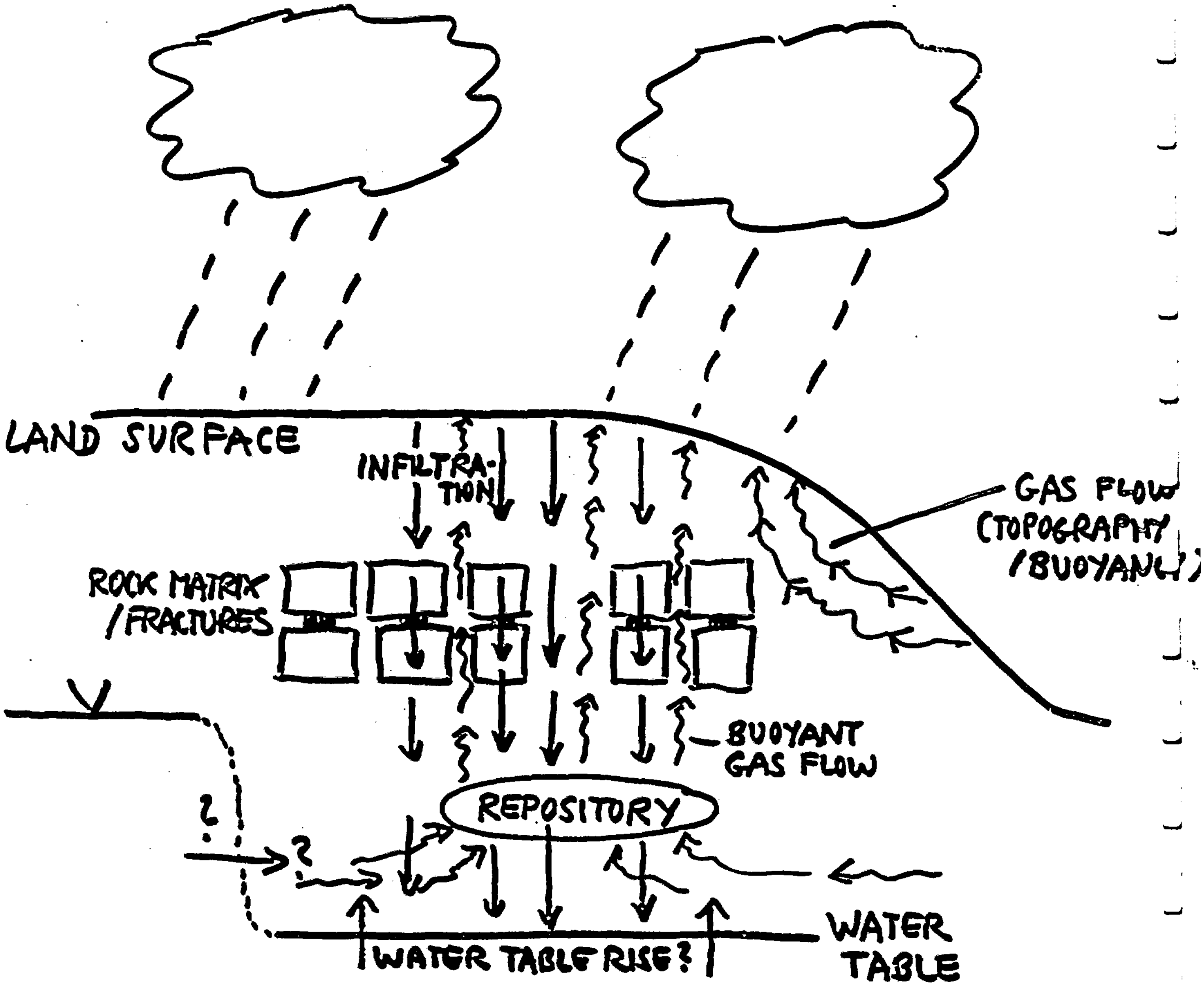
  ★ thermally induced effects on larger scale

  ★ effects of atmospheric forcing (T, P, I)

  ★ role of fractures and faults

  ★ tracer transport

  ★ code verification and validation



LAND SURFACE
INFILTRA-TION
GAS FLOW (TOPOGRAPHY /BUOYANCY)
ROCK MATRIX /FRACTURES
BUOYANT GAS FLOW
REPOSITORY
?
?
WATER TABLE
WATER TABLE RISE?

FAST PATHS?

SITE SUITABILITY —

POTENTIAL WEAK SPOTS

- CAN INFILTRATING GROUNDWATER TRAVEL DOWN THE UNSATURATED ZONE, PAST THE REPOSITORY, AND REACH THE WATER TABLE IN LESS THAN ..... YEARS?

- CAN THE ROCK MATRIX IMBIBE AND THEREBY DRASTICALLY SLOW DOWNWARD WATER MIGRATION?

- CAN MATRIX RETENTION PROCESSES (DIFFUSION, SORPTION) SUBSTANTIALLY RETARD CHEMICAL TRANSPORT?

- CAN THE GROUNDWATER TABLE RISE TO FLOOD THE REPOSITORY?

- CAN NATURAL OR THERMALLY INDUCED FLOW OF FORMATION GAS PROVIDE A "FAST PATH" TO THE ACCESSIBLE ENVIRONMENT?

IMPORTANT CURRENT ISSUES

- relative permeabilities of fractures
- treatment of fractured-porous flow systems
- solution efficiency (3-D problems)
- chemical, mechanical, and thermal couplings
- tracer transport
- code verification
- field observation and experimentation (parameter identification, code validation)

SUMMARY

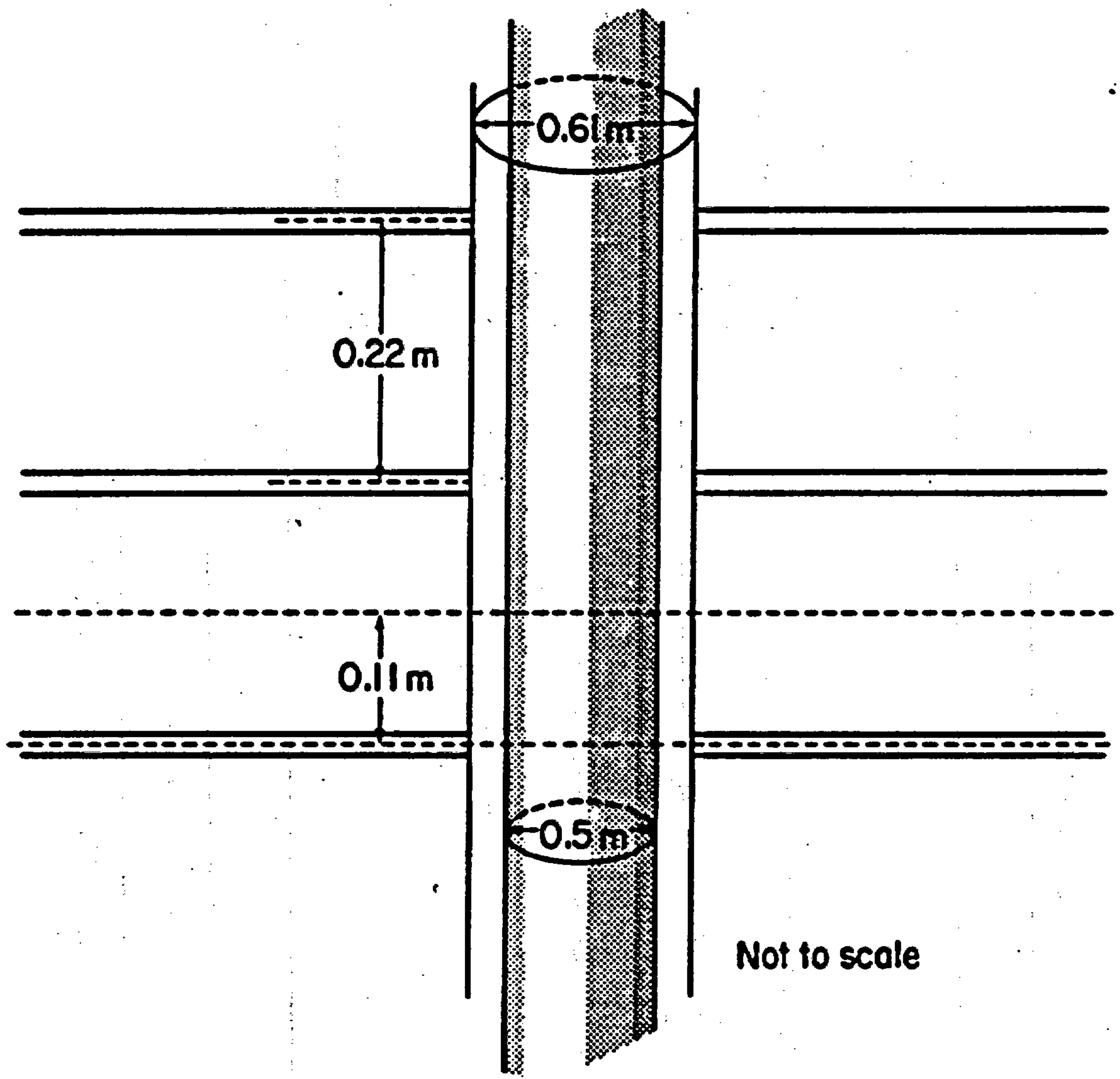
- substantial modeling capabilities exist
  — use them!

- significant limitations are also present
  - — fundamental processes and parameters
  - — field studies

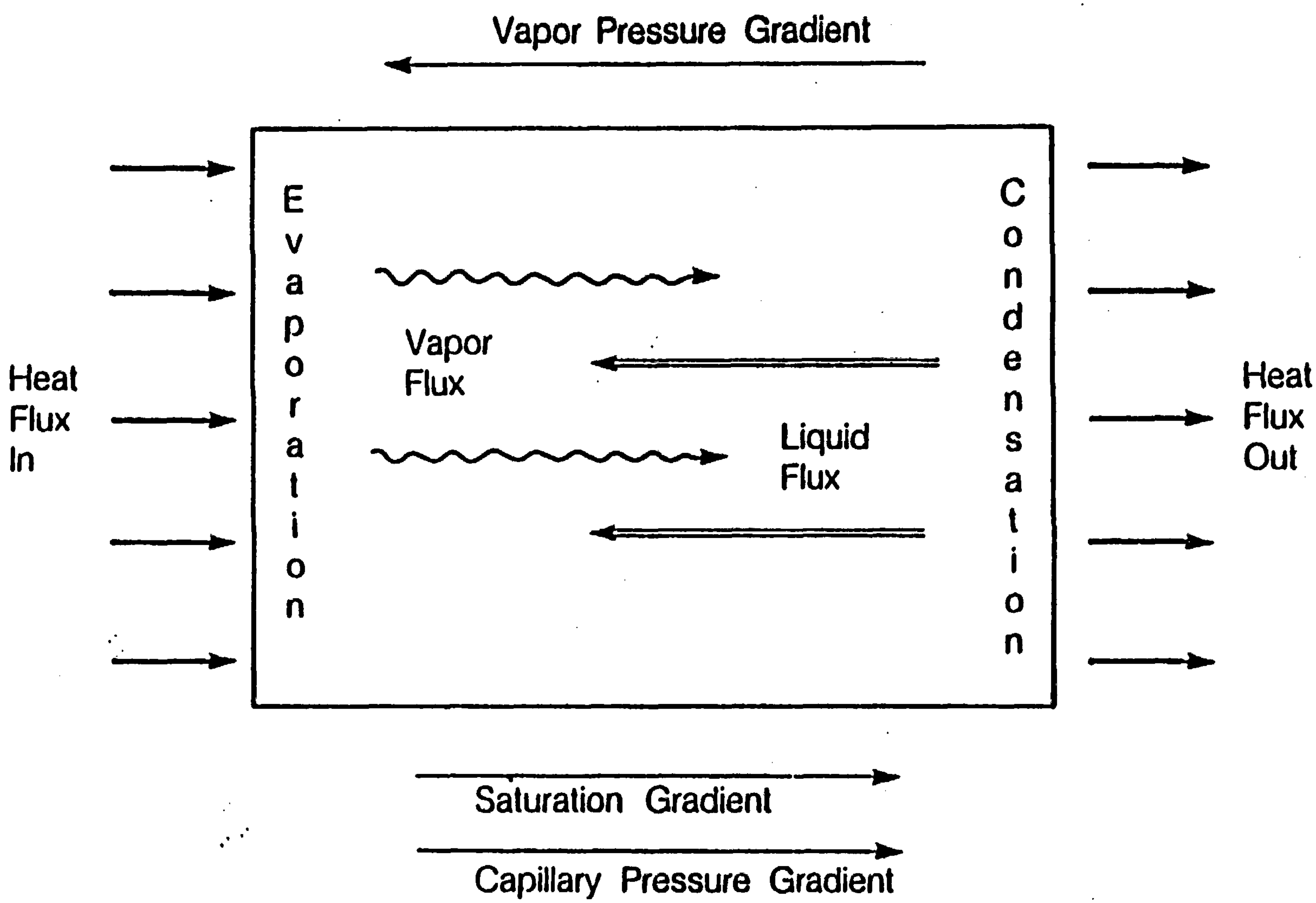
- suitability of Yucca Mountain site remains open

- need a well-focussed research program

TOPICAL STUDIES

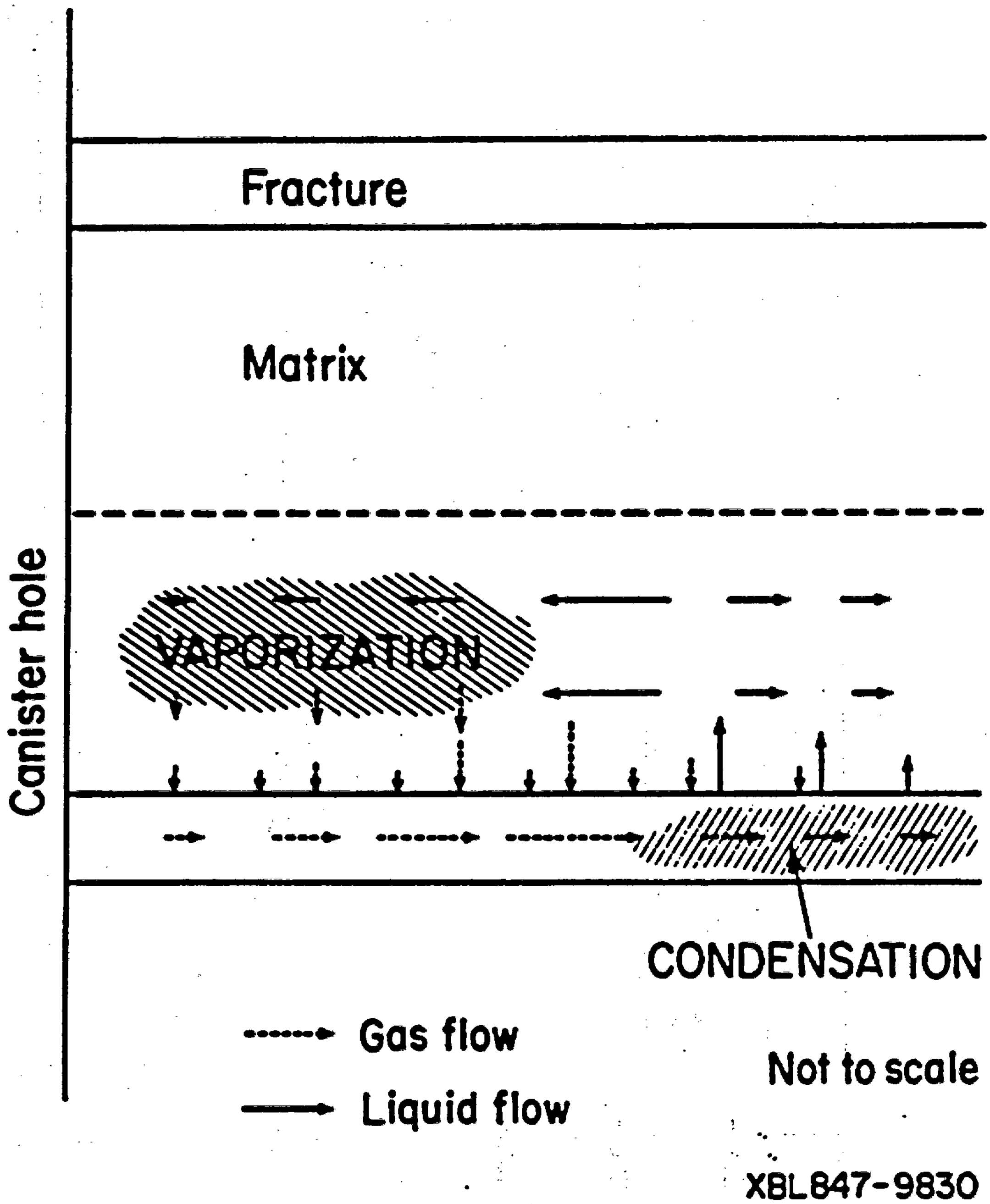


XBL847-9831



XBL 8510-12376

Figure 1. Schematic diagram of a porous heat pipe, after *Jennings* [1984].



Canister hole
Fracture
Matrix
VAPORIZATION
CONDENSATION
Gas flow
Liquid flow
Not to scale
XBL847-9830

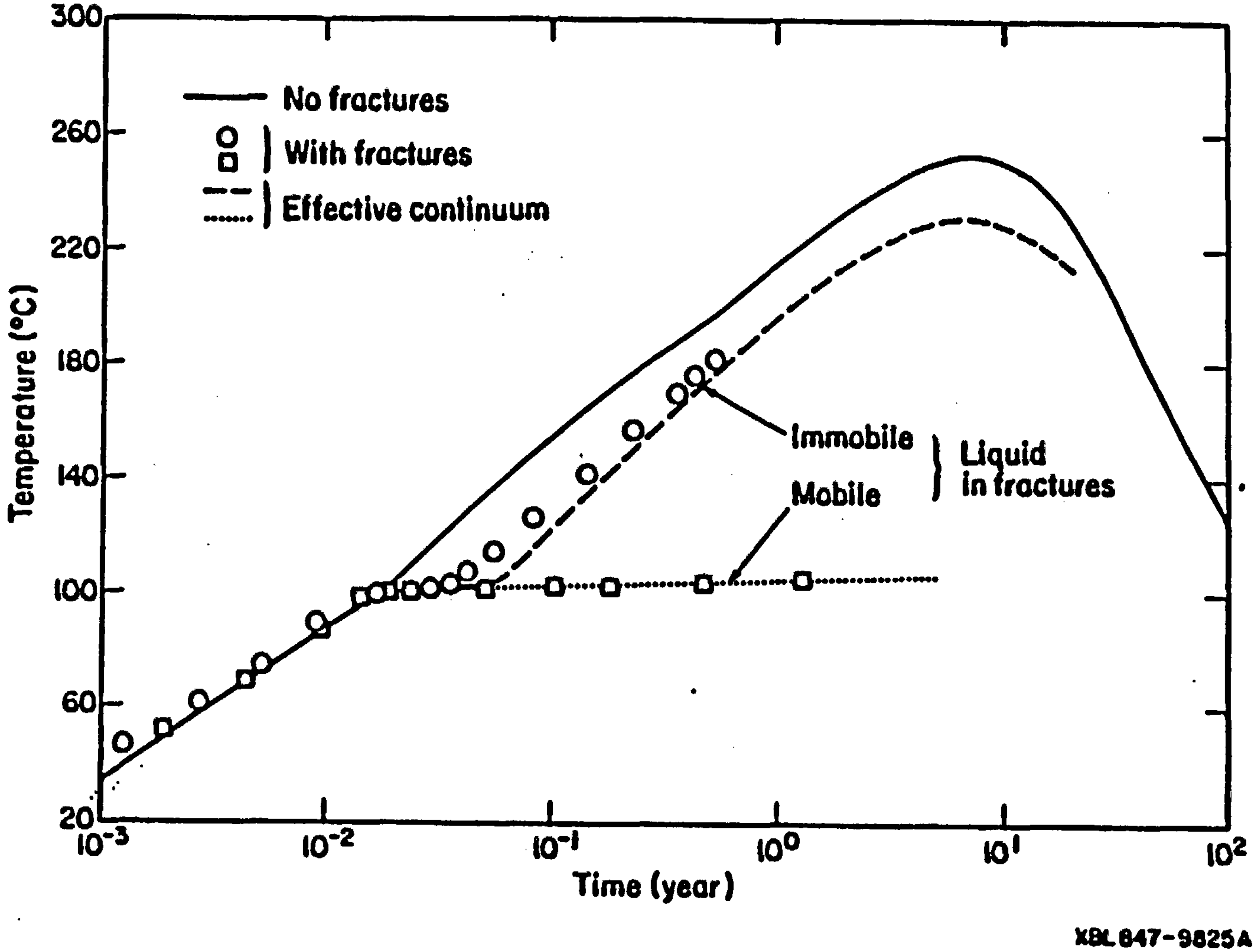
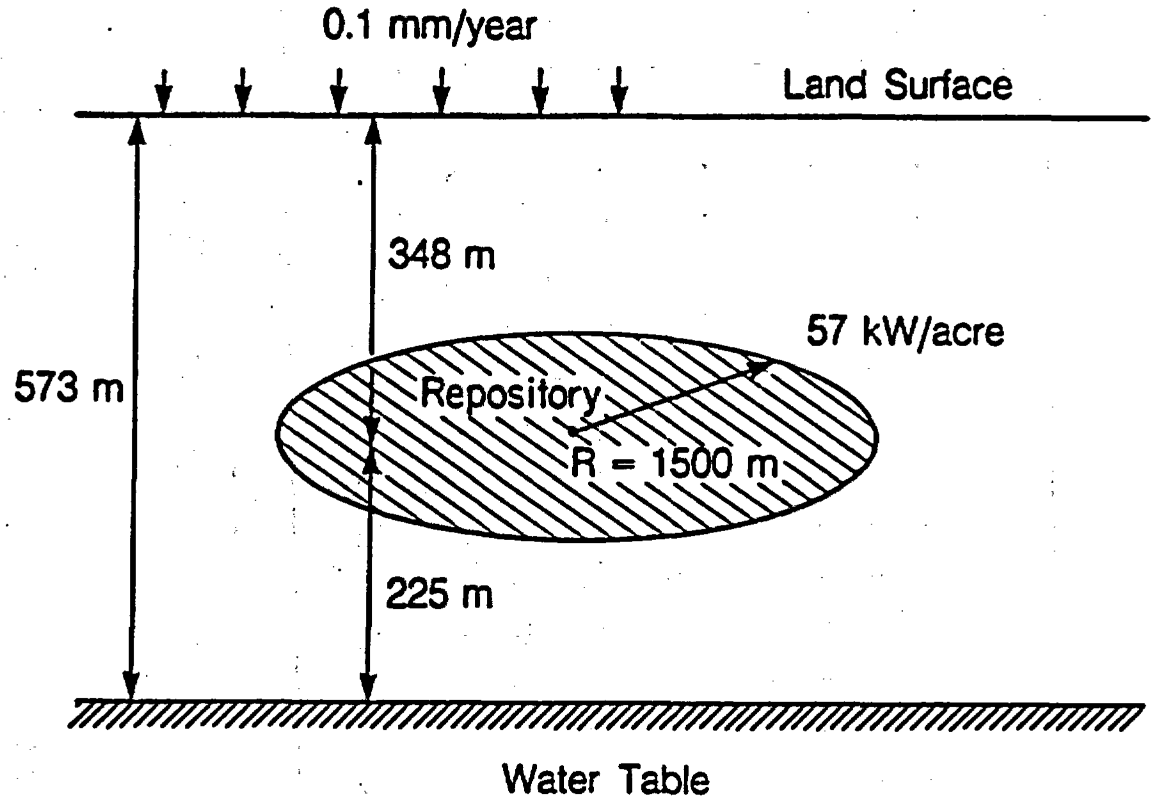
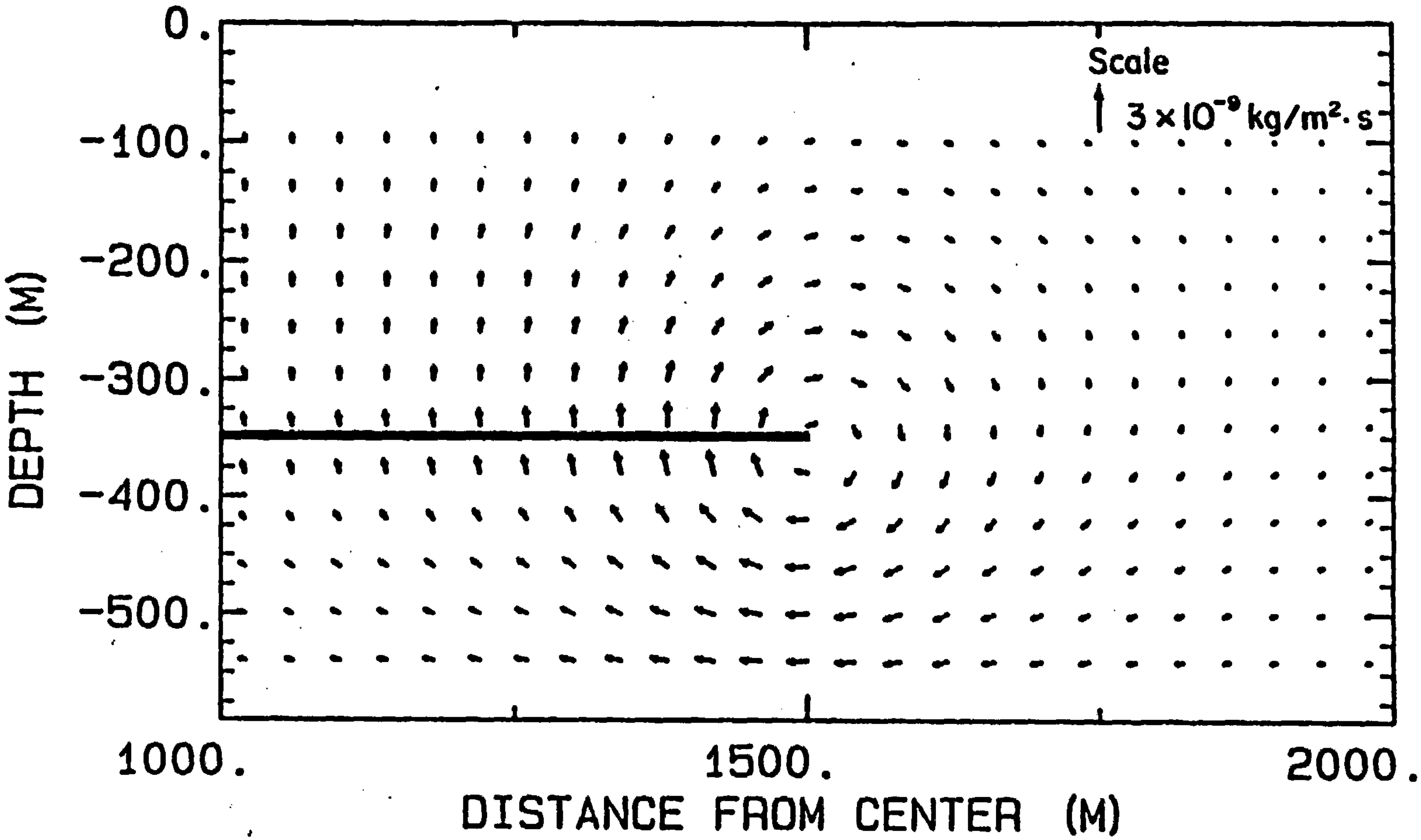


Figure 8. **Simulated temperatures at a distance of 0.34 m from the centerline of the waste packages (after Pruess et al., 1085).**

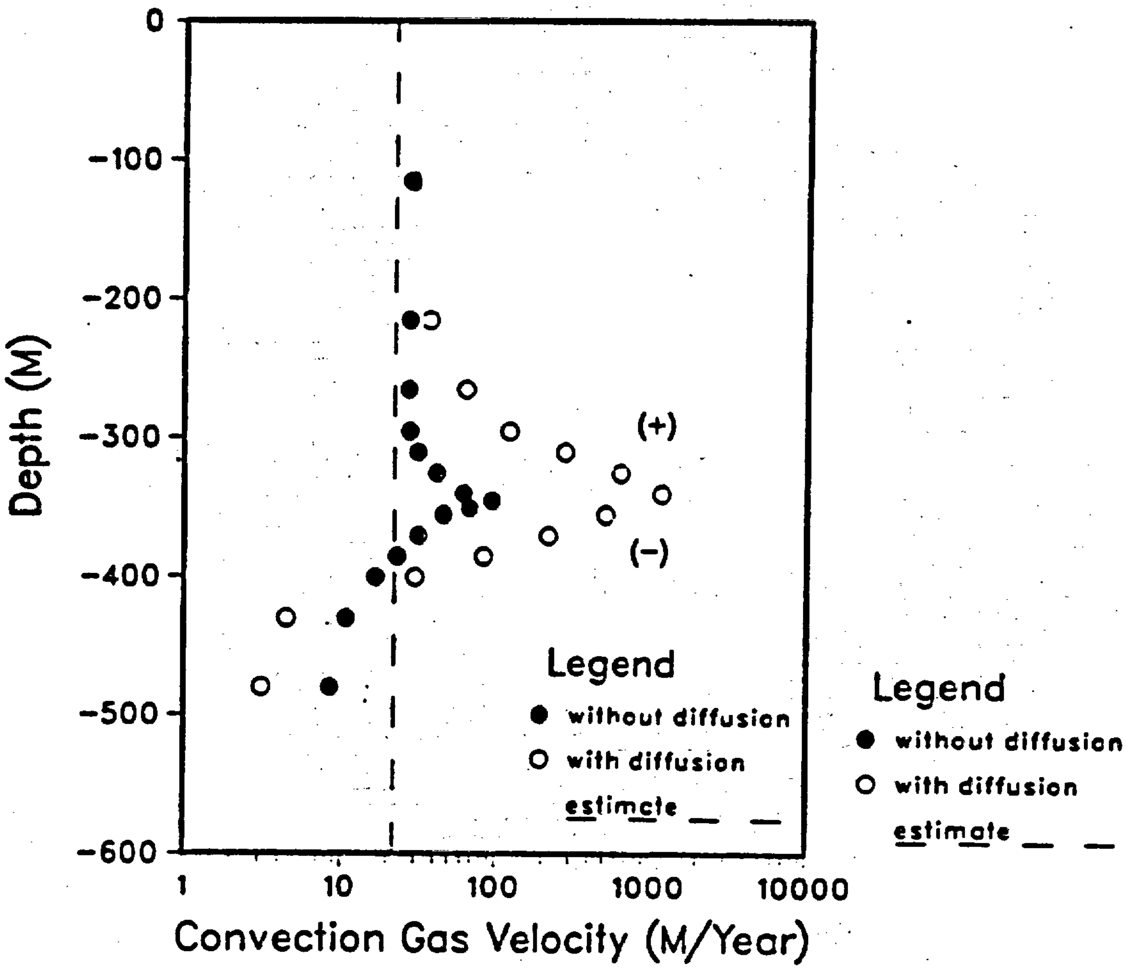


XBL 863-10715



GAS FLUX (NO BINARY DIFFUSION)

XBL 865-1955



XBL 863-10726

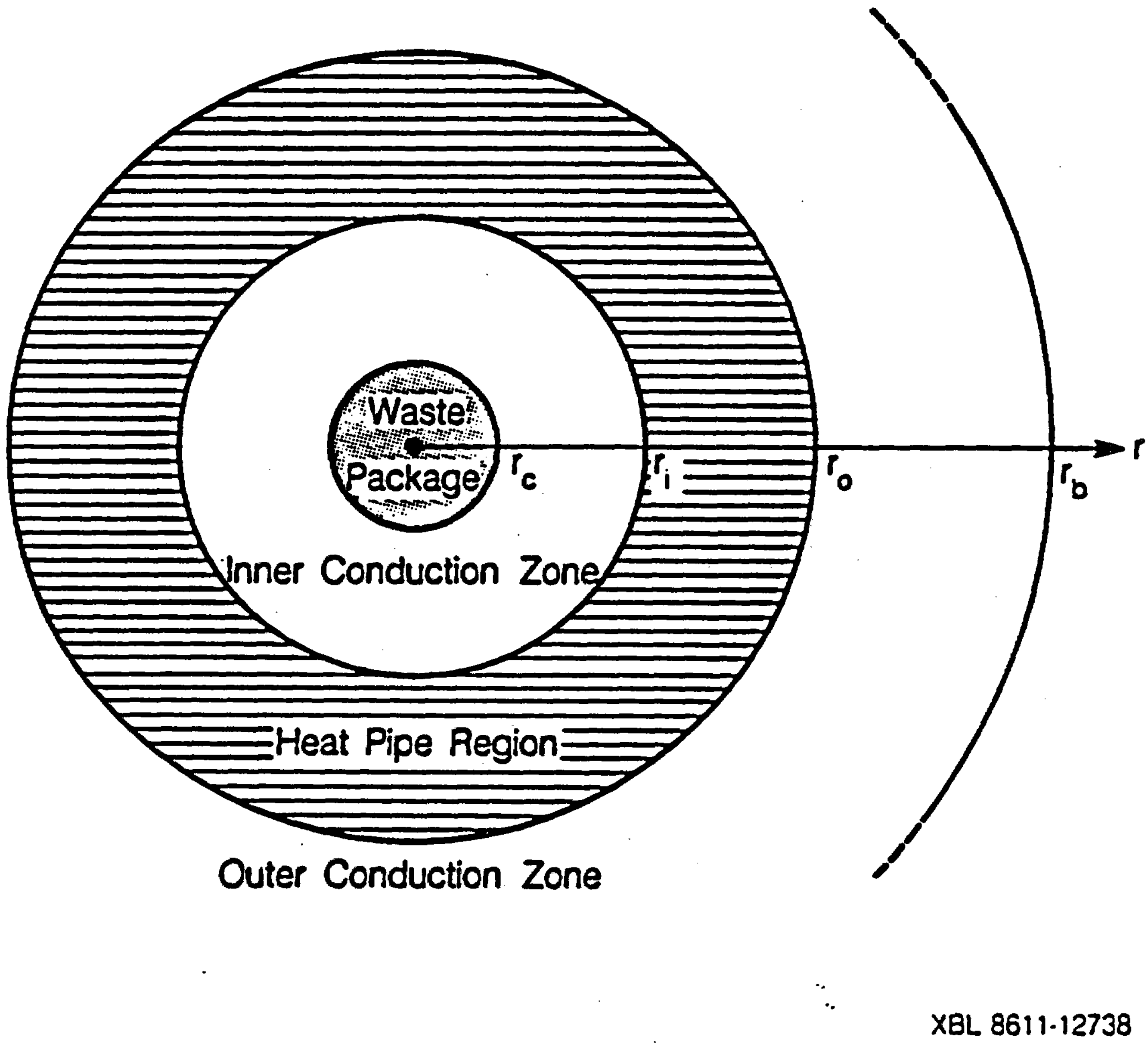
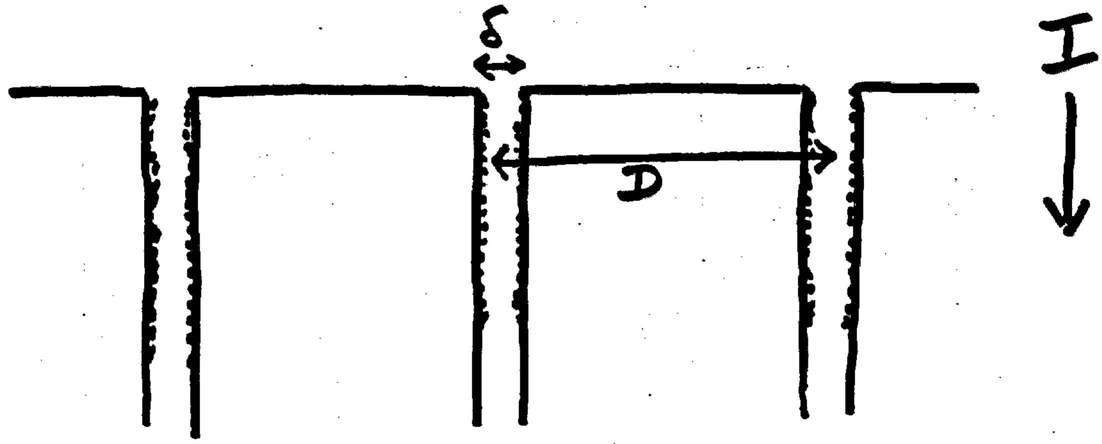


Fig. 1. Schematic of heat transfer regimes in plane perpendicular to the axis of the waste packages (not to scale).

SIMILARITY VARIABLE $r/\sqrt{t}$



$$\phi_f = \delta / D$$

$$v_{pore} = \frac{I}{\phi_f S_\ell}$$

<u>EXAMPLE</u>: $I = 0.1 \text{ mm/yr}$

$$\left.\begin{aligned} D &= 1 \text{ m} \\ \delta &= 100 \mu\text{m} \end{aligned}\right\} \Rightarrow \phi_f = 10^{-4}$$

$$S_\ell = 10\%$$

$$\Rightarrow v_{pore} = \frac{0.1}{10^{-5}} \text{ mm/yr}$$

$$\simeq 10 \text{ m/yr}$$

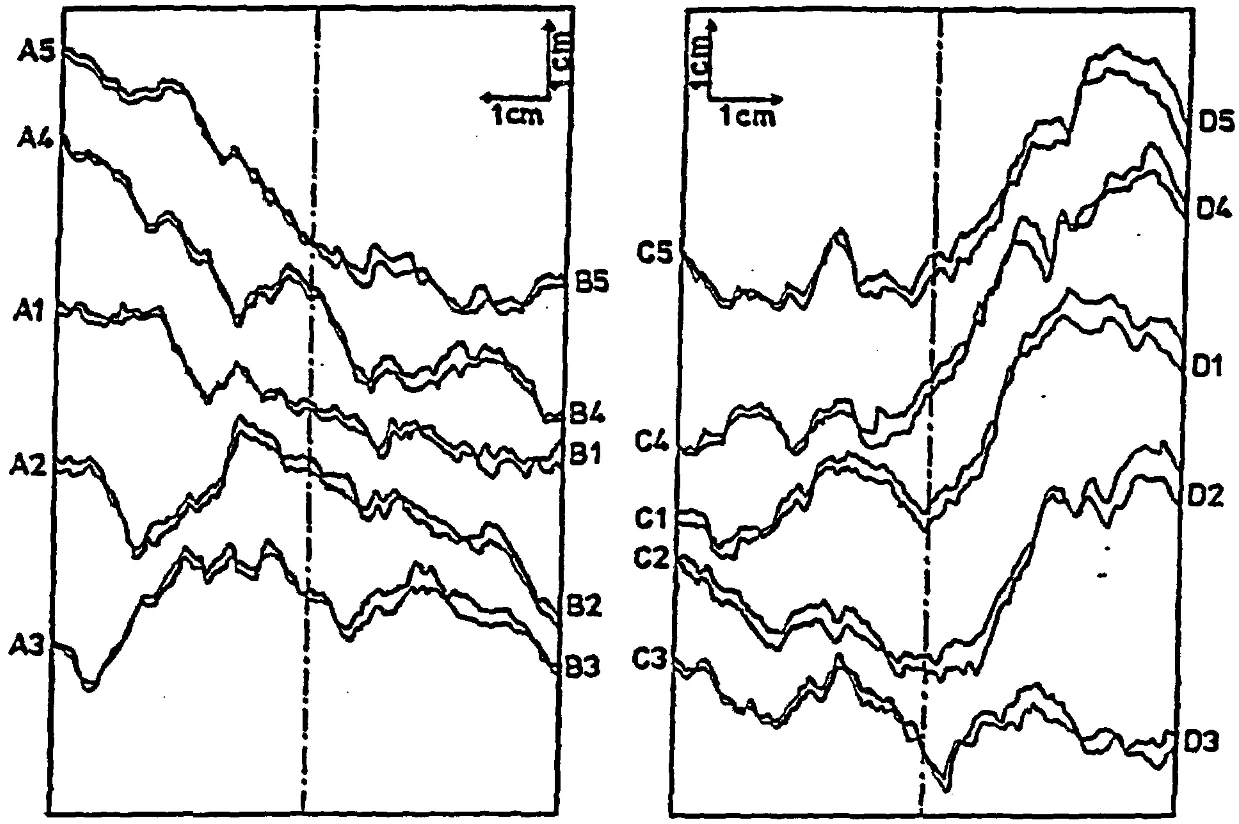
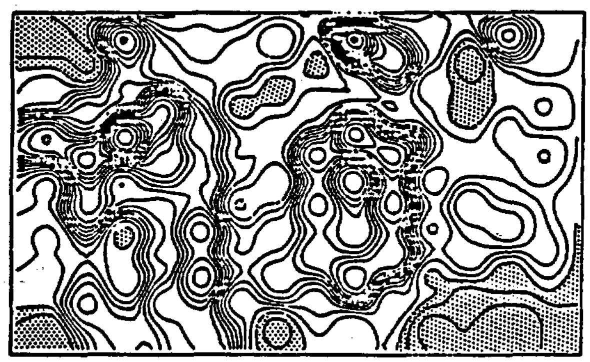


Figure 2.1 Profiles from upper and lower surface of a joint. The profiles AB are perpendicular to CD on the same joint surface. Gentier (1986).

Another technique to reveal the apertures inside a joint has been developed by Gale (1987). The experiments involves injection of an epoxy resin into the joint under normal load. After hardening the joint is cut into sections and the distances between the rock surfaces and the thickness of the resin is measured along the profiles, (Fig. 2.3). In Figure 2.4 the variation in aperture and resin thickness from all profiles is shown by frequency histograms. The joint specimen was obtained from the Stripa test site in Sweden.

a)

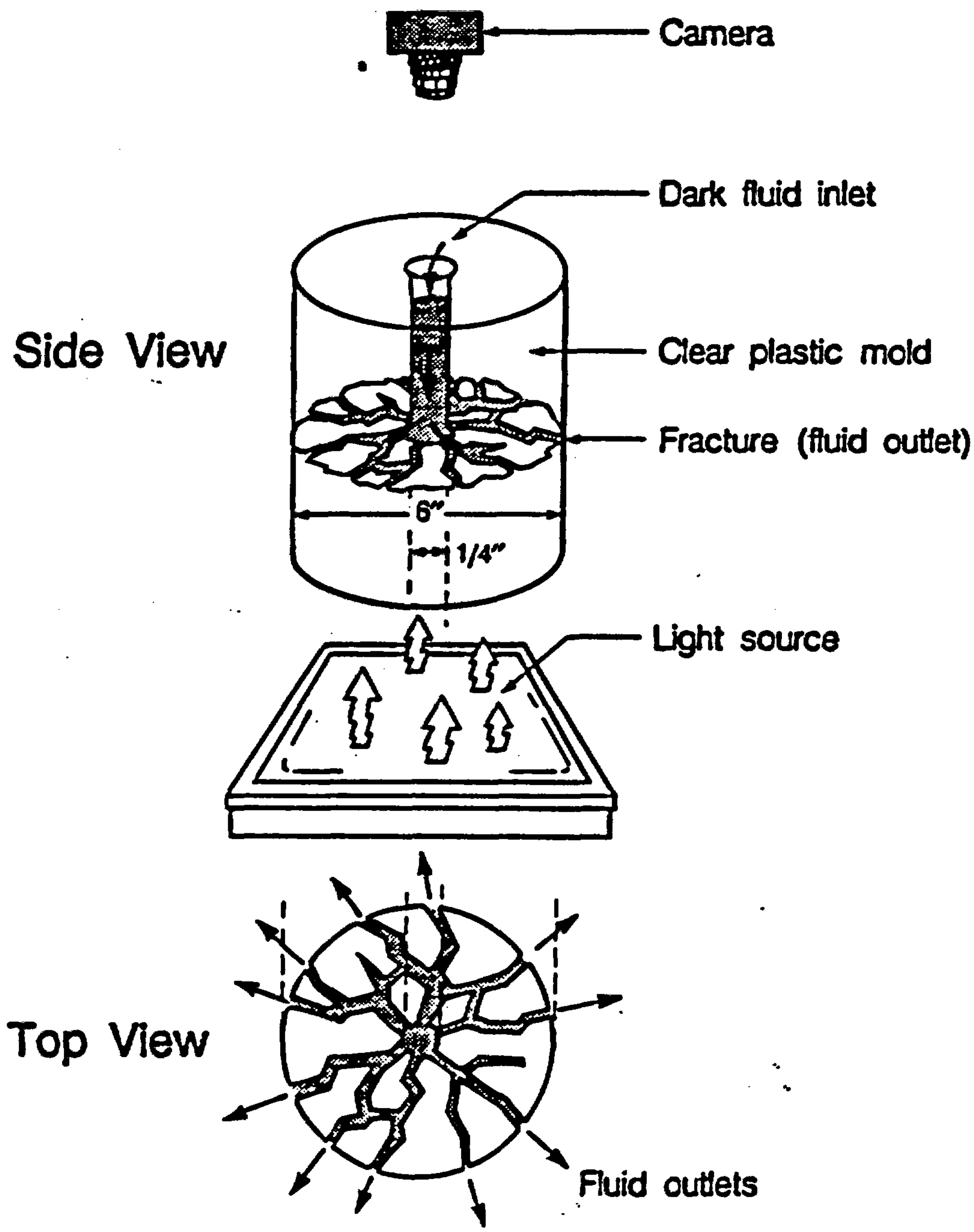


b)

Figure 4.9 Isoplots of the apertures of sample a) S4 and b) S2. The hatched areas correspond to apertures smaller than 250 µm. Equidistance 50 µm. Scale 1:1.5.

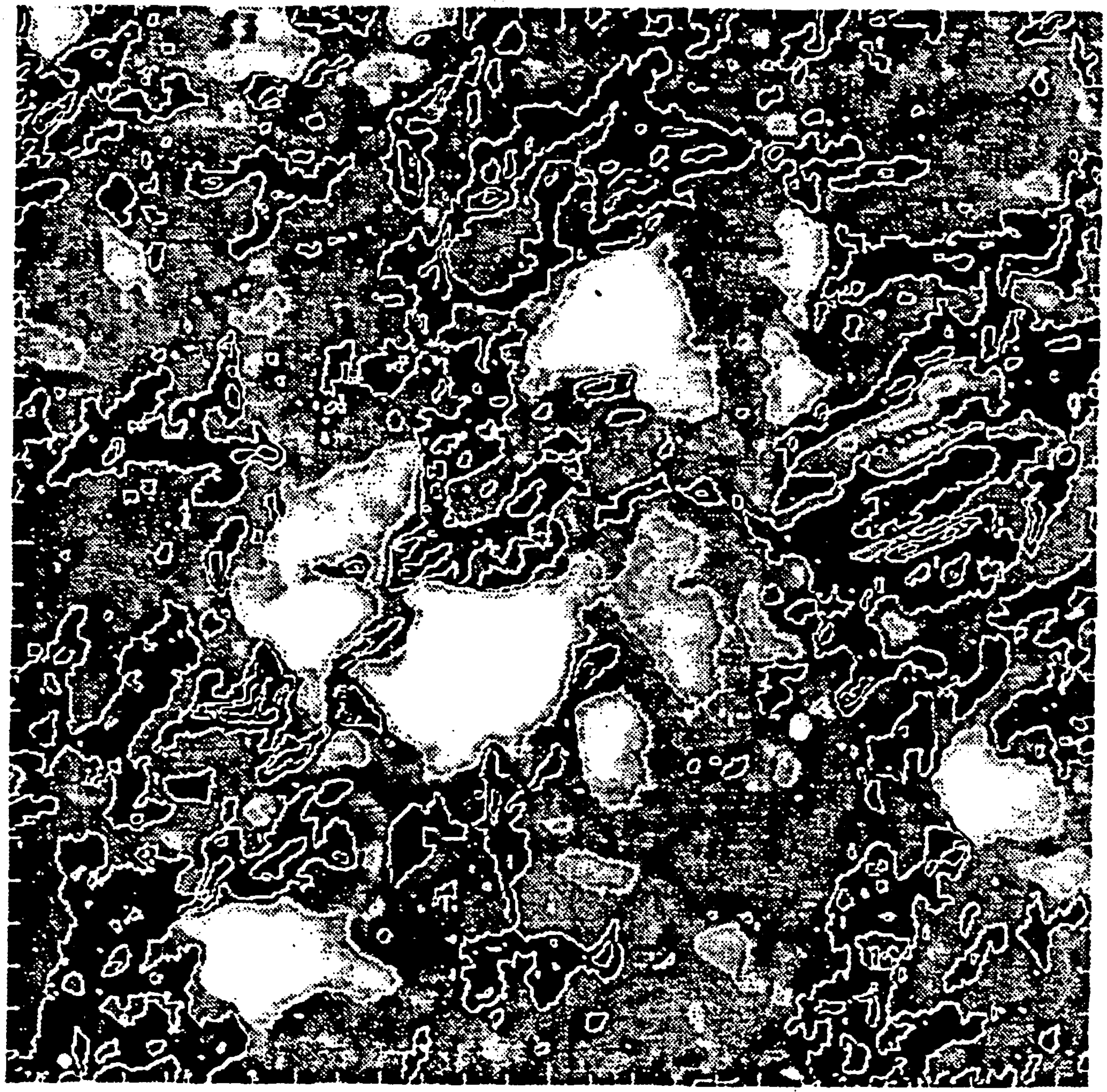
HAKAMI, THESIS, 1988

Flow Visualization Experiment



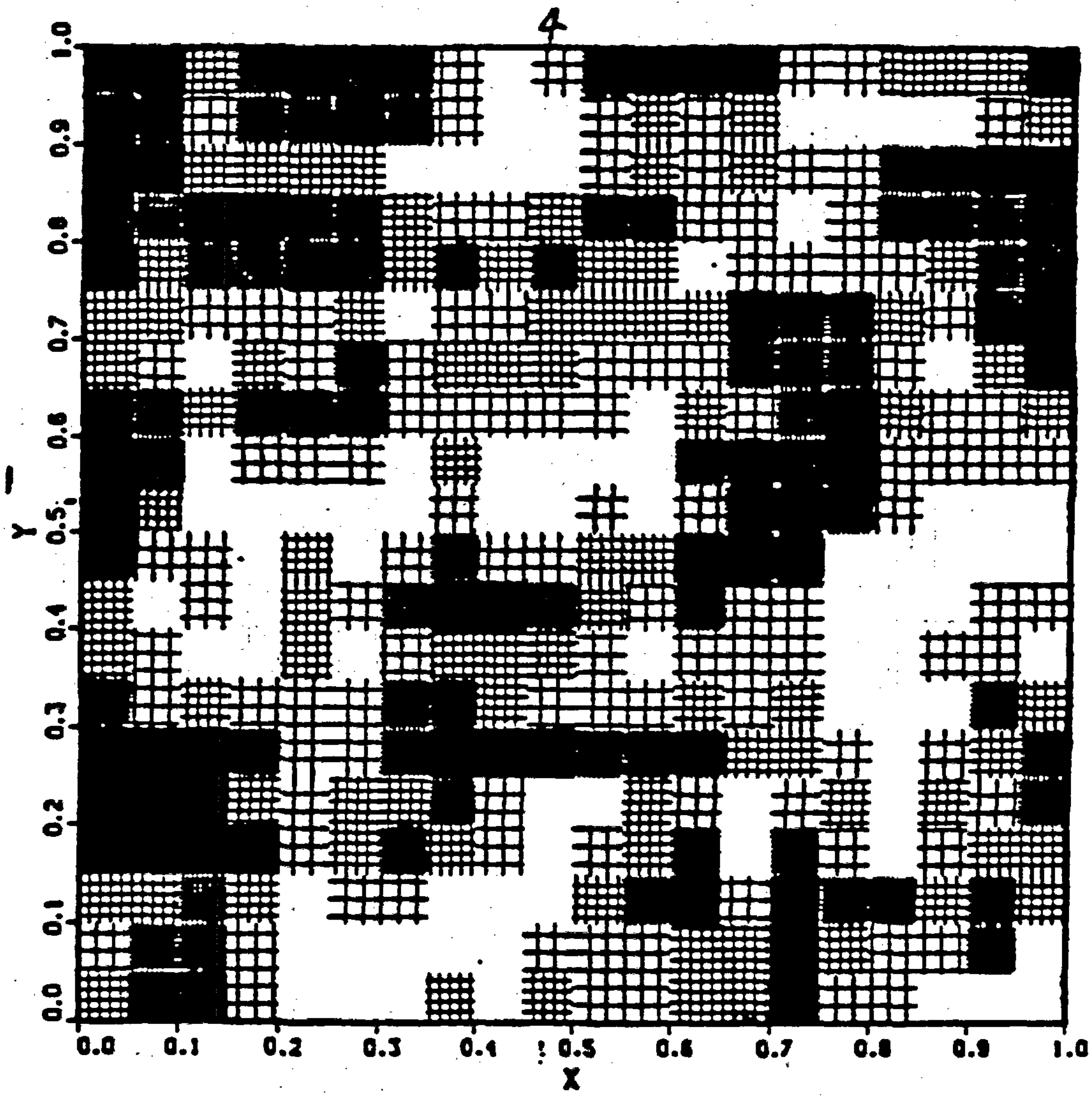
XBL 886-8043

FLOW VISUALIZATION IN EPOXY-RESIN CAST OF ROCK FRACTURE (LBL, 1988

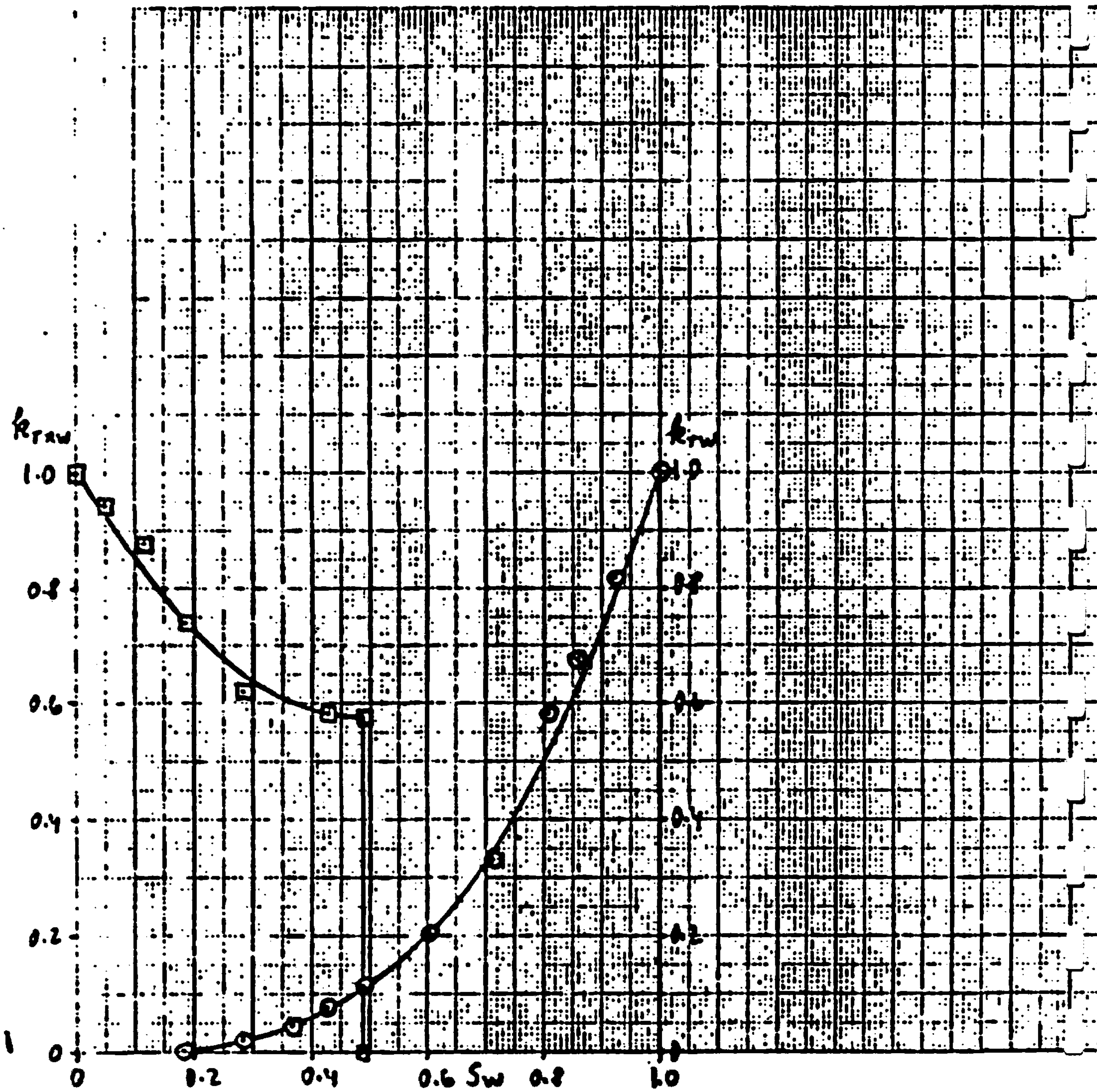


APERTURE CONTOURS FROM DIGITIZED FRACTURE IMAGES (LBL, 1988)

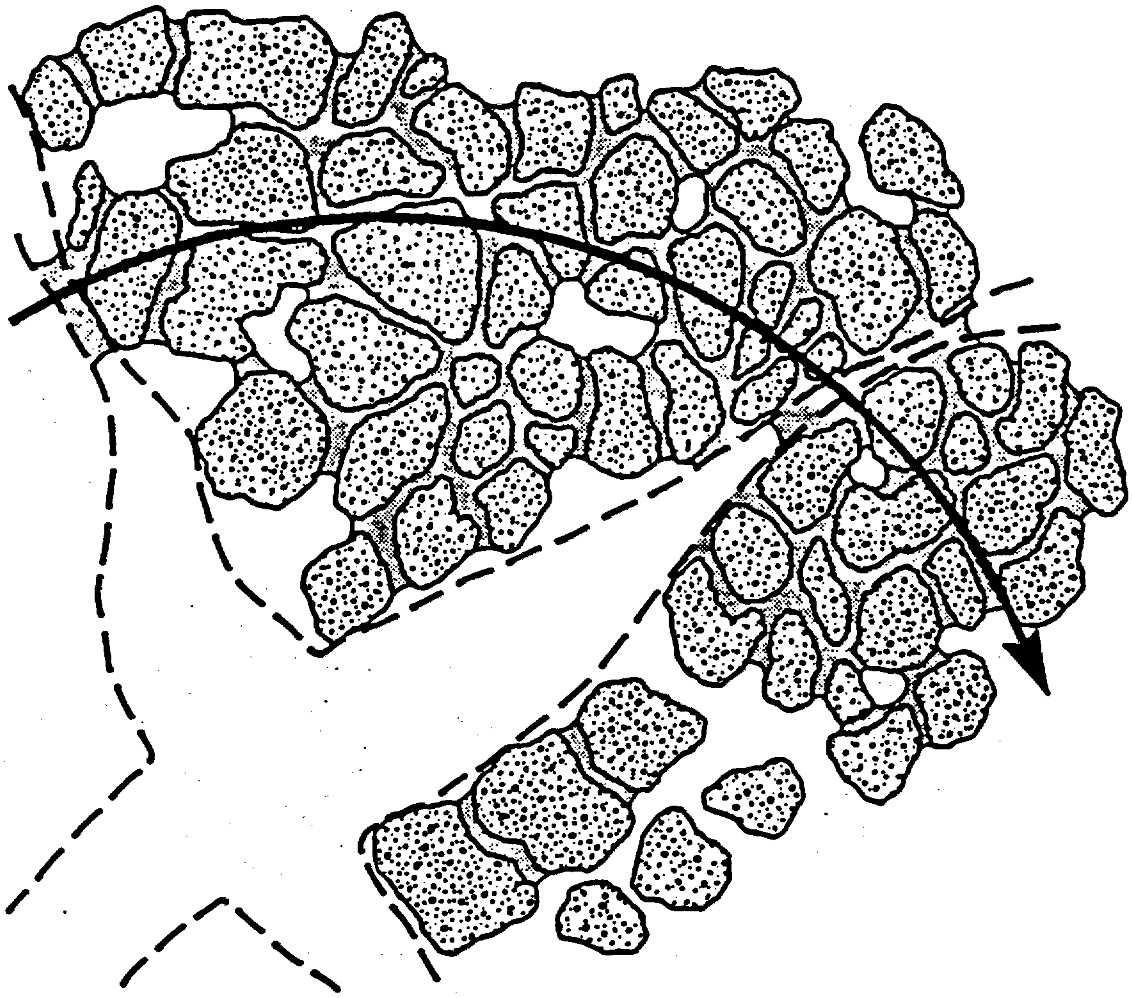
FINITE-DIFFERENCE MODEL
OF ROUGH-WALLED ROCK FRACTURE
(Y. TSANG, 1988)



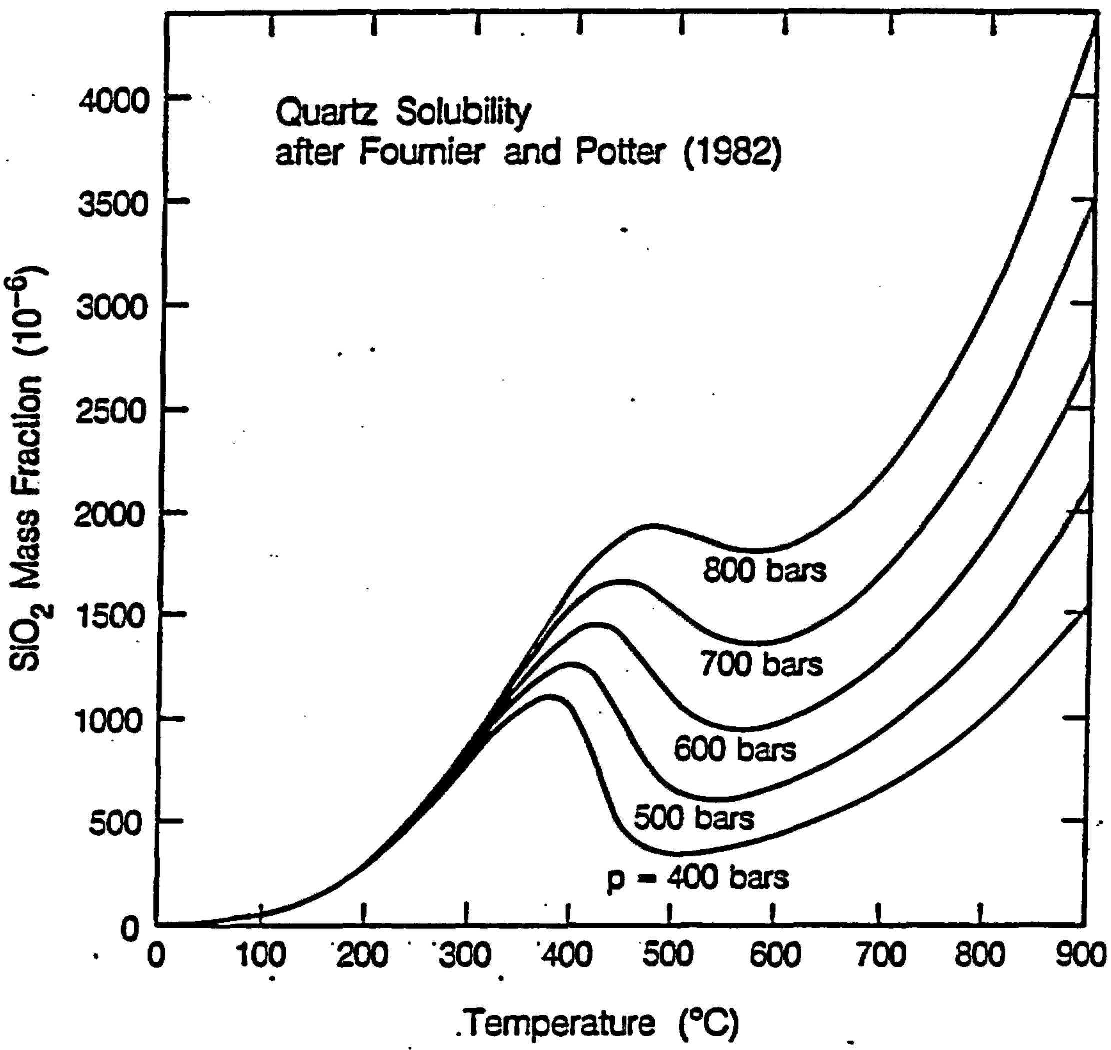
KP127a → h



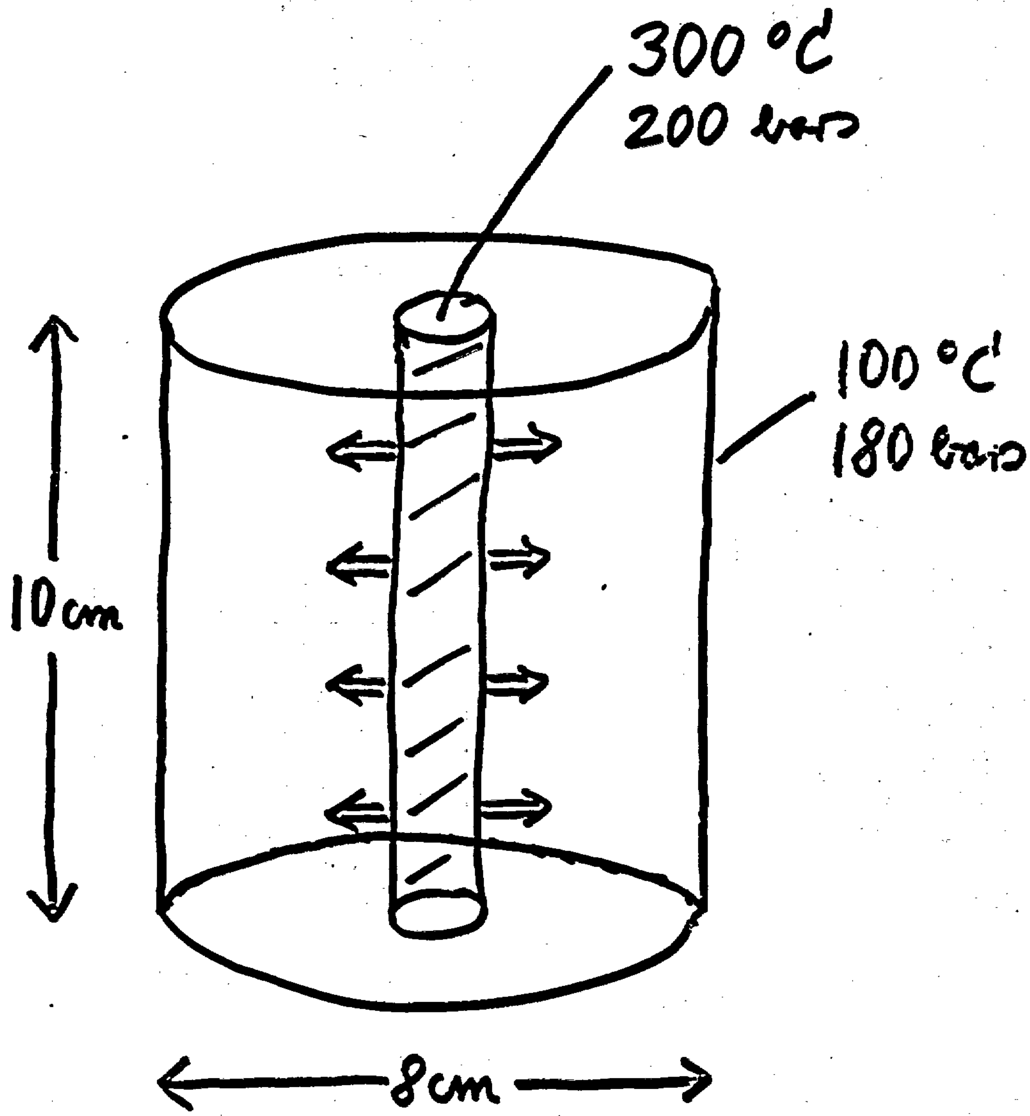
SIMULATED WETTING (k_{rw}) and NONWETTING (k_{rnw}) RELATIVE PERMEABILITIE in ROUGH-WALLED FRACTURE (PRUESS and TSANG, 1988)



XBL 841-9580



XBL 889-10441



USGS SILICA REDISTRIBUTION EXPERIMENT

(after Vaughan, 1987)

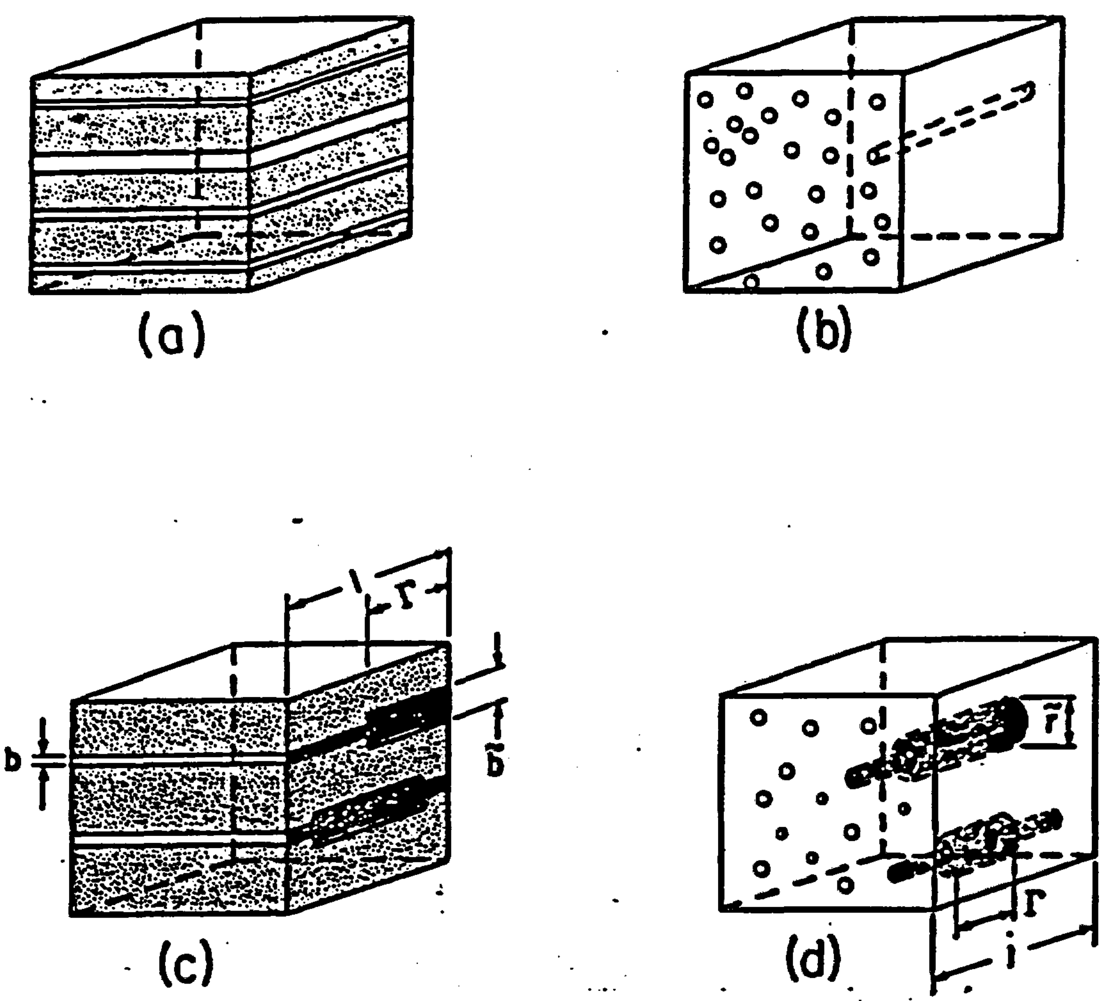


Fig. 1. Idealized models of permeable media. Figures 1*a* and 1*b* represent the straight capillaris models, and Figures 1*c* and 1*d* are the "series" models.

have produced results which differ considerably from each other. For example, while *Mavis and Wilsey* [1937] (as cited by *Scheidegger* [1974]) have found the permeability k to be proportional to ϕ^3 or ϕ^4, *Graham* [1973] found the permeability to be proportional to $(\phi - \phi_c)^{1.8}$ for sintered metallic powders, where ϕ_c represents the critical porosity at which the permeability reduces to zero. Yet another investigator [*Brace*, 1977] found a third power correlation for crystalline rocks. It is therefore obvious that no simple general correlation between porosity and permeability can be applied to all permeable materials because this relationship depends on many complex factors such as geometric details of the pores, their sizes, and their connectivity.

However, what is needed in the current study is not an absolute permeability-porosity correlation but the relationship between their relative changes. Many investigators have proposed such relationships for different materials where the porosity changes were brought about by different physical mechanisms. For example, *Lund* [1974] and *McClure et al.* [1979] proposed an exponential relationship for permeability enhancement of sandstone due to acidizing. *Pearson* [1976] proposed a similar relationship for permeability enhancement of rock in geothermal reservoirs, where the porosity changes are brought about by dissolution of rock minerals in a hydrothermal flow field. *Camp* [1964] proposed the use of the Kozeny-Stein equation in the field of water filtration. This equation is basically a third-power relationship scaled by a factor depending on the net change in porosity. *Graham*'s [1973] equation can be written to correlate relative changes in porosity to corresponding changes in permeability, thus representing a 1.8th power relationship for cases where porosity alterations are caused by grain bonding in the sintering process of metallic powders. *Wyble* [1958] conducted an experimental study on the effects of confining pressure on porosity and permeability for three different types of sandstones and presented his results correlating pressure to porosity and permeability reductions. His results can be restated, by factoring out pressure, to provide a porosity-permeability correlation of the form

$$\frac{k - k_r}{k_0 - k_r} = \left\{\frac{\phi - \phi_r}{\phi_0 - \phi_r}\right\}^{\tau} \qquad (6)$$

where k_r and ϕ_r represent asymptotic values of permeability and porosity, which are the lowest values to which these parameters can be reduced by increasing the confining pressure and k_0, ϕ_0, and τ represent the initial permeability, porosity, and the exponent, respectively, of the correlation (determined

VERMA / PRUESS (1988)

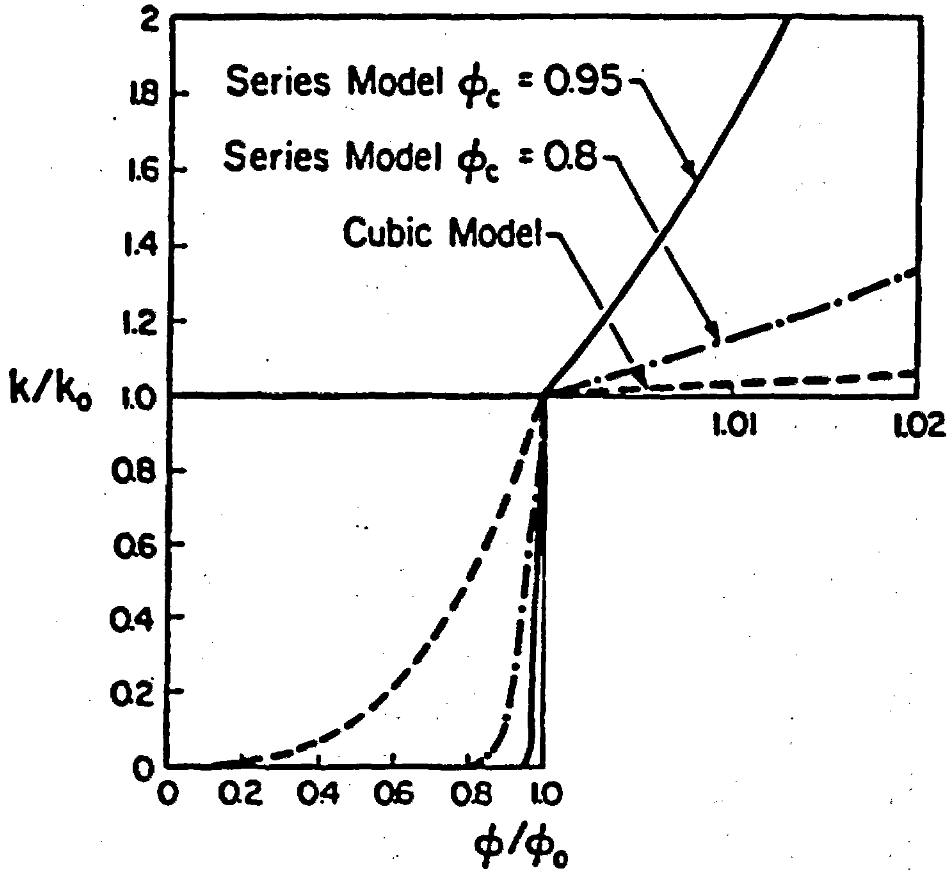


Figure 4. Porosity-permeability relationships for three different models considered in this study.

U.S. DEPARTMENT OF ENERGY

OCRWM

YUCCA MOUNTAIN

YUCCA MOUNTAIN PROJECT

QUANTIFYING UNCERTAINTY IN MODELING UNSATURATED FLOW

PRESENTED TO

UNIV. OF ARIZONA, WORKSHOP IV ON FLOW AND TRANSPORT THROUGH UNSATURATED FRACTURED ROCK RELATED TO A HIGH-LEVEL RADIOACTIVE WASTE REPOSITORY

PRESENTED BY

SCOTT SINNOCK

SUPERVISOR, SANDIA NATIONAL LABORATORIES
DIVISION 6317

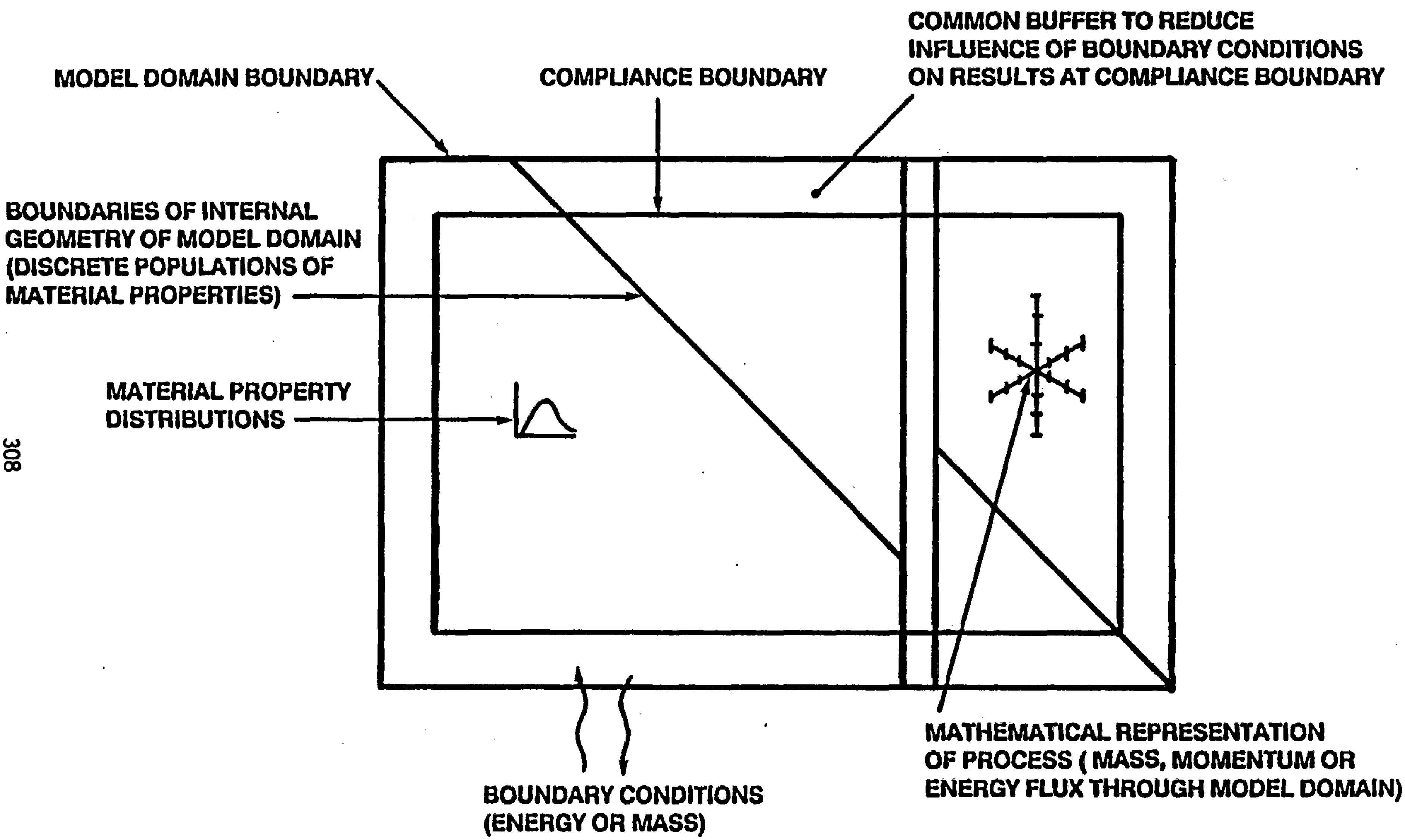
DECEMBER 15, 1988

UNITED STATES DEPARTMENT OF ENERGY
NEVADA OPERATIONS OFFICE/YUCCA MOUNTAIN PROJECT OFFICE

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

PREDICTIONS OF REPOSITORY BEHAVIOR FOR 10,000 OR MORE YEARS

- **MISSION**
  - PROVIDE BASIS FOR JUDGING ACCEPTABILITY
- **APPROACH**
  - USE NUMERICAL MODELS
- **PROBLEM**
  - HOW CAN ANYONE BELIEVE THE RESULTS


MODEL DOMAIN BOUNDARY
COMPLIANCE BOUNDARY
COMMON BUFFER TO REDUCE INFLUENCE OF BOUNDARY CONDITIONS ON RESULTS AT COMPLIANCE BOUNDARY
BOUNDARIES OF INTERNAL GEOMETRY OF MODEL DOMAIN (DISCRETE POPULATIONS OF MATERIAL PROPERTIES)
MATERIAL PROPERTY DISTRIBUTIONS
BOUNDARY CONDITIONS (ENERGY OR MASS)
MATHEMATICAL REPRESENTATION OF PROCESS (MASS, MOMENTUM OR ENERGY FLUX THROUGH MODEL DOMAIN)

SOURCES OF UNCERTAINTY IN PREDICTING REPOSITORY BEHAVIOR

- PARAMETER UNCERTAINTY
- SCALAR UNCERTAINTY
- TEMPORAL UNCERTAINTY
- PROCESS UNCERTAINTY

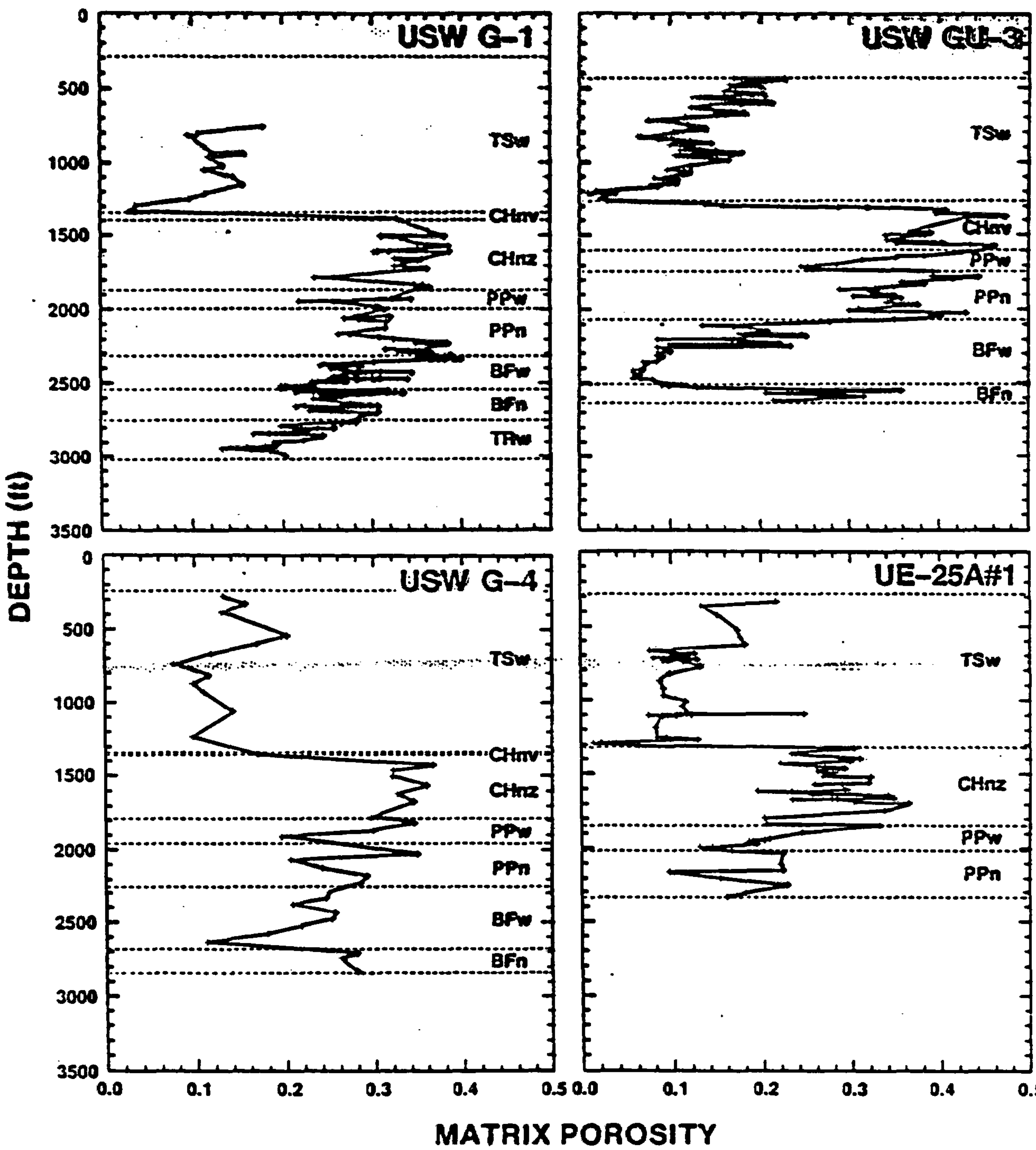
REPBEH.PM3/11-17-88

	TYPE OF UNCERTAINTY			
	PARAMETER	SCALAR	TEMPORAL	PROCESS
MODEL DOMAIN			X	X
BOUNDARY CONDITIONS	X	X	X	X
INTERNAL GEOMETRY OF MODEL DOMAIN	X	X	X	
MATERIAL PROPERTIES IN MODEL DOMAIN	X	X	X	
PROCESS REPRESENTATION			X	X

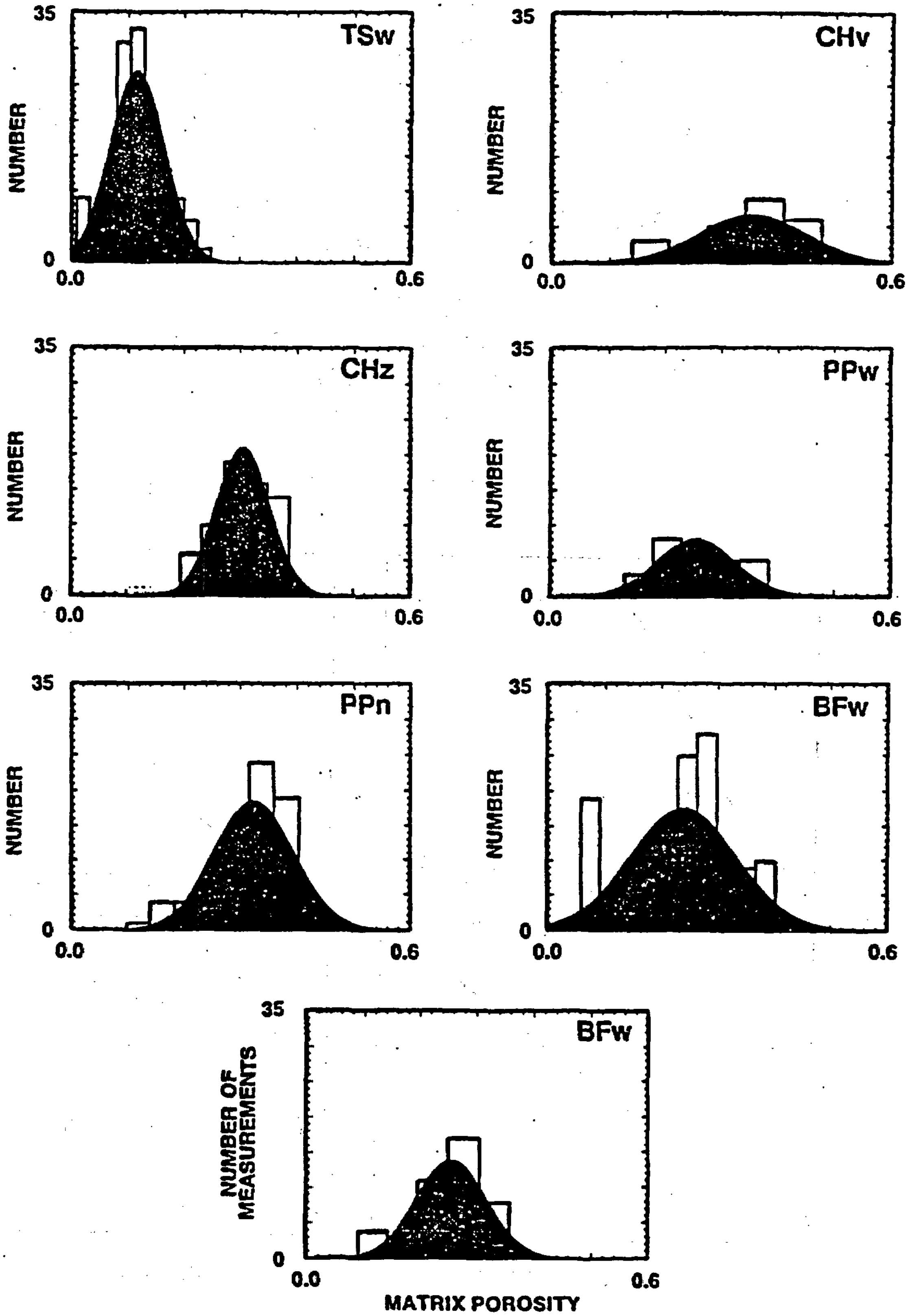
UAZSNDIA1P.A01/12-15-88

PARAMETER UNCERTAINTY

- LIMITS TO KNOWLEDGE ABOUT VALUES OF INPUT VARIABLES
- GENERALLY CAN BE TREATED WITH FREQUENTIST STATISTICS
- ASSUMES ABILITY TO DEFINE DISCRETE "POPULATIONS"



USW G-1
USW GU-3
USW G-4
UE-25A#1
DEPTH (ft)
MATRIX POROSITY
TSw
CHnv
CHnz
PPw
PPn
BFw
BFn
TRw
0
500
1000
1500
2000
2500
3000
3500
0.0
0.1
0.2
0.3
0.4
0.5

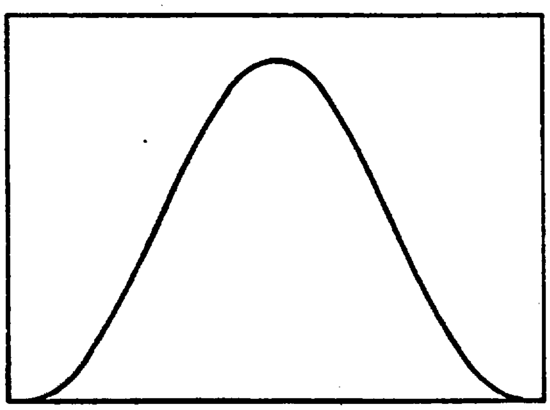

TSw
CHv
CHz
PPw
PPn
BFw
BFw
35
0
NUMBER
0.0
0.6
NUMBER OF MEASUREMENTS
MATRIX POROSITY

EXAMPLE OF NEED FOR CONCEPTUAL ASSUMPTIONS AT PARAMETER LEVEL OF CONCERN

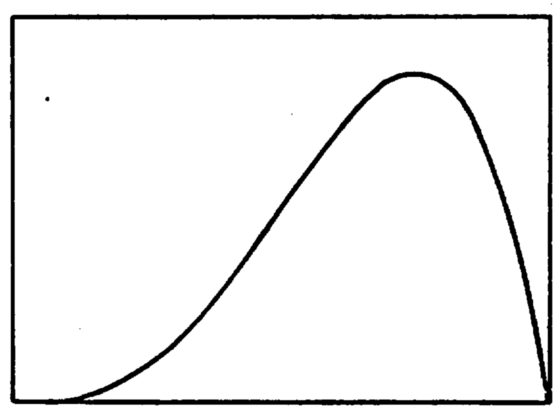
BETA DISTRIBUTION OF ANY SHAPE CAN BE DEFINED BY FOUR VALUES

- MEAN ($\bar{x}$)
- STANDARD DEVIATION (σ)
- MINIMUM VALUE
- MAXIMUM VALUE

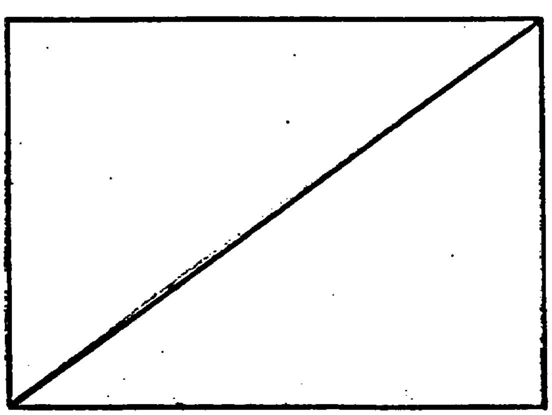
WHERE COEFFICIENT OF VARIATION = $\frac{\sigma}{\bar{x}}$



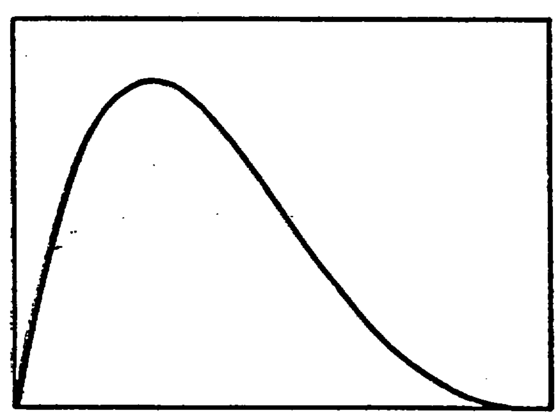
SYMMETRICAL DISTRIBUTION



SKEWED DISTRIBUTION



TRIANGULAR DISTRIBUTION



SKEWED DISTRIBUTION

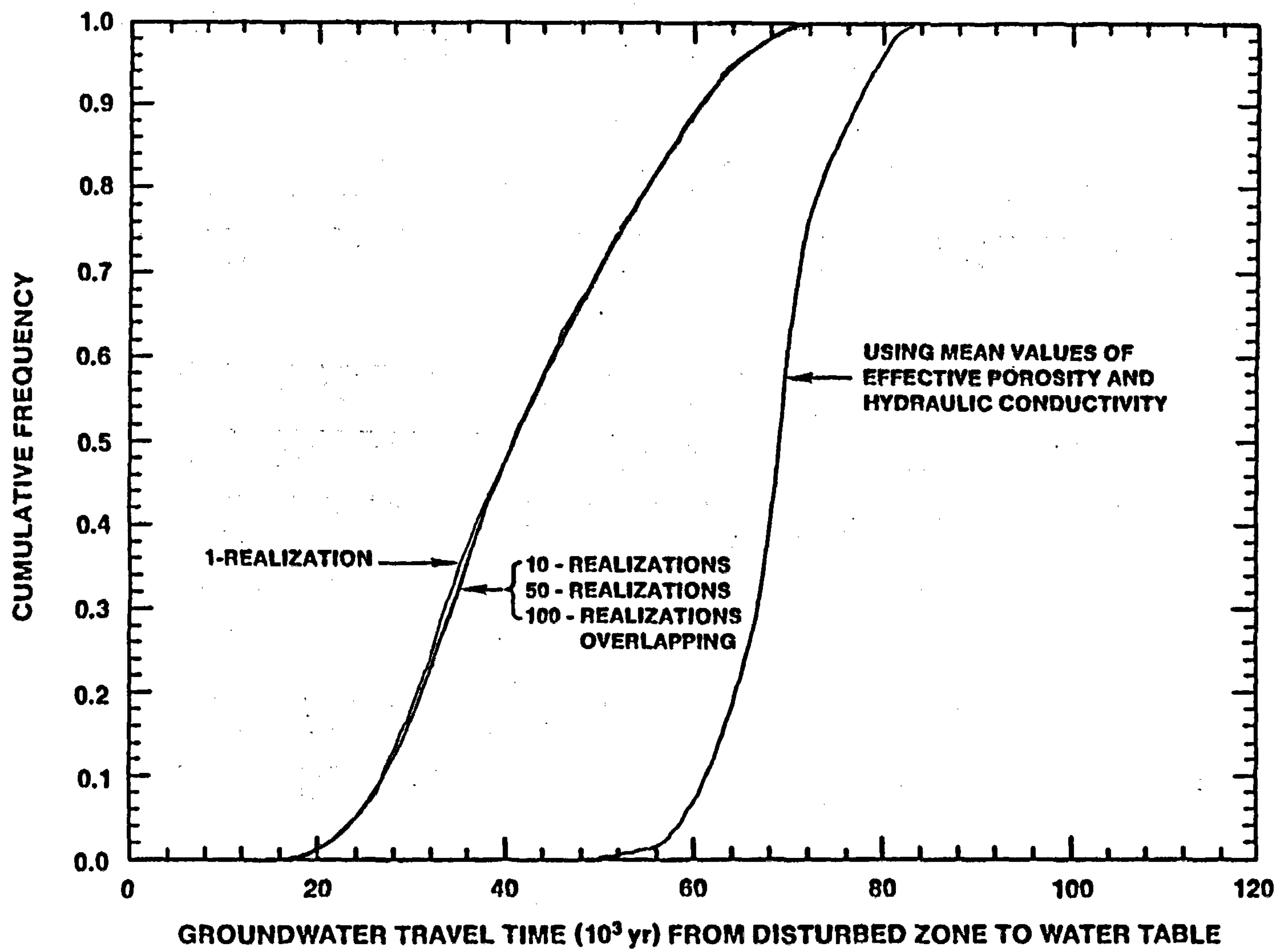


Figure 10. Cummulative distribution curves for 1, 10, 50, and 100 realizations based on randomly selected values Ks and ne and a deterministic curve based on mean values of affective porosity and hydraulic conductivity, for a flux of 0.5 mm/yr using 10-foot-thick calculational elements.

SCALAR UNCERTAINTY

- LIMITS TO KNOWLEDGE ABOUT SCALE-DEPENDENCY OF PROPERTIES
- CAN BE PARTIALLY TREATED WITH NON-STATIONARY GEOSTATISTICS, FOURIER ANALYSIS, FRACTALS (?), OR THE MARKOVIAN PROCESSES
- ASSUMES ABILITY TO DISCRIMINATE TRENDS FROM DISCONTINUITIES
- ASSUMES HETEROGENEITY IS HOMOGENEOUS

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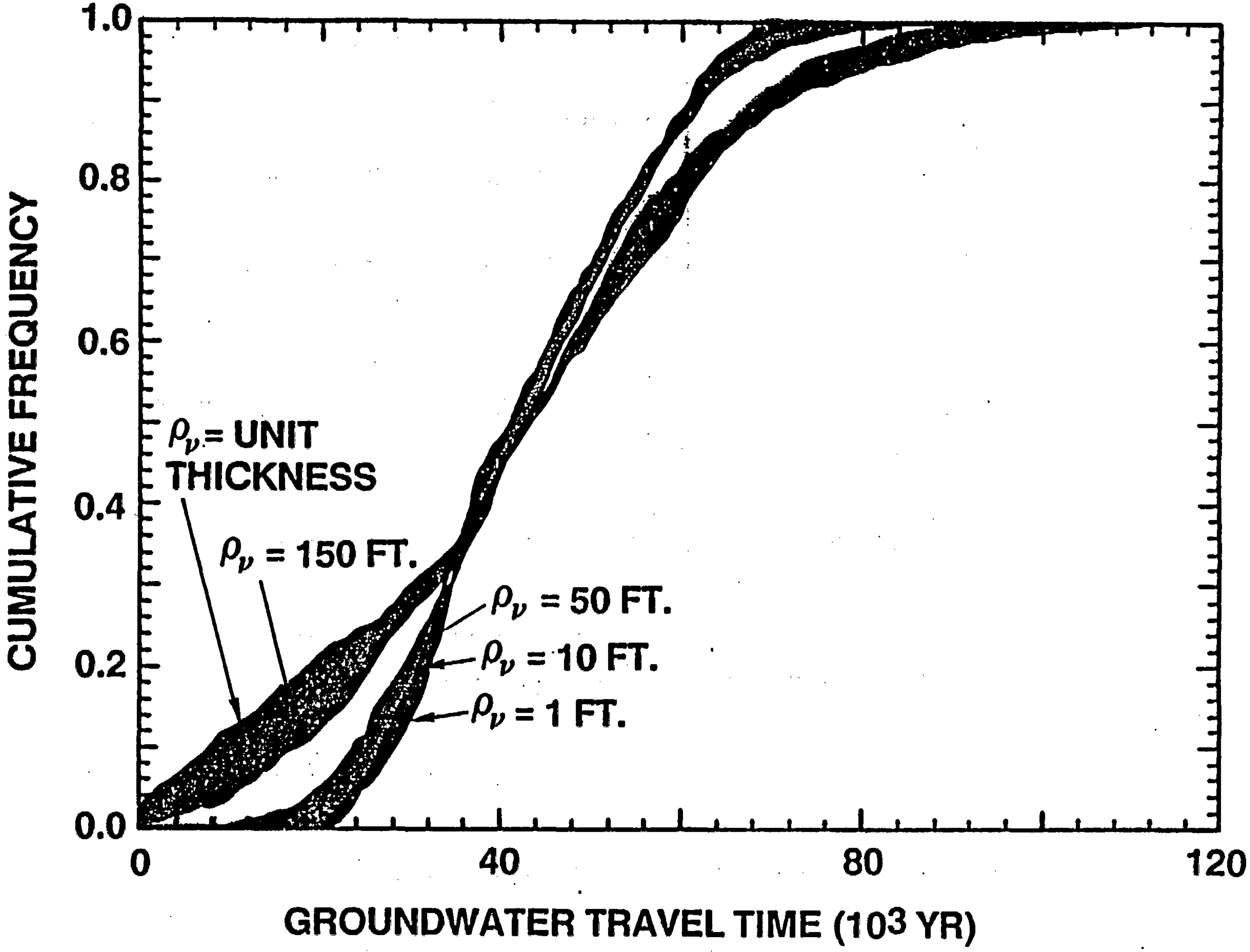


CUMULATIVE FREQUENCY
1.0
0.8
0.6
0.4
0.2
0.0
0
40
80
120
GROUNDWATER TRAVEL TIME (10^3 YR)
ρ_ν = UNIT THICKNESS
ρ_ν = 150 FT.
ρ_ν = 50 FT.
ρ_ν = 10 FT.
ρ_ν = 1 FT.

TREATMENT OF PARAMETER UNCERTAINTY

SENSITIVITY ANALYSIS

- TREAT SENSITIVE INPUT VARIABLES AS RANDOM DISTRIBUTIONS
- IDENTIFY MOST INFLUENTIAL VARIABLES

UNCERTAINTY ANALYSIS

- PROBABALISTIC PREDICTION OF PERFORMANCE
  - MONTE CARLO
  - DIRECT STOCHASTIC SIMULATION

TEMPORAL UNCERTAINTY

- LIMITS TO KNOWLEDGE ABOUT FUTURE CONDITIONS
- MUST BE TREATED AS CONDITIONAL "SCIENTIFIC" OPINION (BAYSEAN STATISTICS)
- DELPHI-LIKE METHODS

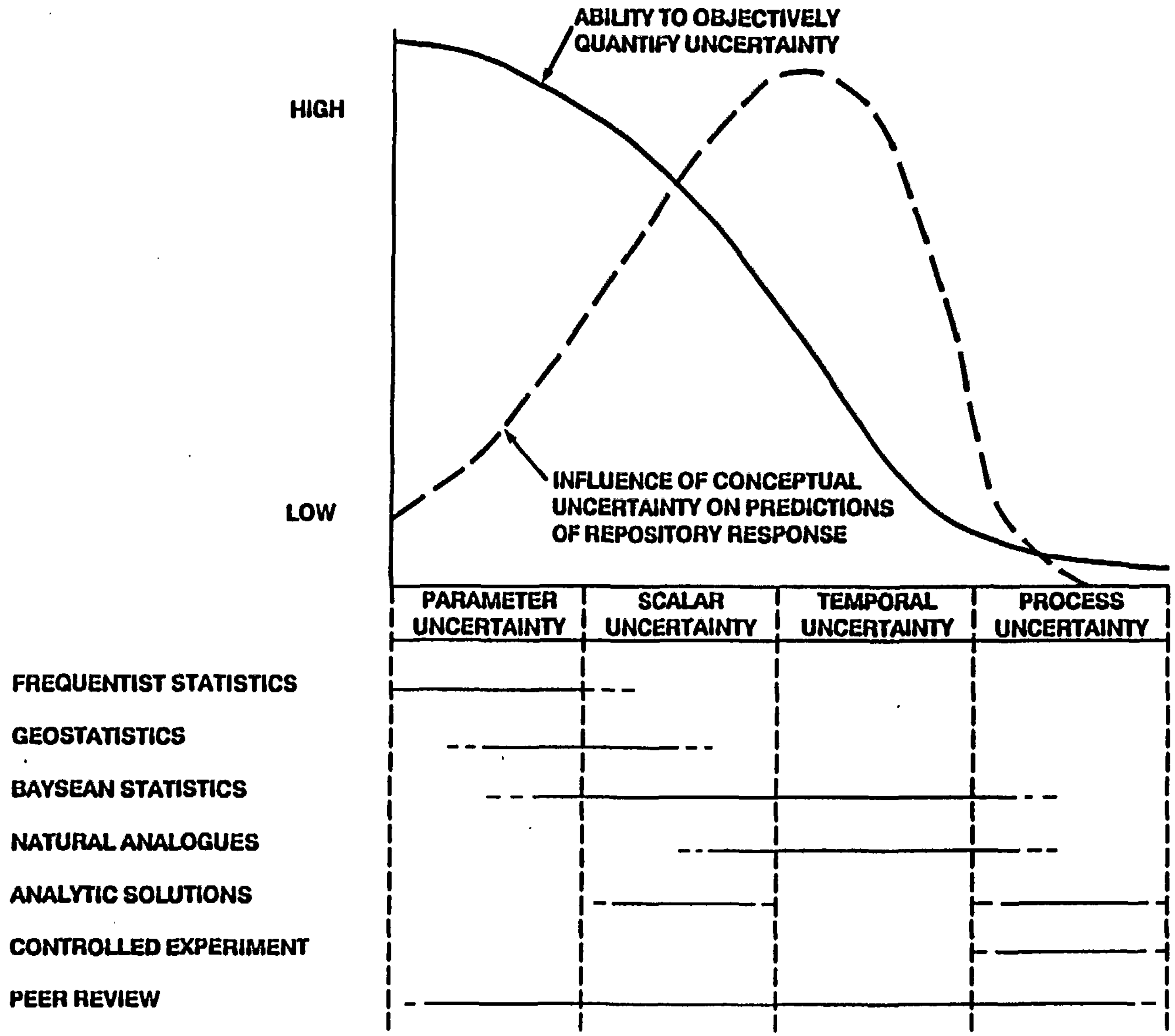
PROCESS UNCERTAINTY

- LIMITS TO KNOWLEDGE ABOUT MASS, MOMENTUM, AND ENERGY TRANSFER THROUGH PHYSICAL SYSTEM
- ALSO TREATED AS CONDITIONED SCIENTIFIC OPINION
- PEER REVIEW

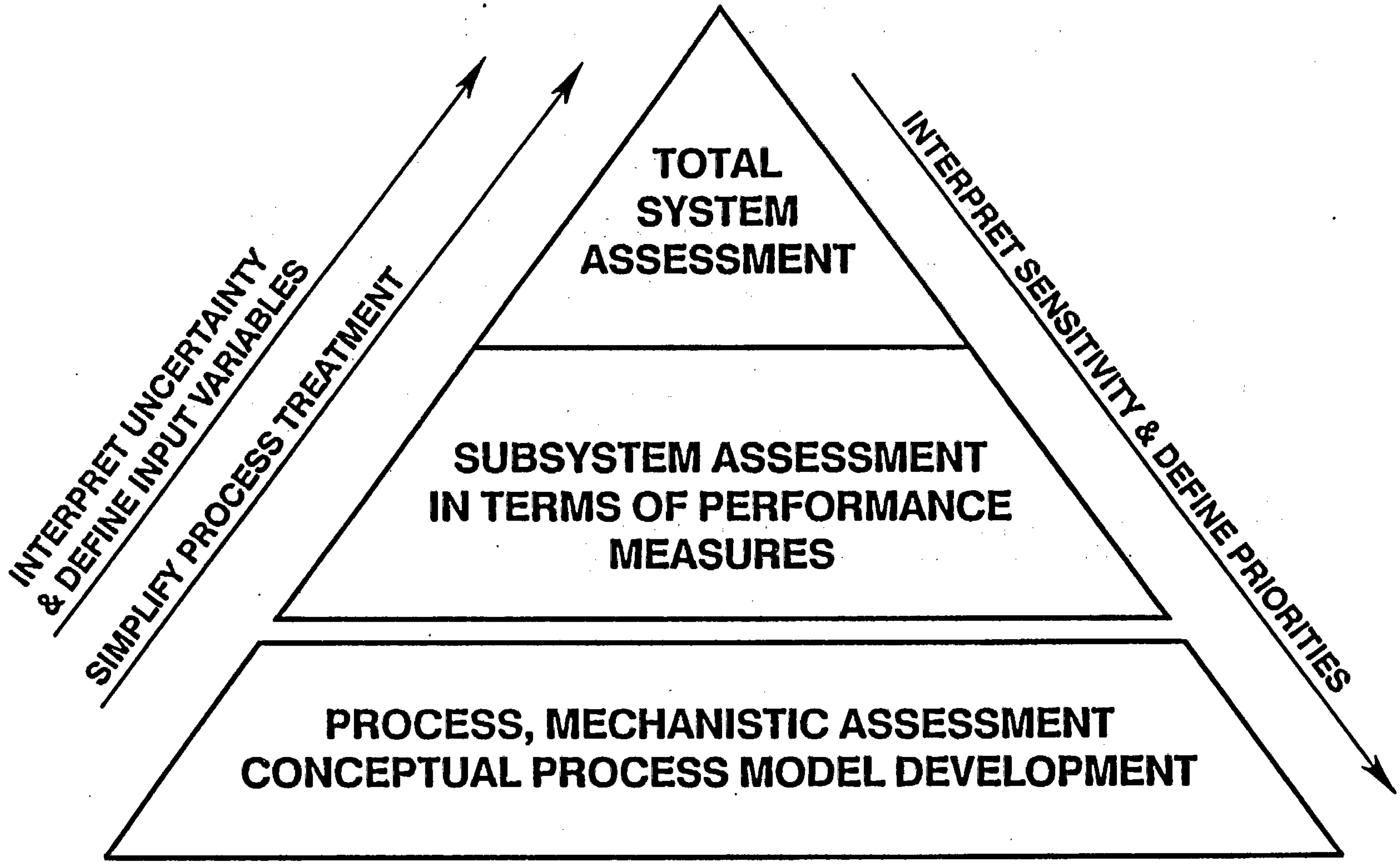
REPBEH.PM3/11-17-88

TREATMENT OF CONCEPTUAL UNCERTAINTY

- Less Amenable to Quantification
- Addressed by Consideration of Alternative Concepts
  - Weighting by Professional Judgment, DELPHI, or Bounding Calculations
  - Extensive Dialogue with State, NRC, Expert Consultants
- Validation of Modeling Approaches
  - Calibration with respect to field observations (ψ, S, $\delta h/\delta \ell$)
  - Comparison to controlled field experiments
  - Comparison to controlled laboratory experiments
  - Periodic Formal Peer Review


ABILITY TO OBJECTIVELY QUANTIFY UNCERTAINTY
HIGH
LOW
INFLUENCE OF CONCEPTUAL UNCERTAINTY ON PREDICTIONS OF REPOSITORY RESPONSE
PARAMETER UNCERTAINTY
SCALAR UNCERTAINTY
TEMPORAL UNCERTAINTY
PROCESS UNCERTAINTY
FREQUENTIST STATISTICS
GEOSTATISTICS
BAYSEAN STATISTICS
NATURAL ANALOGUES
ANALYTIC SOLUTIONS
CONTROLLED EXPERIMENT
PEER REVIEW

TREATMENT OF UNCERTAINTY THROUGH MODELING HIERARCHY



REPBEH.PM3/11-17-88

STRATEGY FOR ENCOMPASSING UNCERTAINTY

- DEFENSE-IN-DEPTH
- QUANTIFY PARAMETER UNCERTAINTY
- SIMPLIFY MODELS
- STRESS UNCERTAINTY ABOUT COMPLIANCE RATHER THAN ACTUAL BEHAVIOR
- ACKNOWLEDGE RELIANCE ON PROFESSIONAL JUDEMENT

REPBEH.PM3/11-17-88

UNSATURATED FLOW
IN SPATIALLY VARIABLE AND ANISOTROPIC MEDIA

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Princeton University
(Water Resources Program)

WORKSHOP IV -- FLOW AND TRANSPORT THROUGH UNSATURATED FRACTURED ROCK AS RELATED TO A HIGH-LEVEL RADIOACTIVE DISPOSAL

University of Arizona, Tucson
Dec. 12-15, 1988

UNSATURATED FLOW IN SPATIALLY VARIABLE AND ANISOTROPIC MEDIA

Rachid Ababou
Princeton University

SUMMARY:

An overview of heterogeneous unsaturated flow processes is presented, based on analytical solutions, detailed numerical simulations, and physical arguments. Starting with idealized cases such as low-rate steady flow in uniformly layered or "periodic" media, we progressively incorporate more complex features such as slanted stratification, imperfect or random stratification, transient effects, and fractures. For steady flow in horizontally layered or stratified media, the unit gradient assumption appears generally valid in the mean (not locally). Detailed simulation of steady infiltration in a randomly heterogeneous medium with horizontal stratification shows a strongly anisotropic moisture pattern with wet zones perched over dryer zones (3D simulation with 300,000 grid points). A simple analysis shows that streamlines will bend slopewise, in the mean, if the strata are tilted. Possible consequences on the migration and dispersion of solutes are briefly discussed. Spatial variability and uncertainty are distinguished based on the scale of observation, using concepts of self-similarity and spectral conditioning. Finally, we analyze transient effects in the case of a periodic forcing at the upper boundary, and relate this to a possible scenario for the space-time response of a vertically fractured porous medium submitted to sparse but intense rainfalls in arid climate.

Note: A schematic outline of this talk and a few figures illustrating some of the main points are attached.

OUTLINE:

1. STEADY FLOW IN DRY POROUS FORMATIONS:

   - Homogeneous, Layered, and Case of Tilted Layers (Some Analytical Solutions)
   - Comparison with Imperfectly Stratified Random Medium (3D Simulation)
   - Possible Consequences for Solute Transport, Issues of Variability and/or Uncertainty

2. SCALE ISSUES IN QUANTIFYING VARIABILITY AND UNCERTAINTY:

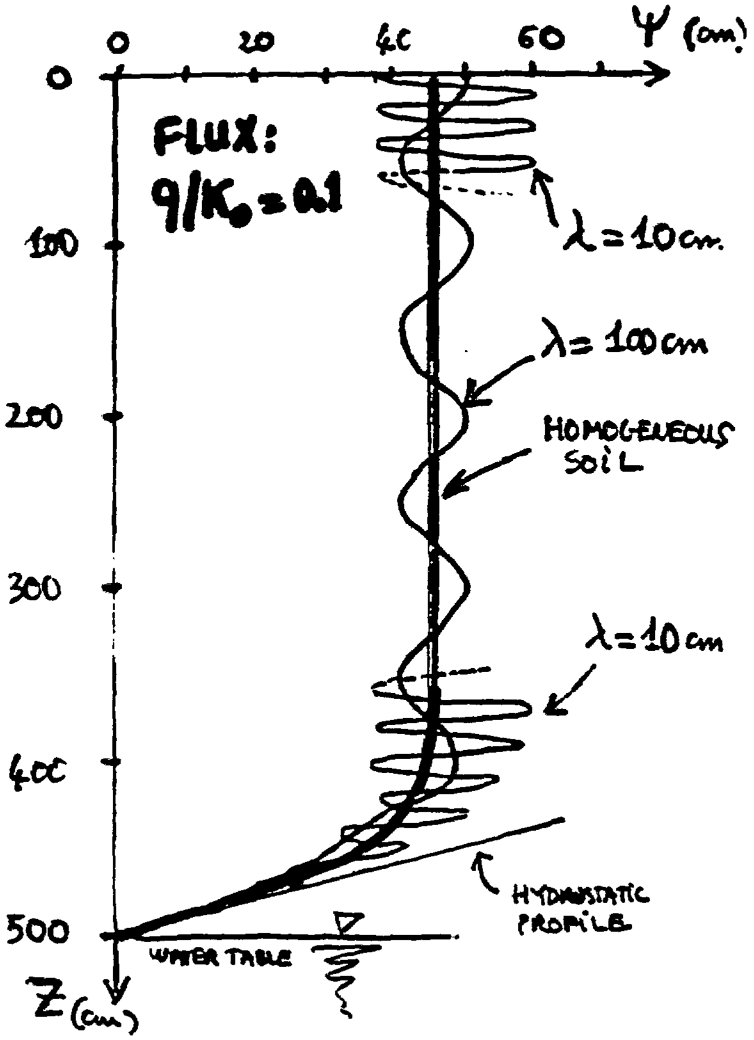
   - Self-Similarity
   - Uncertainty versus Effective Spatial Variability (Conceptual Approach Illustrated in the Case of a Growing Contaminant Plume)

3. TRANSIENT EFFECTS AND SPACE-TIME HETEROGENEITY:

   - Case of Periodic Flux Conditions (Analytical Solution)
   - More Realistic Types of Climatic Forcing, and Possible Role of Vertical Fractures
   - Some Transient Simulations of Unsaturated Flow (Horizontally Stratified Random Media, and Case of Vertically Layered Medium).

I

ANALYTICAL SOLUTIONS FOR INFILTRATION IN SOILS WITH PERIODIC STRATIFICATION; COARSE SOIL ($\alpha_0 = 0.05\ cm^{-1}$):



λ = wavelength of conductiv. fluctuations

$\sigma_k \simeq 0.6$

$\sigma_\alpha = 0.1$

PERIODIC STRATIFICATION:

AMPLITUDE

AMPLITUDE

$$K(\Psi; z) = \underbrace{K_s \exp\left(\sigma_k \sin\left(\frac{2\pi z}{\lambda}\right)\right)}_{K_s(z)} \cdot \exp\left\{\underbrace{\alpha_0 \cdot \exp\left(\sigma_\alpha \sin\frac{2\pi z}{\lambda}\right)}_{\alpha(z)} \cdot \Psi\right\}$$

$$K(\Psi, z) = K_s(z) \cdot \exp\{\alpha(z) \cdot \Psi\}$$

II

CASE OF HETEROGENEOUS + STRATIFIED SOILS:

FLUCTUATIONS OF PRESSURE IN THE "UNIT GRADIENT" ZONE

691

VERTICAL TRANSECT

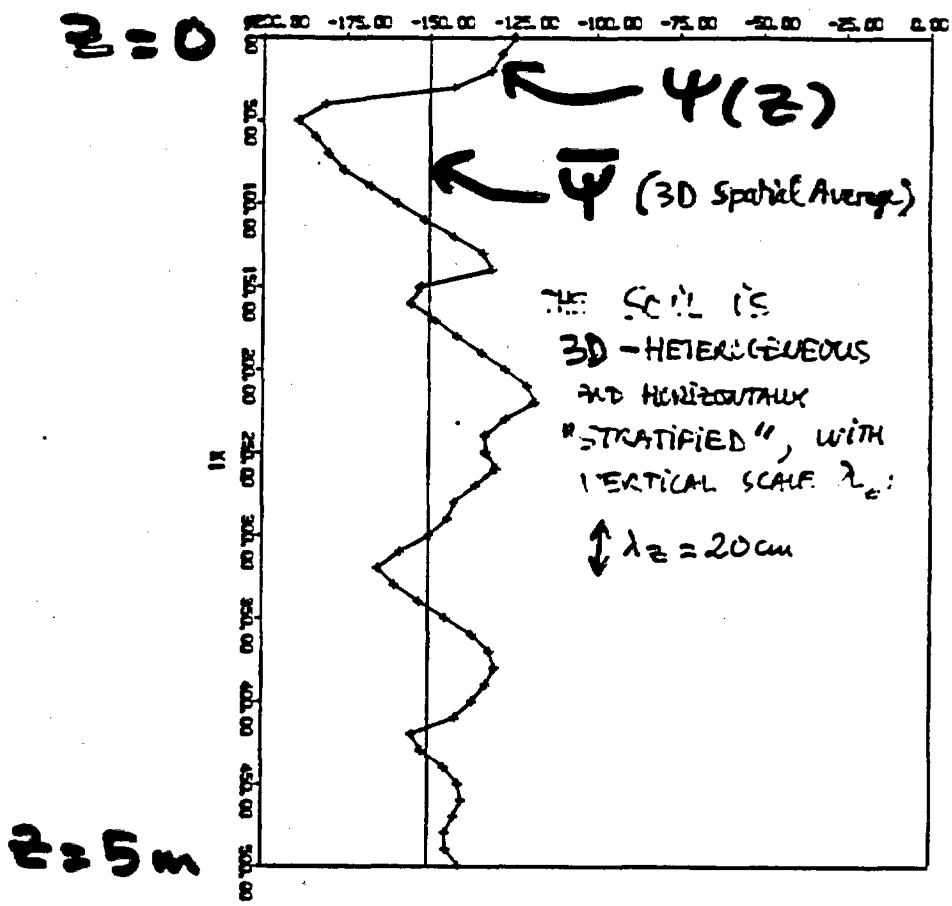
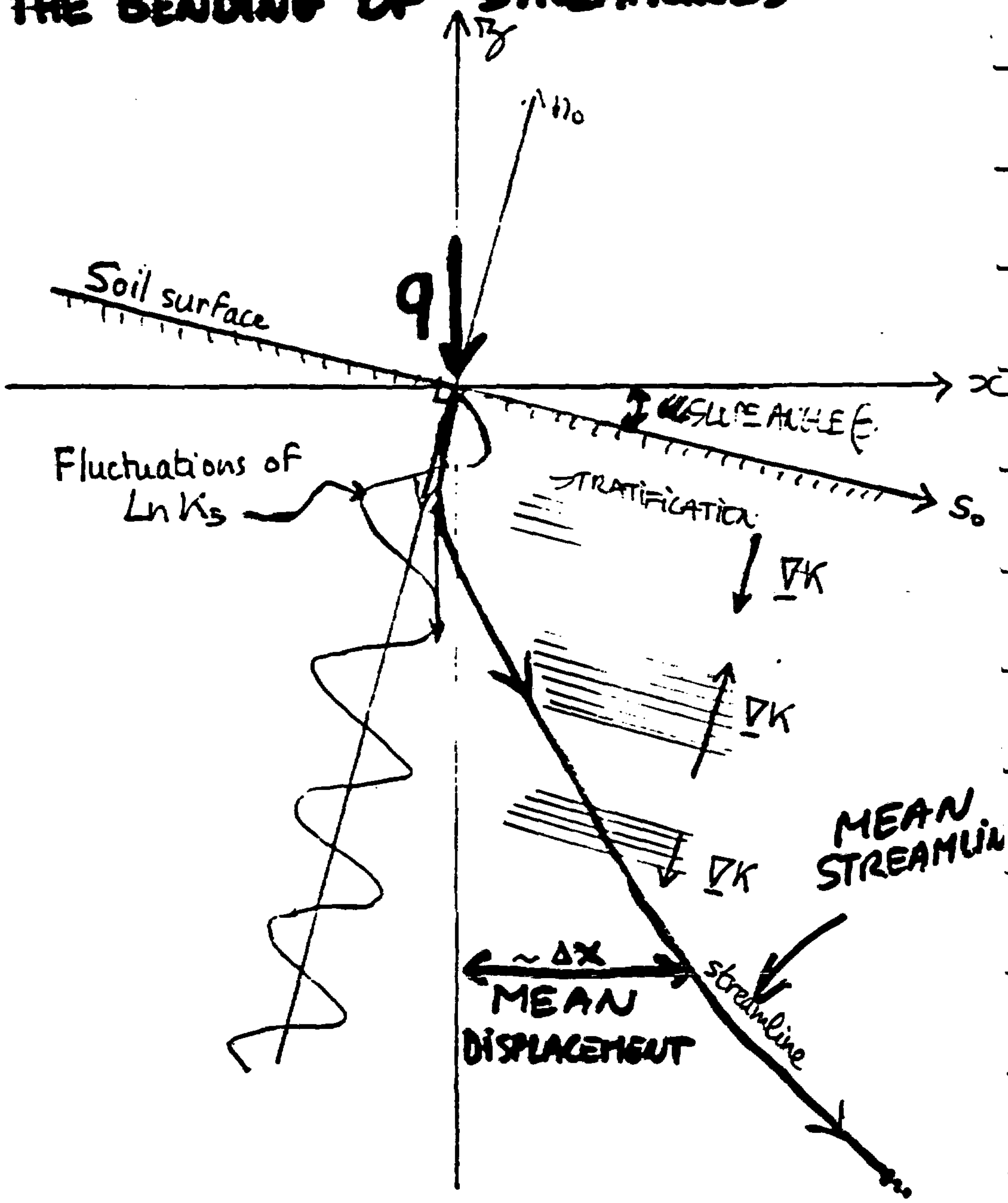


Figure 7.25 Pressure head profile in the vertical direction for the steady state "rainfall" infiltration simulation. The transect is located near the geometric center of the domain (X = 0, Y = 7.4m).

TILTED STRATIFICATION: THE BENDING OF STREAMLINES

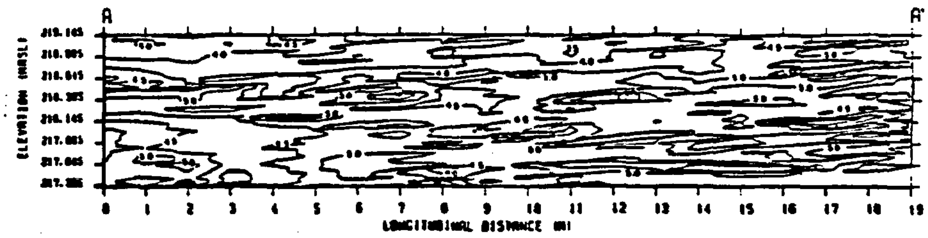
FIGURE 5



IV

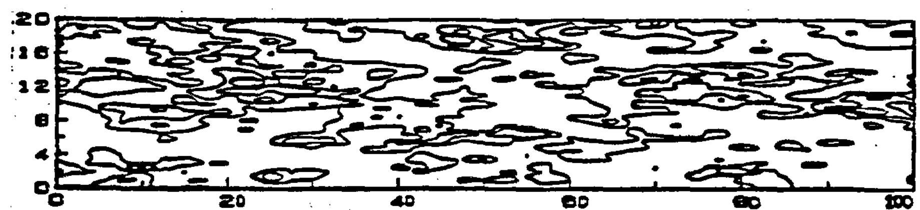
VERTICAL SECTIONS OF
3D LOG-CONDUCTIVITY CONTOURS IN STATISTICALLY ANISOTROPIC FORMATIONS

(b): LnK contours below K_G ($\ln K_G = 0$) in the vertical plane (x_1, x_3); ANISOTROPY RATIO $\lambda_3/\lambda_1 = 1/5$.



Location of measurements and distribution of -ln(K) along A-A' (contour interval = 0.5; vertical exaggeration = 2; K < 10^{-3} cm/s in stippled zones).

(a): Measured

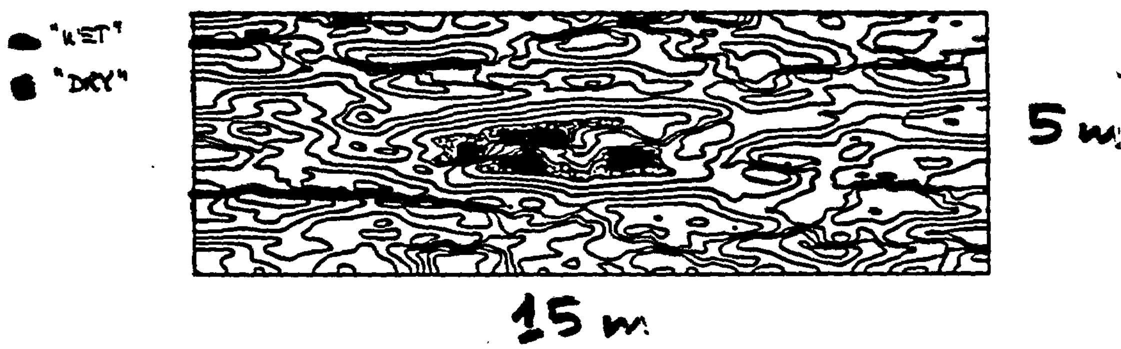


(b): Simulated by the Turning Band Method

Figure 2: Log-conductivity contours in a vertical plane. The upper part is reproduced from Sudicky, 1985 (measured at the Borden tracer site). The lower part of the figure was obtained by simulation, using the Turning Band Method with an anisotropic spectrum.

SUCTION HEAD IN 3D RANDOM SOIL WITH HORIZONTAL "STRATIFICATION"

VERTICAL SLICE



$\ln K_s(z)$, $\ln \alpha(z)$ RANDOM FIELDS $\Rightarrow$ $\boxed{K(\psi, z) = K_s(z) \ldots \alpha(z) \cdot \psi)}$ CONDUCTIVITY CURVE IS DIFFERENT AT EACH GRID POINT $\Rightarrow$ i.e.: THE MODEL INCLUDES 300,000 KC CURVES... BUT FEW PARAMETERS.

Figure 7.23 Pressure head contour lines in a vertical slice for the steady state "rainfall" infiltration in a statistically anisotropic soil (300,000 nodes). The slice approximately crosses the geometric center of the domain (Y = 7.4m).

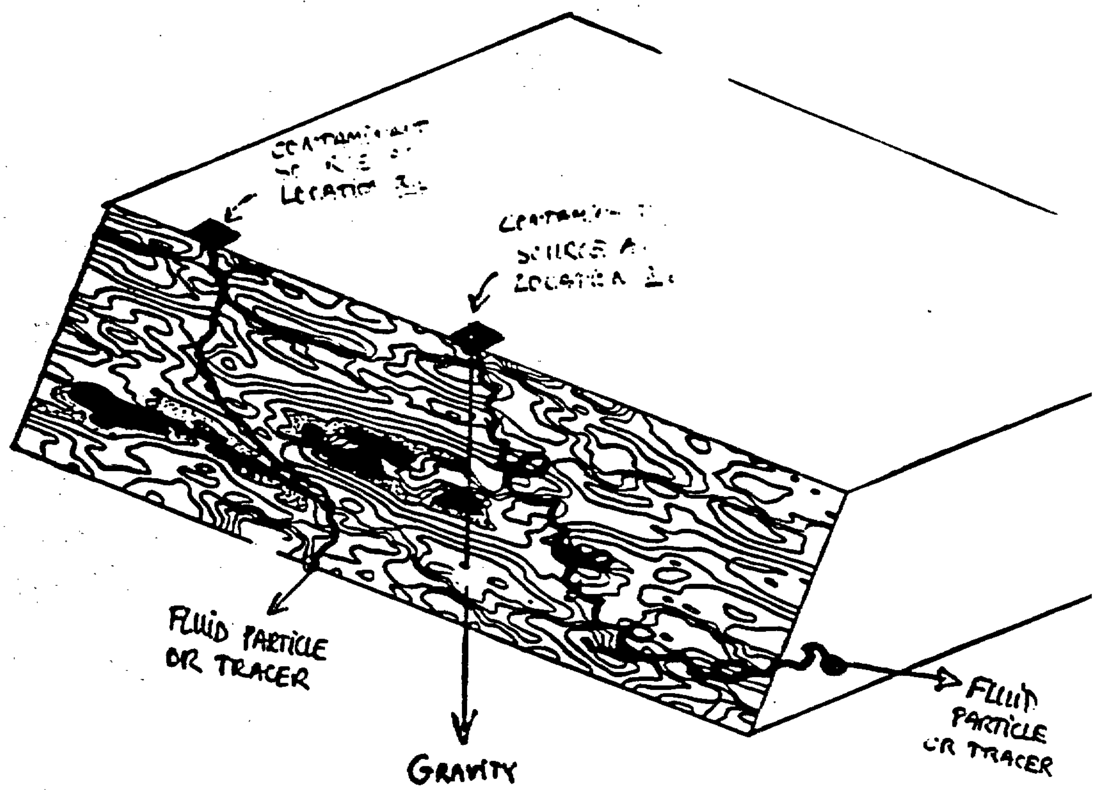
MEAN FLUX: $\bar{q} \simeq 213$ mm/year $\simeq 8.5$ inch/year

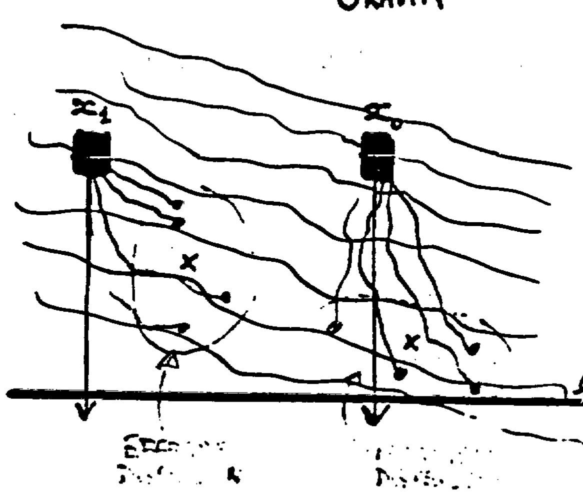
SUCTION FLUCTUATIONS: $\sigma_\psi \simeq 20$ cm (observed)

MEAN SUCTION: $\bar{\psi} \simeq 150$ cm

VI

3D RANDOM SOIL WITH TILTED STRATA: FLUID PATHWAYS AND CONTAMINANT MIGRATION

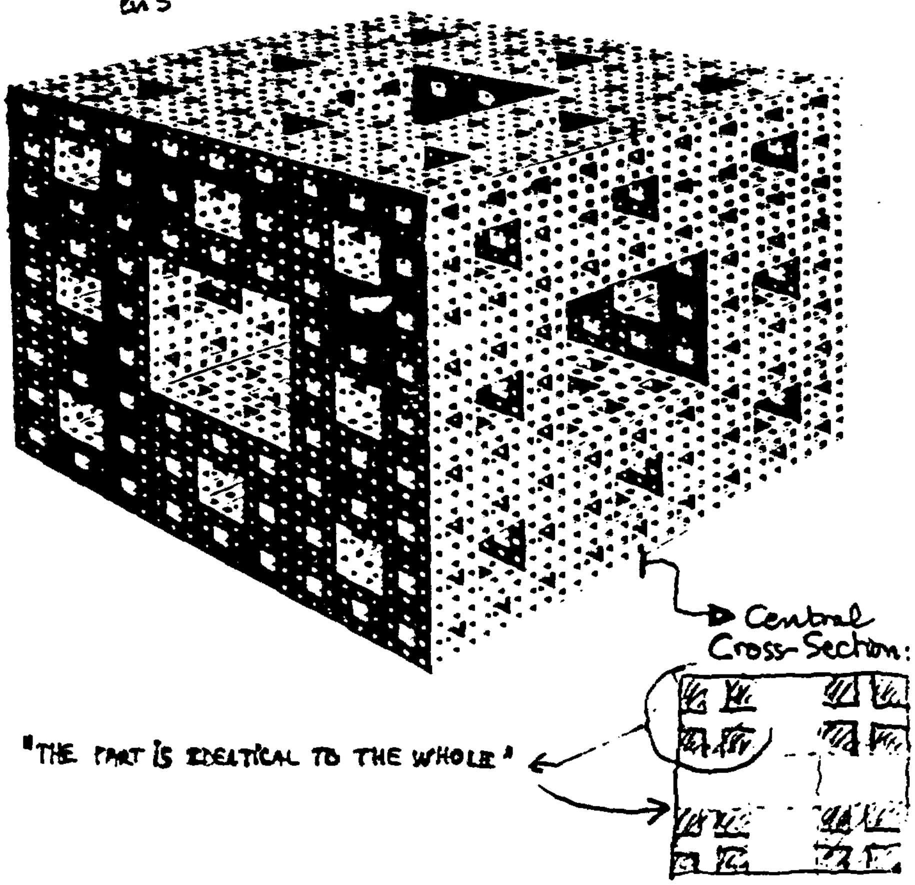




MEAN DISPLACEMENT AS WELL AS DISPERSION REQUIRES MULTIPLE SIMULATIONS.

EXAMPLE OF A DETERMINISTIC FRACTAL SET:
THE MENGER SPONGE
(from B. Mandelbrot, 1983).

Fractal Dimension of "pores":
$D_F = \frac{\ln 7}{\ln 3}$



VIII

SCALE ISSUES:

ILLUSTRATION OF FINITE SIZE EFFECTS; UNCERTAINTY VERSUS SPATIAL VARIABILITY.

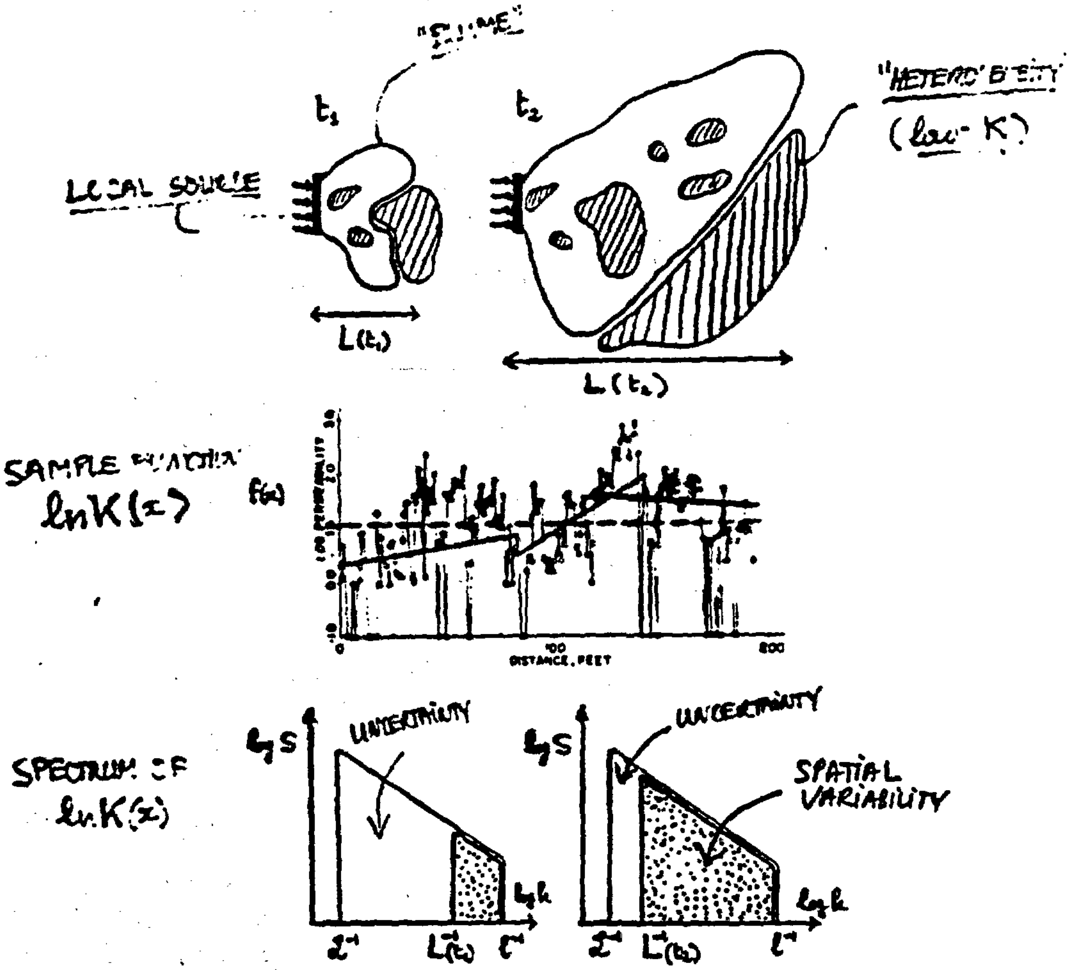
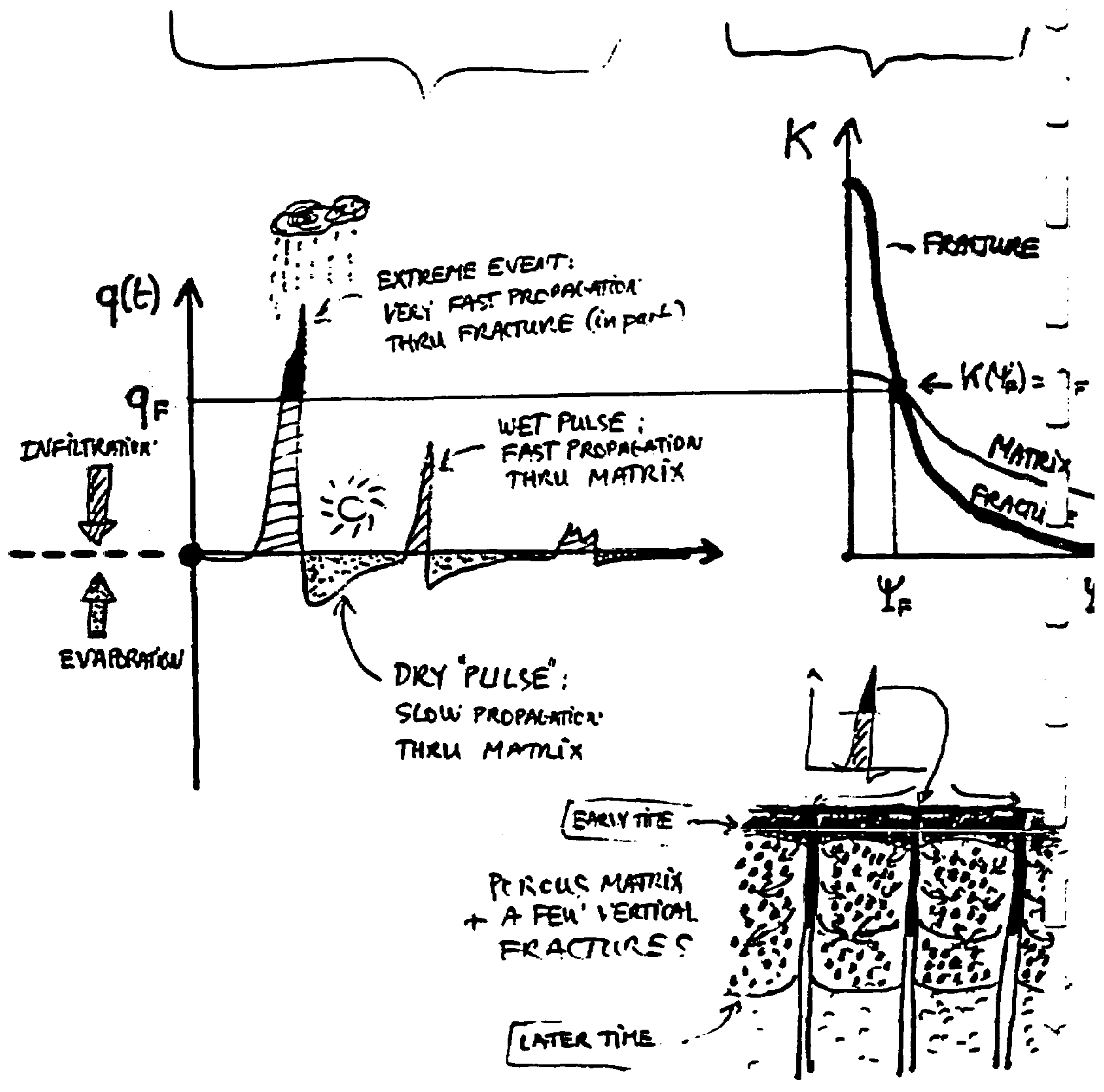


Figure 4.3: Illustration of finite-size effects:
(a) Contamination plume
(b) Log-conductivity field sample function
(c) Band-pass self-similar spectrum

TRANSIENT EFFECTS;
A MORE REALISTIC PICTURE (?)

ERRATIC RAINFALL EVENTS + FRACTURED MATRIX

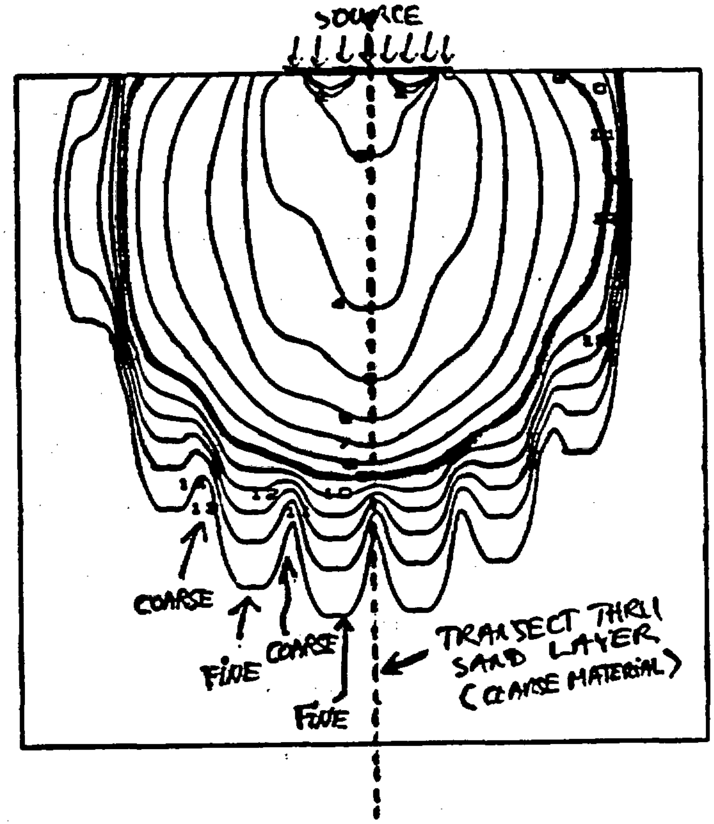


X

2D STRIP-SOURCE INFILTRATION IN MULTILAYER SAND/SILT SYSTEM WITH

473

VERTICAL LAYERS :



NOTE: THE RED CONTOUR IS SUCH THAT $K(h)_{SAND} \approx K(h)_{SILT}$

Figure 5.26 Vertically layered sand/silt soil system (strip source infiltration-time = 1day).

REMARKS: • VERTICAL LAYERS WERE ARRANGED IN SUCH A WAY THAT SYMMETRY IS BROK

• THE **RED** PRESSURE CONTOUR IS SMOOTHEST, AND SEPARATES THE WET ZONE IN TWO REGIONS :
$K_{sand} > K_{silt}$ INSIDE, but $K_{sand} < K_{silt}$ OUTSIDE.

Variably Saturated Fracture Flow Modeling

Using the Boundary Integral Method

Todd C. Rasmussen
Department of Hydrology & Water Resources

The characterization of water flow through variably saturated fractured rock presents unusual challenges to both experimentalists and modelers. The presence of multiple porosities with different geometric properties results in flow equations which differ in both dimensionality and parametric representation. Also, at low matric suctions the presence of air-water interfaces yields uncertain saturation and pressure head distributions within fractures.

To examine and understand some of the hydraulic properties of variably saturated fractured rock, a series of simulation experiments have been performed using the boundary integral method. Laboratory experiments have been conducted using parallel glass plates (Hele-Shaw Model), as well as a porous rock with an embedded fracture. The challenge addressed in this study is the reproduction of observed hydraulic behavior using a numerical scheme which incorporates as many of the physical processes as are needed to accurately describe the observed hydraulic behavior.

The boundary integral method takes advantage of Gauss' theorem to reduce by one the dimensionality of a steady homogeneous boundary value problem. For example, a two-dimensional flow field can be solved by discretizing the one-dimensional boundary around the flow domain. For fractured rock, fracture flow occurs within a two-dimensional flow domain embedded within a three-dimensional rock matrix flow domain. This problem can be reduced to a two-dimensional boundary around the rock matrix with an embedded one-dimensional fracture flow domain.

The effect of variable saturation within a fracture is modeled by defining a discrete air-water interface. The interface is a one-dimensional boundary which replaces the original fracture boundary. The position of the interface is determined by recursively approaching a position where the pressure head along the interface is equal to the capillary head. To aid the positioning process, each node along the interface is required to maintain the same total head from one iteration to the next. Also, a Newton-Raphson iteration scheme is used to more rapidly converge to the correct position.

Once the flow domain has been defined, the position of streamlines within the flow domain are determined by using the Cauchy-Riemann conditions. Travel times and breakthrough curves can then be generated by summing the integrated inverse velocity along a streamline over all streamlines.

Simulated flow and breakthrough curves in response to a step injection of solute are obtained for saturated, variably saturated, and unsaturated fractures. Three zones are found in a variably saturated fracture corresponding to non-wetted regions, regions wetted under suction, and regions wetted under pressure.

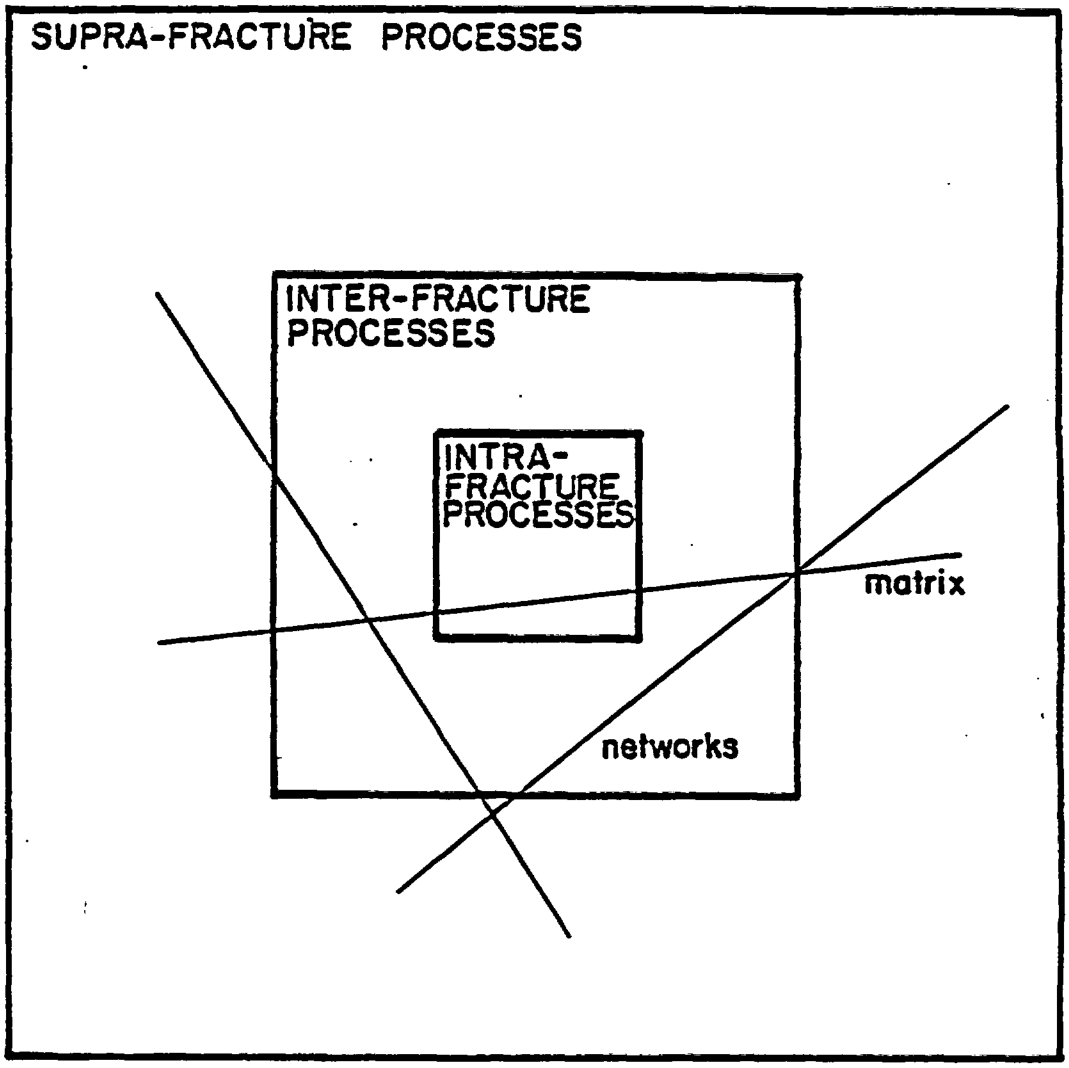


Figure 1 Nesting of fluid flow and solute transport processes in fractured rock.

From: Rasmussen, T.C. and D.D. Evans, 1988, Fluid Flow and Solute Transport Modeling Through Three-Dimensional Networks of Variably Saturated Discrete Fractures, NUREG/CR-5239.

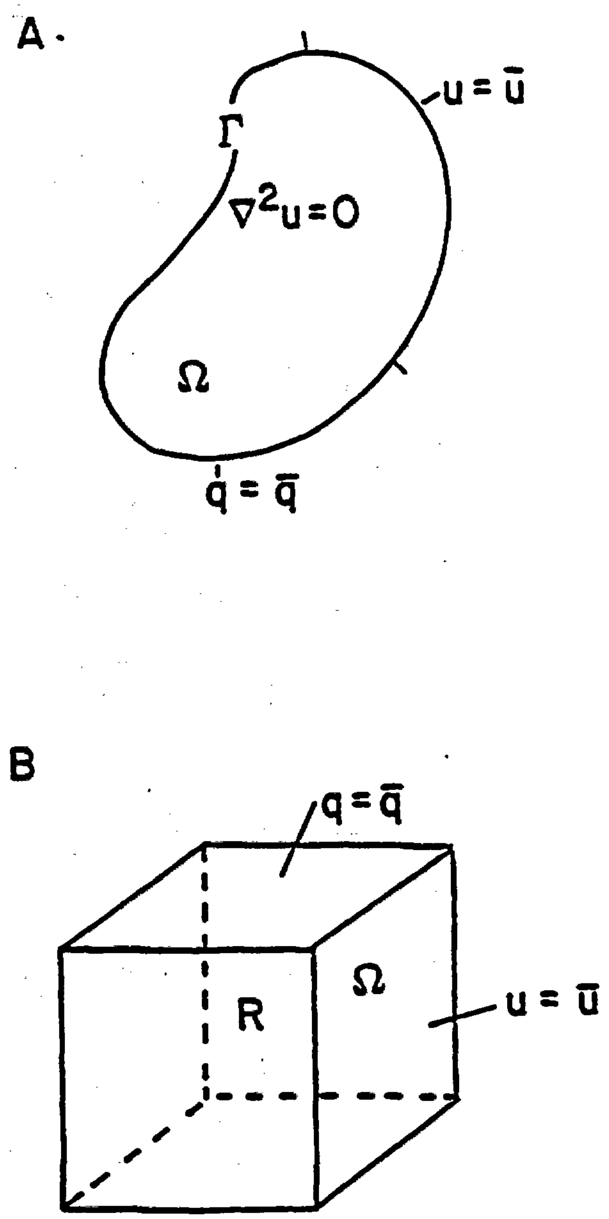


Figure 2   Flow domain and boundary conditions for two dimensional (A) and three dimensional (B) porous media. Symbols are defined in text.

From: Rasmussen, T.C. and D.D. Evans, 1988, Fluid Flow and Solute Transport Modeling Through Three-Dimensional Networks of Variably Saturated Discrete Fractures, NUREG/CR-5239.

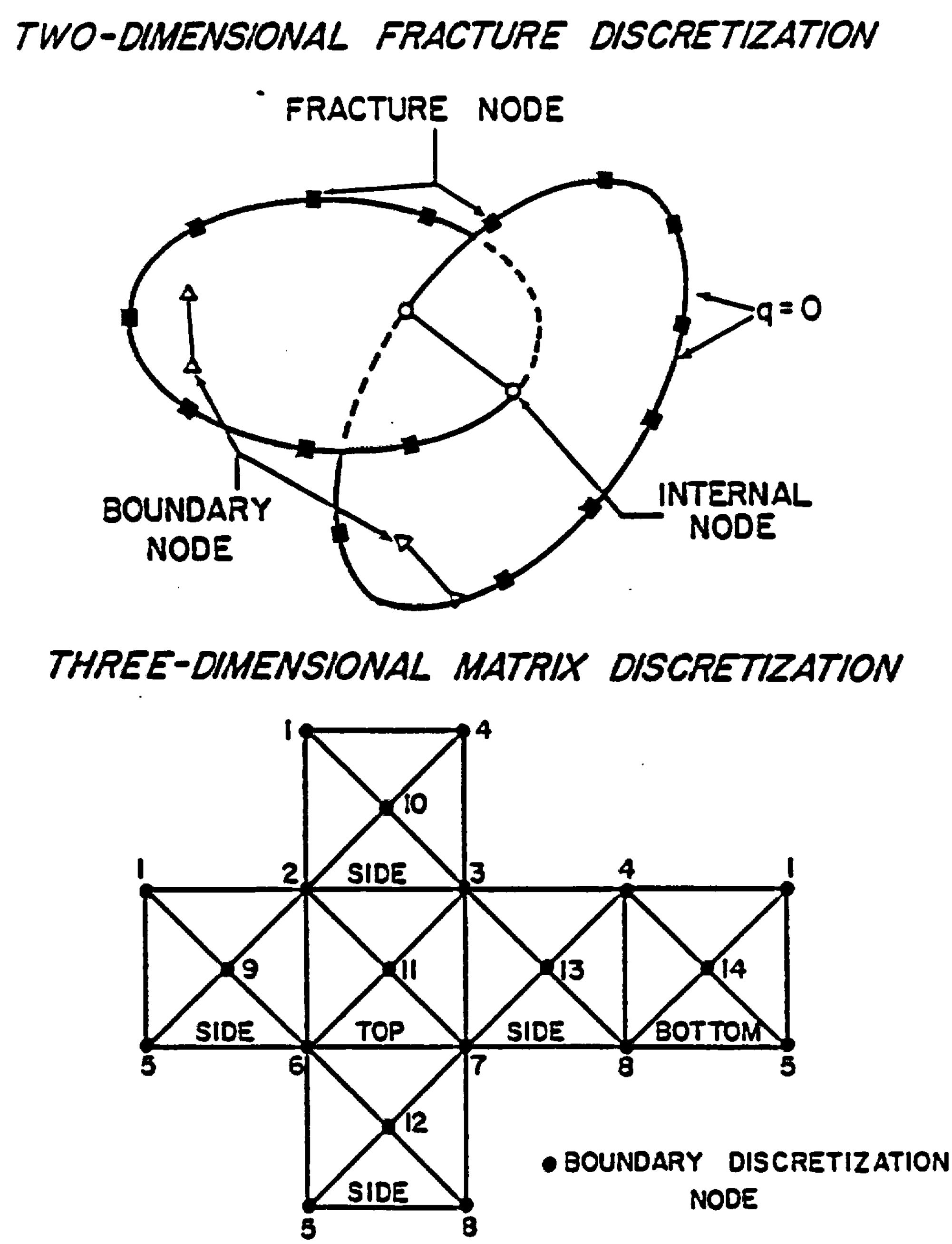


Figure 3 Boundary discretization schemes for two dimensional planar fractures (A) and three dimensional rock matrix (B).

From: Rasmussen, T.C. and D.D. Evans, 1988, Fluid Flow and Solute Transport Modeling Through Three-Dimensional Networks of Variably Saturated Discrete Fractures, NUREG/CR-5239.

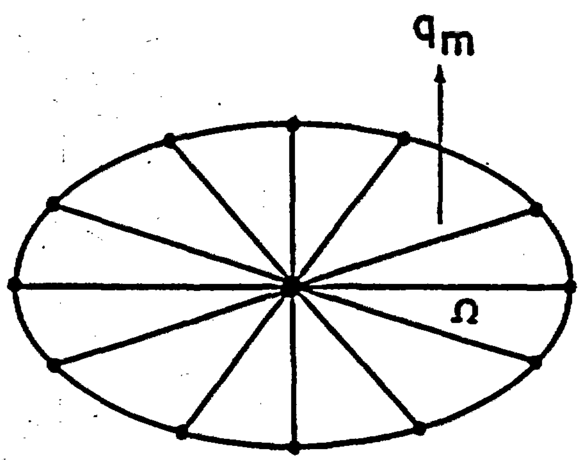
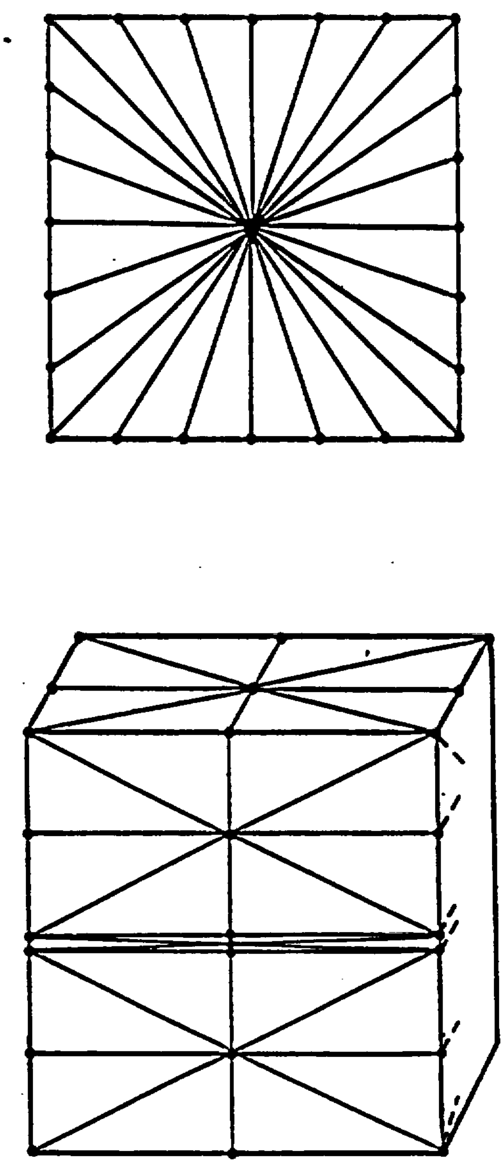


Figure 4 Fracture surface discretization geometry showing net flux term, q_m, representing flow between the fracture and the matrix.

From: Rasmussen, T.C. and D.D. Evans, 1988, Fluid Flow and Solute Transport Modeling Through Three-Dimensional Networks of Variably Saturated Discrete Fractures, NUREG/CR-5239.

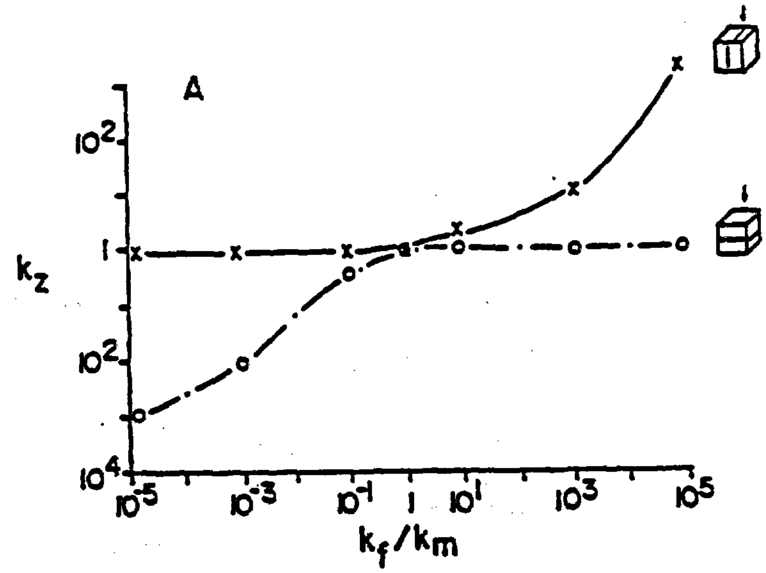
A



B

Figure 5 Three dimensional flow geometry showing fracture (A) and matrix (B) boundary surface discretization strategies.

From: Rasmussen, T.C. and D.D. Evans, 1988, Fluid Flow and Solute Transport Modeling Through Three-Dimensional Networks of Variably Saturated Discrete Fractures, NUREG/CR-5239.



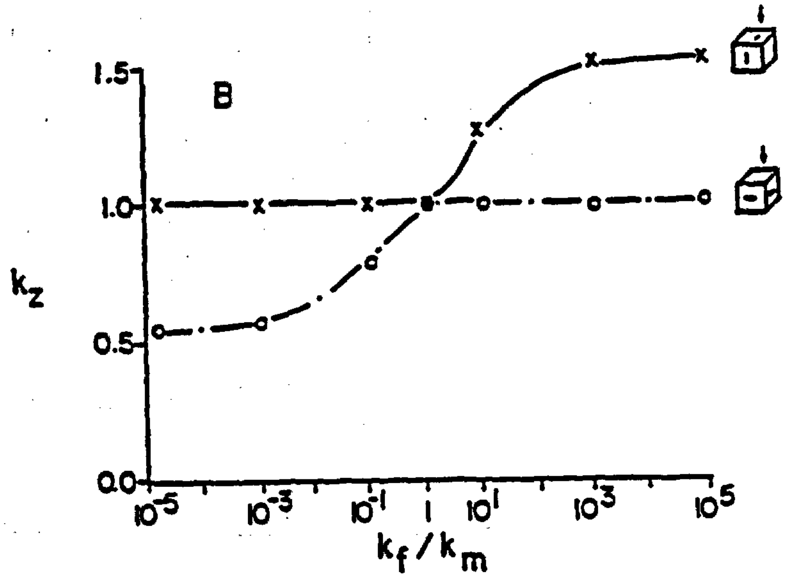


Figure 6 **Results of simulations performed using the three dimensional flow geometry for fractures fully (A) and partially (B) dividing the flow domain.**

From: Rasmussen, T.C. and D.D. Evans, 1988, Fluid Flow and Solute Transport Modeling Through Three-Dimensional Networks of Variably Saturated Discrete Fractures, NUREG/CR-5239.

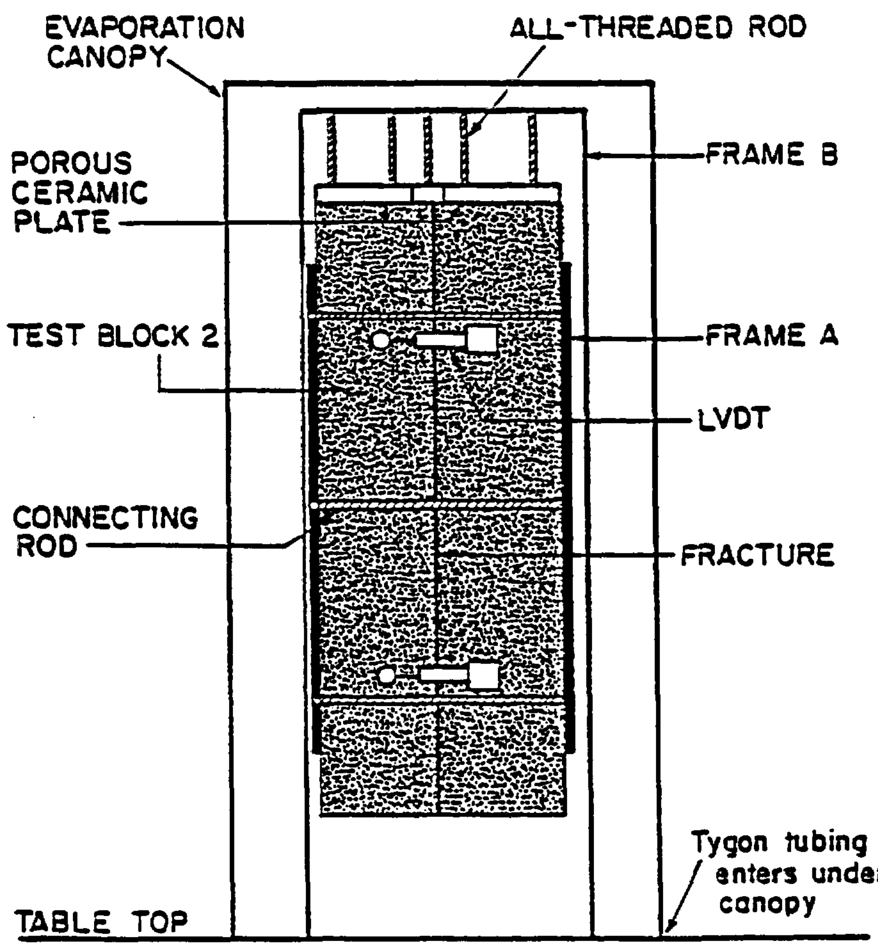


Figure 7 Test block number 2 experimental setup. Frame A is held by hooks from frame B.

From: Haldeman, William R., 1988, Water Flow Through Variably Saturated Fractured Tuff: A Laboratory Study, Unpublished M.S. Thesis, Department of Hydrology and Water Resources, 219 pp.

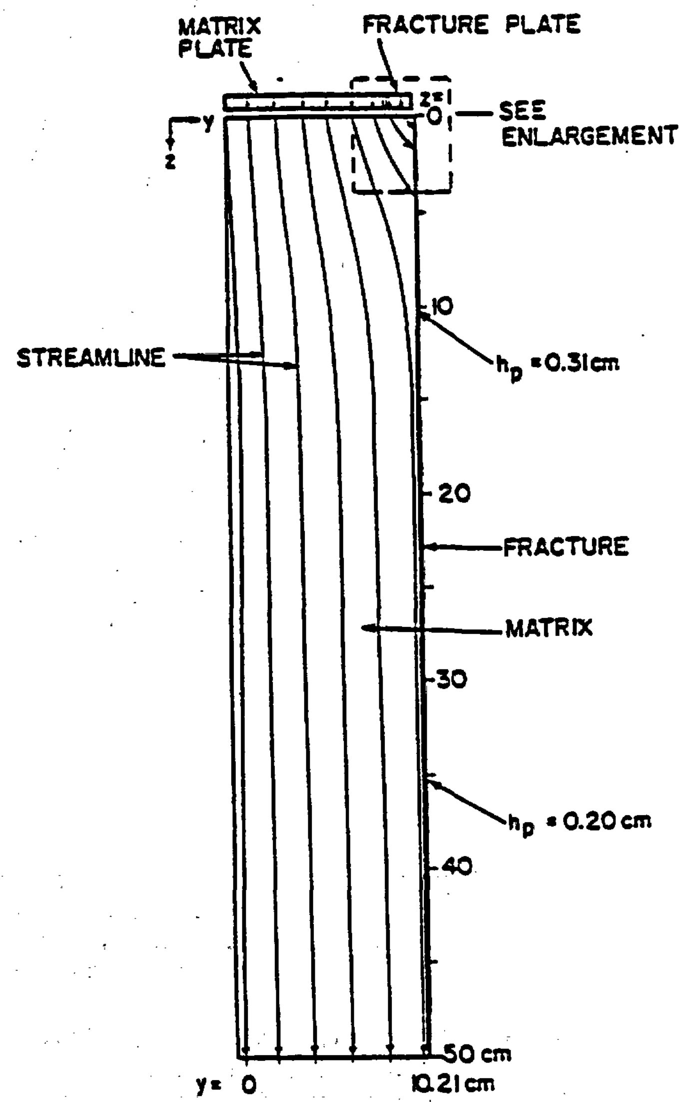


Figure 8 Simulated results for test block number 1 showing streamlines and pressure head at the sampling ports.

From: Haldeman, William R., 1988, Water Flow Through Variably Saturated Fractured Tuff: A Laboratory Study, Unpublished M.S. Thesis, Department of Hydrology and Water Resources, 219 pp.

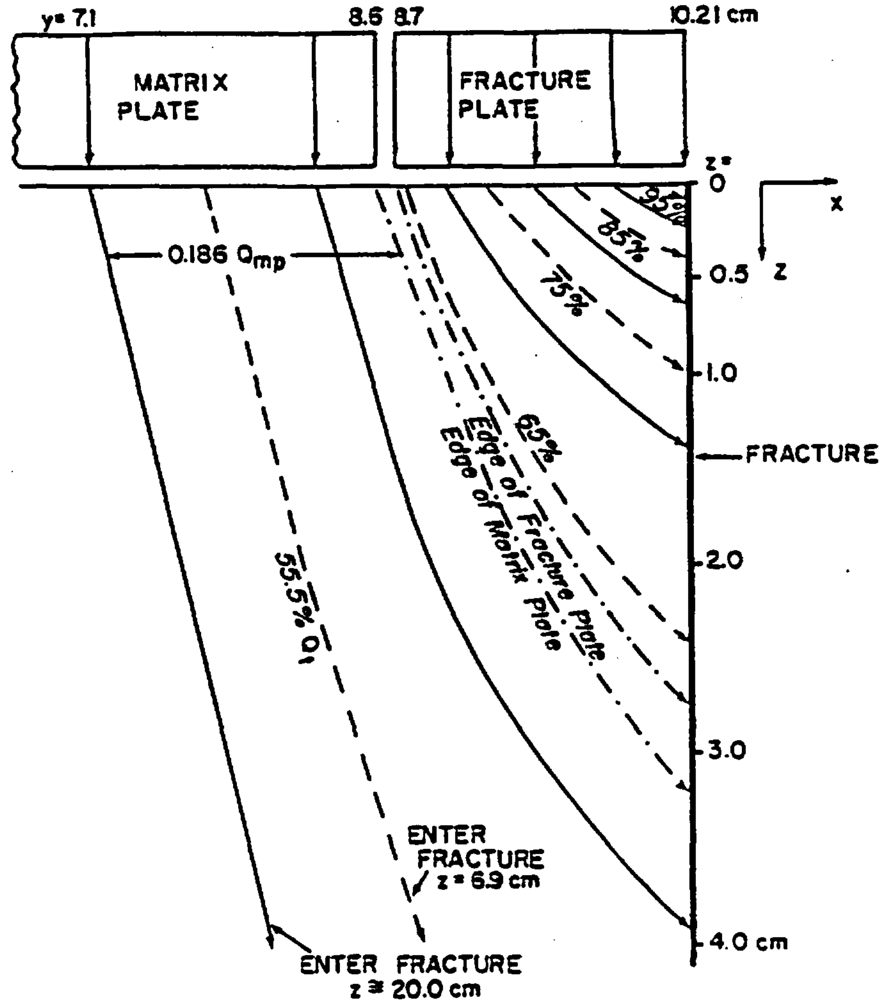


Figure 9 Enlargement of Figure 5.10 showing the fracture-plate-matrix intersection. Streamlines of Figure 5.10 are shown as solid lines and other streamlines of interest are dashed.

From: Haldeman, William R., 1988, Water Flow Through Variably Saturated Fractured Tuff: A Laboratory Study, Unpublished M.S. Thesis, Department of Hydrology and Water Resources, 219 pp.

Table 1 Saturated Matrix Conductivity and Fracture Transmissivity Test Block Number 1

	Matrix K (m/s)	Fracture T(1) (m^2/s)	Fracture T(2) (m^2/s)
median	6.19×10^{-8}	7.47×10^{-9}	5.38×10^{-9}
mean	5.91×10^{-8}	7.16×10^{-9}	5.12×10^{-9}
std. dev.	2.29×10^{-8}	1.68×10^{-9}	1.54×10^{-9}
coef. var.	0.387	0.235	0.301
high	1.33×10^{-7}	1.07×10^{-8}	8.64×10^{-9}
low	2.85×10^{-8}	3.52×10^{-9}	2.11×10^{-9}

From: Haldeman, William R., 1988, Water Flow Through Variably Saturated Fractured Tuff: A Laboratory Study, Unpublished M.S. Thesis, Department of Hydrology and Water Resources, 219 pp.

Table 2 A comparison of flow and pressure head data obtained from using the computer model, and those measured or calculated from experimental data(1).

	Model	Experimental
Matrix Plate Flow, $Q_{mp} \times 10^9$ (m^2/s)	6.33	6.65
Fracture Plate Flow, $Q_{fp} \times 10^9$ (m^2/s)	3.77	3.15(2)
Flow Exiting Fracture, $Q_f \times 10^9$ (m^2/s)	5.06	NDM(3)
Flow Exiting Matrix, $Q_m \times 10^9$ (m^2/s)	5.15	NDM
Pressure Head under Matrix Plate, h_{mp} (cm)	+2.6 to +3.7 (mean = +3.2)	-3.9 to +5.9(4)
Pressure Head under Fracture Plate, h_{fp} (cm)	-1.7 to +3.2(5) (mean = +0.1)	-12.6 to +7.4(4)
Pressure Head in Fracture (cm)		
at z = 10 cm	+0.3	-1.8 to -5.6
at z = 35 cm	+0.2	-3.1 to -8.4
Pressure Head in Matrix (cm)		
at x = 4 cm and z = 5 cm	+1.7	-0.4 to +1.0
at x = 4 cm and z = 30 cm	+0.3	+0.6 to +1.9

(1) Experimental data are from Haldeman (1988).
(2) Fracture plate flow is half the actual observed because the model divides the test block into two identical halves with the fracture as the plane of symmetry.
(3) NDM - not directly measured.
(4) Pressure head calculated using equation 3.2.
(5) The pressure head directly over the fracture opening is -1.7 cm (suction of 1.7 cm).

From: Chuang, Yueh, 1988, Solute Transport Measurement by Ion-Selective Electrodes in Fractured Tuff, Unpublished M.S. Thesis, Department of Hydrology and Water Resources, 246 pp.

Table 3 Case study of idealized test block system: a comparison of computer model input parameters and experimental data[1].

Input Parameters	Model	Experimental
Average Matrix Hydraulic Conductivity, $K_m \times 10^9$ (m/s)	50	59.1
Average Fracture Transmissivity, $T_f \times 10^9$ (m^2/s)	5	7.16[2] 5.12[3]
Fracture Half-Aperture, e_b (µm)	100	NA[4]
Average Matrix Plate Conductivity, $K_{mp} \times 10^9$ (m/s)	2	1.80
Applied Head above Matrix Plate, H_{mp} (cm)	28.3	27.2 to 30.0[5]
Average Fracture Plate Conductivity, K_{fp} (m/s)	5	3.77
Applied Head above Fracture Plate, H_{fp} (cm)	36.3	35.5 to 36.8[5]

(1) Experimental data are from Haldeman (1988).
(2) Transmissivity is calculated assuming all the flow from fracture plate and no flow from the matrix plate enter the fracture; mean = 7.16×10^{-9} m^2/s and Std = 1.68×10^{-9} m^2/s (Haldeman, 1988).
(3) Transmissivity is calculated assuming flow from fracture plate is split between fracture and rock matrix; mean = 5.12×10^{-9} m^2/s and Std = 1.54×10^{-9} m^2/s (Haldeman, 1988). Proportion of flow in matrix is calculated using an average K_m, and subtracted from the total flow to determine T_f.
(4) NA - Not applicable.
(5) Period monitored is between 6-13-88 and 8-3-88.

From: Chuang, Yueh, 1988, Solute Transport Measurement by Ion-Selective Electrodes in Fractured Tuff, Unpublished M.S. Thesis, Department of Hydrology and Water Resources, 246 pp.

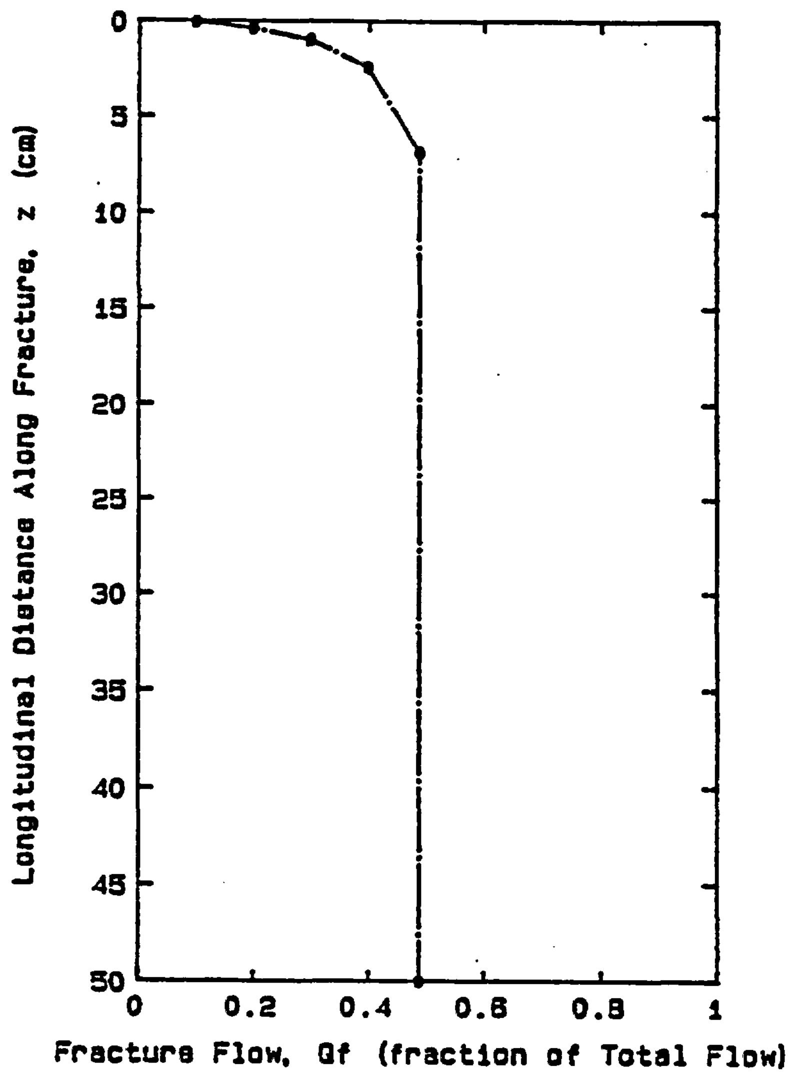


Figure 10 Profile of fracture flow, Q_f (fraction of total flow), as a function of longitudinal distance along fracture, z (cm).

From: Chuang, Yueh, 1988, Solute Transport Measurement by Ion-Selective Electrodes in Fractured Tuff, Unpublished M.S. Thesis, Department of Hydrology and Water Resources, 246 pp.

Table 4 Travel time calculations of selected streamlines contributing to fracture flow.

Stream Tube No.	Streamline[1] (Percent Q_t)	Streamline[1] z (cm)	Travel Distance Δz (cm)	Average Head Change ΔH (cm)	Average[2] Travel Velocity $u_t \times 10^7$ (m/s)	Travel[3] Time t_t (hr)
	100	0.00	0.00	0.0	NA[4]	0.000
1	95	0.085	0.22	2.0	25.7	0.238
	90	0.22	0.44	2.9	18.6	0.657
2	85	0.40	0.70	3.7	14.9	1.302
	80	0.64	0.99	4.4	12.6	2.183
3	75	0.99	1.41	5.0	10.0	3.910
	70	1.40	1.86	5.5	8.35	6.188
4	65	2.44	2.83	6.2	6.19	12.70
	60	3.94	4.36	6.9	4.47	27.09
5	55.5	6.90	7.34	9.6	3.93	51.88
	51	20.0	20.2	52.4	7.31	76.88

(1) The average streamline of each stream tube is chosen to represent the properties of the stream tube, e.g., travel time and concentration of 95-percent streamline represents those of stream tube no. 1 bounded by 90- and 100-percent streamlines.
(2) Average travel velocity, $u_t = (K_m/n_e)(\Delta H/\Delta z)$.
(3) Travel time, $t_t = \Delta z/u_t$.
(4) NA - Not applicable.

From: Chuang, Yueh, 1988, Solute Transport Measurement by Ion-Selective Electrodes in Fractured Tuff, Unpublished M.S. Thesis, Department of Hydrology and Water Resources, 246 pp.

Table 5 Relative concentrations in the fracture as functions of time and distance along the fracture.

Elapsed Time, t_E (hr)	Stream[(1)] Tube No.	Stream Tube z (cm)	Concentration, C x $1/C_0$[(2)] instant. increase	Concentration, C x $1/C_0$ plate effect	Relative Conc., C* instant. increase	Relative Conc., C* plate effect
0.238	1	0.11	1.000	0.069	1.000	0.060
	2	0.43	0.010	0.010	0.000	0.000
	3	1.02	0.010	0.010	0.000	0.000
	4	2.67	0.010	0.010	0.000	0.000
	5	11.97	0.010	0.010	0.000	0.000
	-	50.00	0.010	0.010	0.000	0.000
1.302	1	0.11	1.000	0.208	1.000	0.200
	2	0.43	1.000	0.208	1.000	0.200
	3	1.02	0.670	0.142	0.667	0.133
	4	2.67	0.505	0.109	0.500	0.100
	5	11.97	0.431	0.091	0.425	0.082
	-	50.00	0.010	0.010	0.000	0.000
3.910	1	0.11	1.000	1.000	1.000	1.000
	2	0.43	1.000	1.000	1.000	1.000
	3	1.02	1.000	1.000	1.000	1.000
	4	2.67	0.753	0.753	0.750	0.750
	5	11.97	0.616	0.616	0.612	0.612
	-	46.94	0.431	0.431	0.425	0.425
	-	50.00	0.010	0.010	0.000	0.000
12.70	1	0.11	1.000	1.000	1.000	1.000
	2	0.43	1.000	1.000	1.000	1.000
	3	1.02	1.000	1.000	1.000	1.000
	4	2.67	0.943	0.943	0.942	0.942
	5	11.97	0.771	0.771	0.769	0.769
	-	50.00	0.616	0.616	0.612	0.612
$\geq$ 14.81	1	0.11	1.000	1.000	1.000	1.000
	2	0.43	1.000	1.000	1.000	1.000
	3	1.02	1.000	1.000	1.000	1.000
	4	2.67	0.943	0.943	0.942	0.942
	5	11.97	0.771	0.771	0.769	0.769
	-	50.00	0.771	0.771	0.769	0.769

(1) The midpoint of each stream tube along the z-direction is chosen for plotting, which is different from where the average streamline enters the fracture.

(2) Concentrations are measured as fractions of the tracer solution concentration, C_0.

From: Chuang, Yueh, 1988, Solute Transport Measurement by Ion-Selective Electrodes in Fractured Tuff, Unpublished M.S. Thesis, Department of Hydrology and Water Resources, 246 pp.

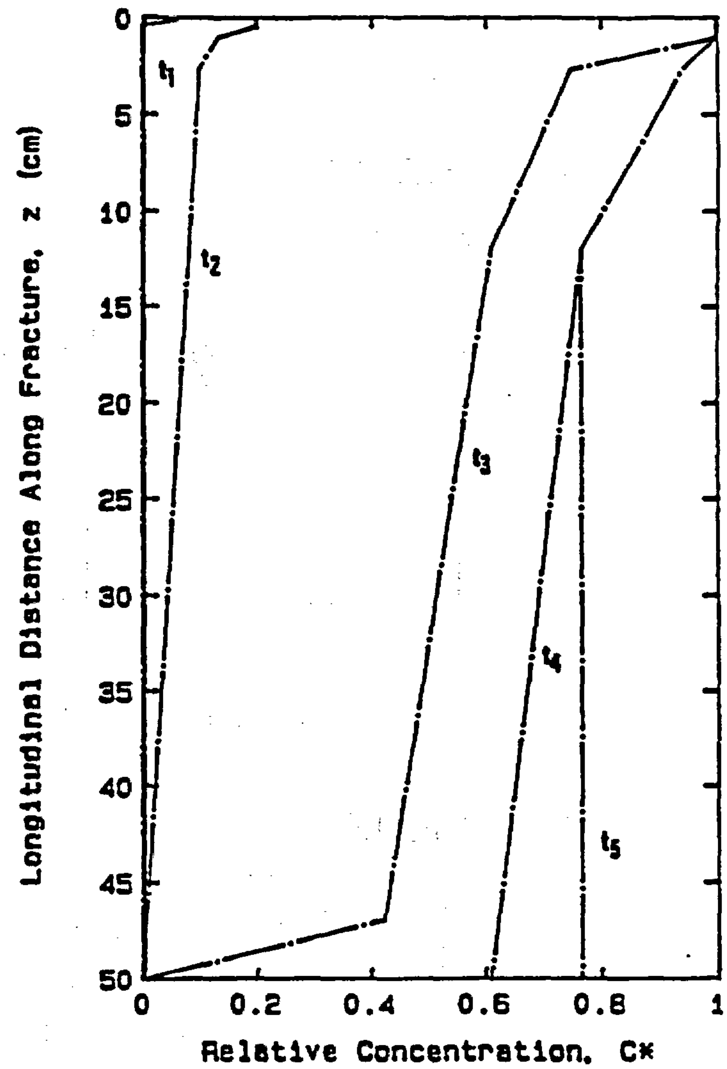


Figure 11 Profile of relative concentration, C^*, as a function of longitudinal distance along the fracture, z (cm), taking into account the chloride breakthrough characteristic of the fracture plate. The time increments are $t_1 = 0.238$ hrs, $t_2 = 1.302$ hrs, $t_3 = 3.910$ hrs, $t_4 = 12.70$ hrs, and $t_5 \geq 14.81$ hrs.

From: Chuang, Yueh, 1988, Solute Transport Measurement by Ion-Selective Electrodes in Fractured Tuff, Unpublished M.S. Thesis, Department of Hydrology and Water Resources, 246 pp.

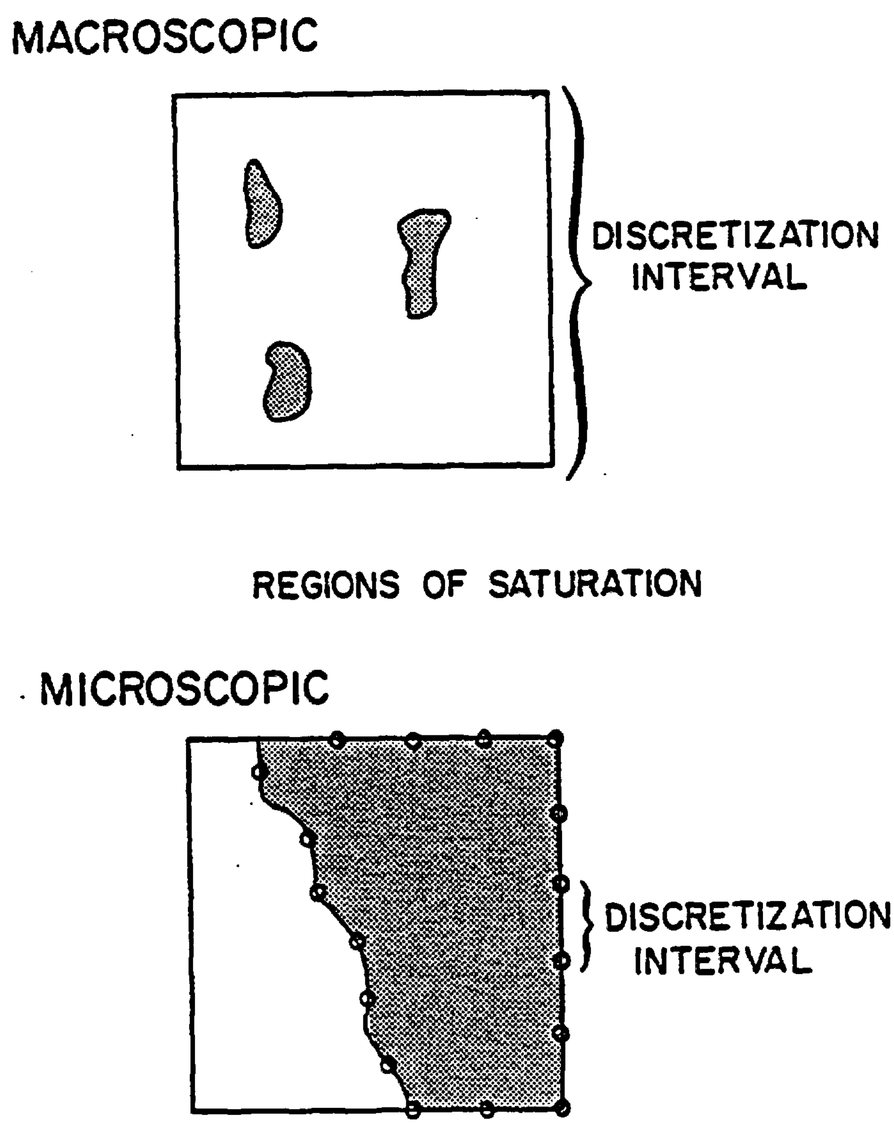


Figure 12. Macroscopic and microscopic formulations of unsaturated flow through fractured rock.

From: Rasmussen, T.C. and D.D. Evans, 1988, Fluid Flow and Solute Transport Modeling Through Three-Dimensional Networks of Variably Saturated Discrete Fractures, NUREG/CR-5239.

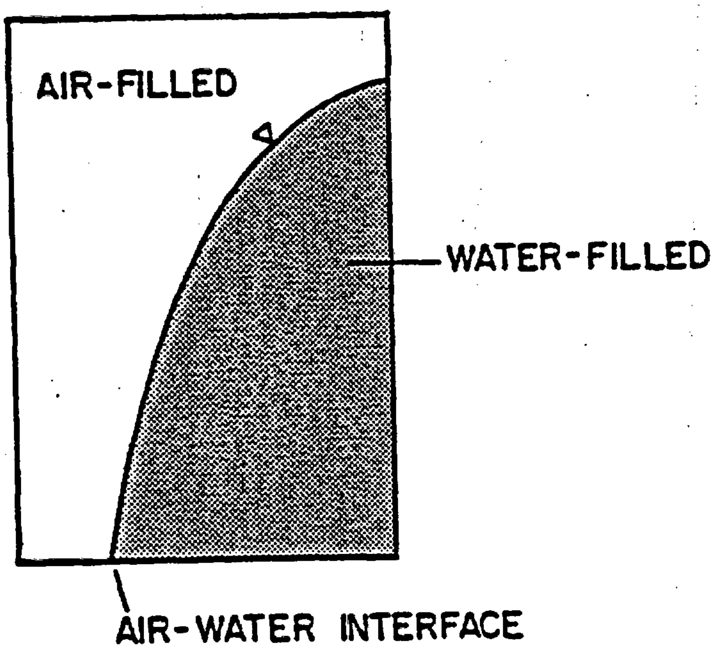


Figure 13 Conceptual model of zone of saturation within an unsaturated fracture.

From: Rasmussen, T.C. and D.D. Evans, 1988, Fluid Flow and Solute Transport Modeling Through Three-Dimensional Networks of Variably Saturated Discrete Fractures, NUREG/CR-5239.

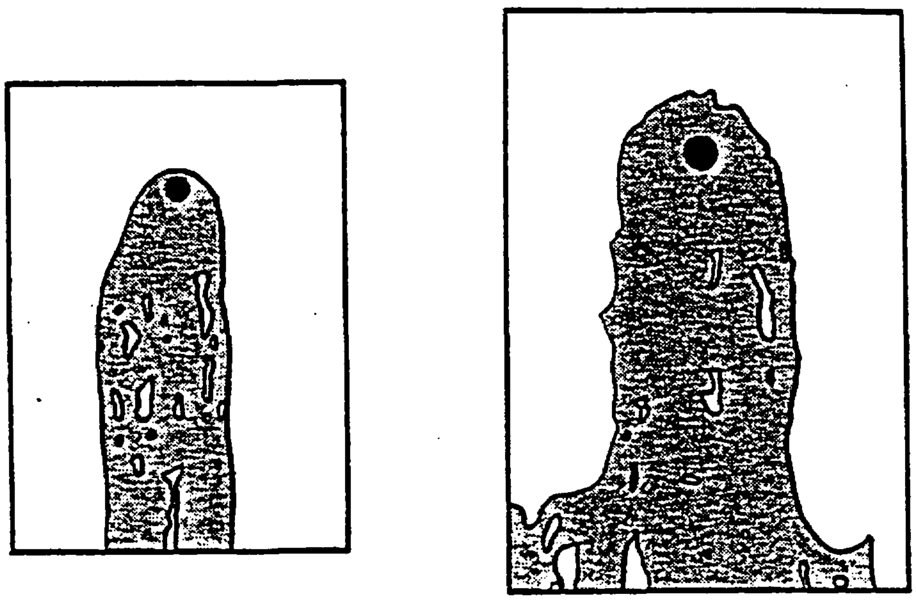


Figure 14 Flow visualization experiment for two input pressure head boundary conditions.

From: Rasmussen, T.C. and D.D. Evans, 1988, Fluid Flow and Solute Transport Modeling Through Three-Dimensional Networks of Variably Saturated Discrete Fractures, NUREG/CR-5239.

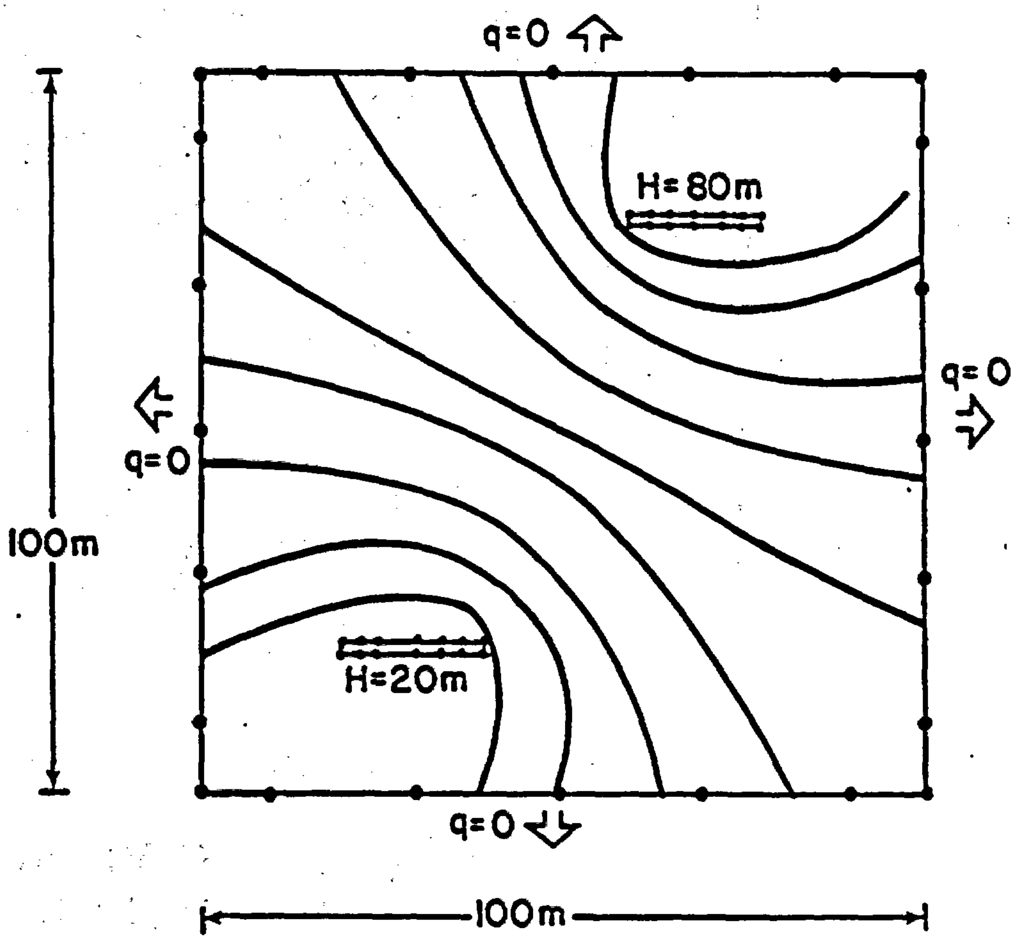


Figure 15 Contours of total head within the plane of a horizontal fracture.

From: Rasmussen, T.C. and D.D. Evans, 1988, Fluid Flow and Solute Transport Modeling Through Three-Dimensional Networks of Variably Saturated Discrete Fractures, NUREG/CR-5239.

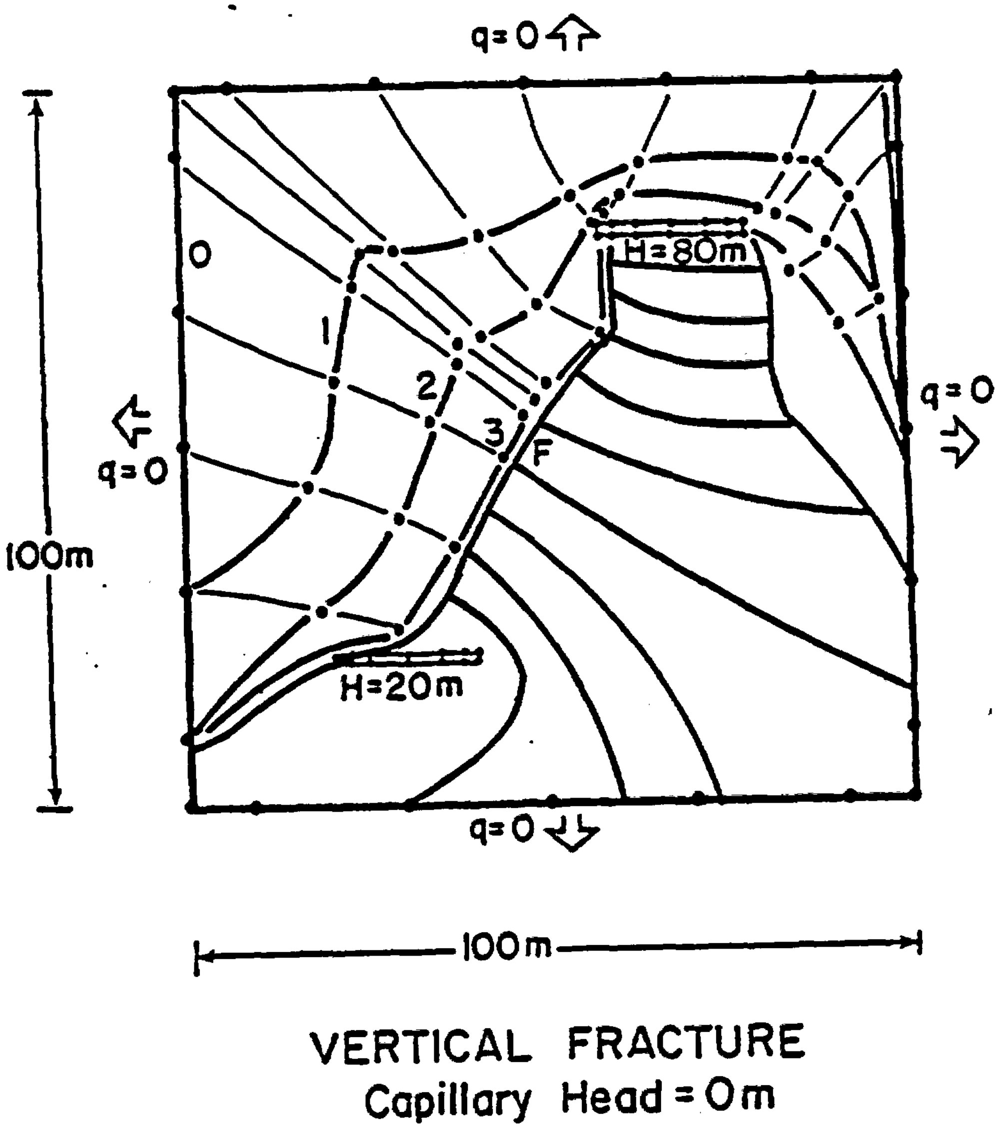


Figure 16 Contours of total head and free surface position after successive iterations and after the final iteration within the plane of a vertical fracture allowing air entry.

From: Rasmussen, T.C. and D.D. Evans, 1988, Fluid Flow and Solute Transport Modeling Through Three-Dimensional Networks of Variably Saturated Discrete Fractures, NUREG/CR-5239.

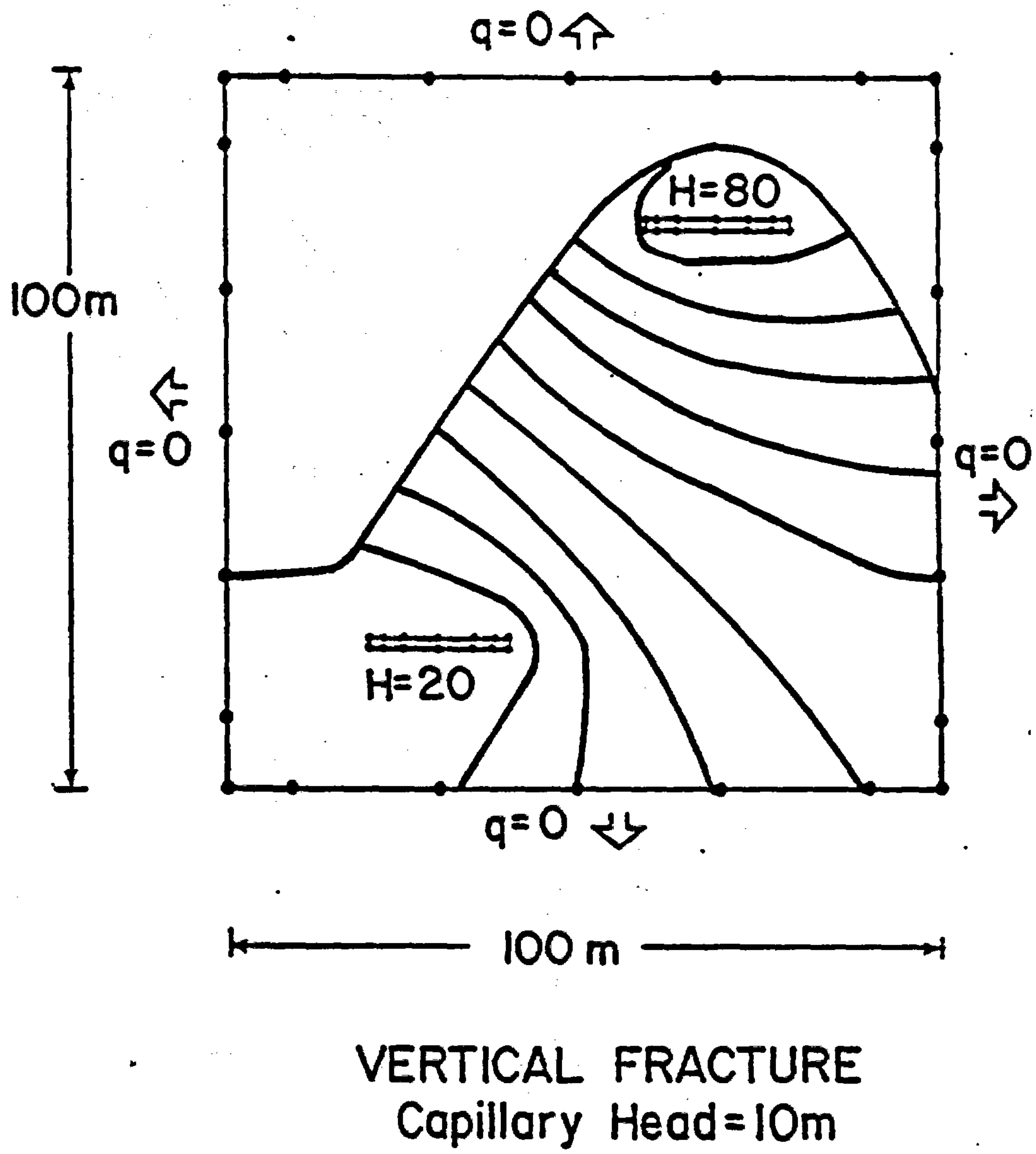


Figure 17 Contours of total head and interface position after the final iteration within the plane of a vertical fracture allowing air entry. A capillary head of 10 m was used.

From: Rasmussen, T.C. and D.D. Evans, 1988, Fluid Flow and Solute Transport Modeling Through Three-Dimensional Networks of Variably Saturated Discrete Fractures, NUREG/CR-5239.

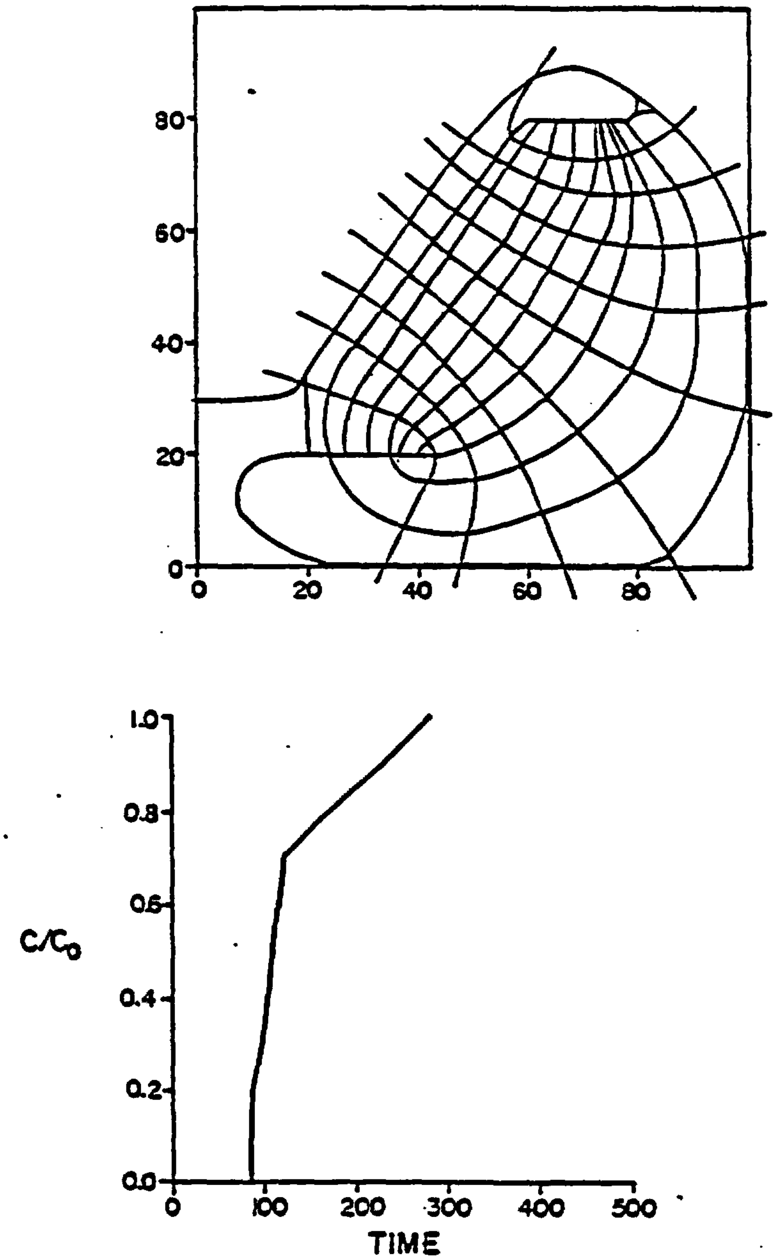


Figure 18 Flow geometry, boundary conditions, calculated total head contours, and calculated stream function contours for a vertical fracture with two intersecting fractures and a capillary head of 10 m (A) and calculated breakthrough curves at the outflow boundary for a step injection at the inflow boundary.

From: Rasmussen, T.C. and D.D. Evans, 1988, Fluid Flow and Solute Transport Modeling Through Three-Dimensional Networks of Variably Saturated Discrete Fractures, NUREG/CR-5239.

LICENSING RESEARCH NEEDS

Dr. Donald L. Chery, Jr., Section Leader

1) Consideration of DOE Research
2) Consideration of CNWRA Recommendations
3) Consideration of NMSS/RES Independent Modeling Endeavors

Licensing Staff Assessment and Determination of Needs (User Need Memo)

Selection of NRC technical work that needs research support is based on:

- o Special technical evaluations needed to support NRC regulations, reg. guides, or technical positions.
- o Poorly understood processes important to repository performance that are anticipated to require independent NRC assessment, or
- o Viability of unconventional methods used by DOE to collect data or develop models.

BROAD AREAS OF LICENSING RESEARCH NEEDS

Waste Form & Package

Repository Design & Rock Mechanics

o Earth Sciences

System Performance

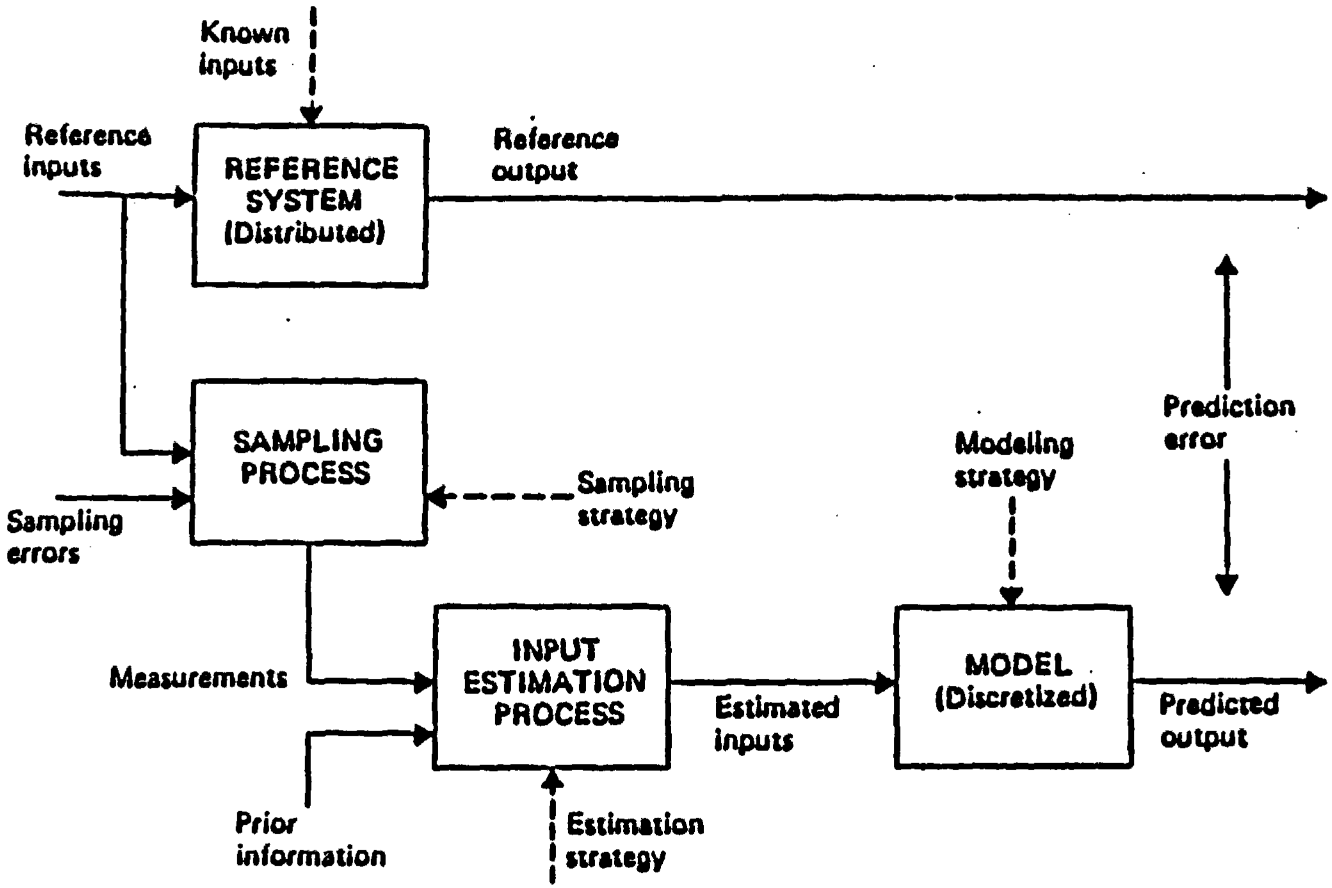
EARTH SCIENCES

Carry-over from Previous User Need Retaining Generic Activities

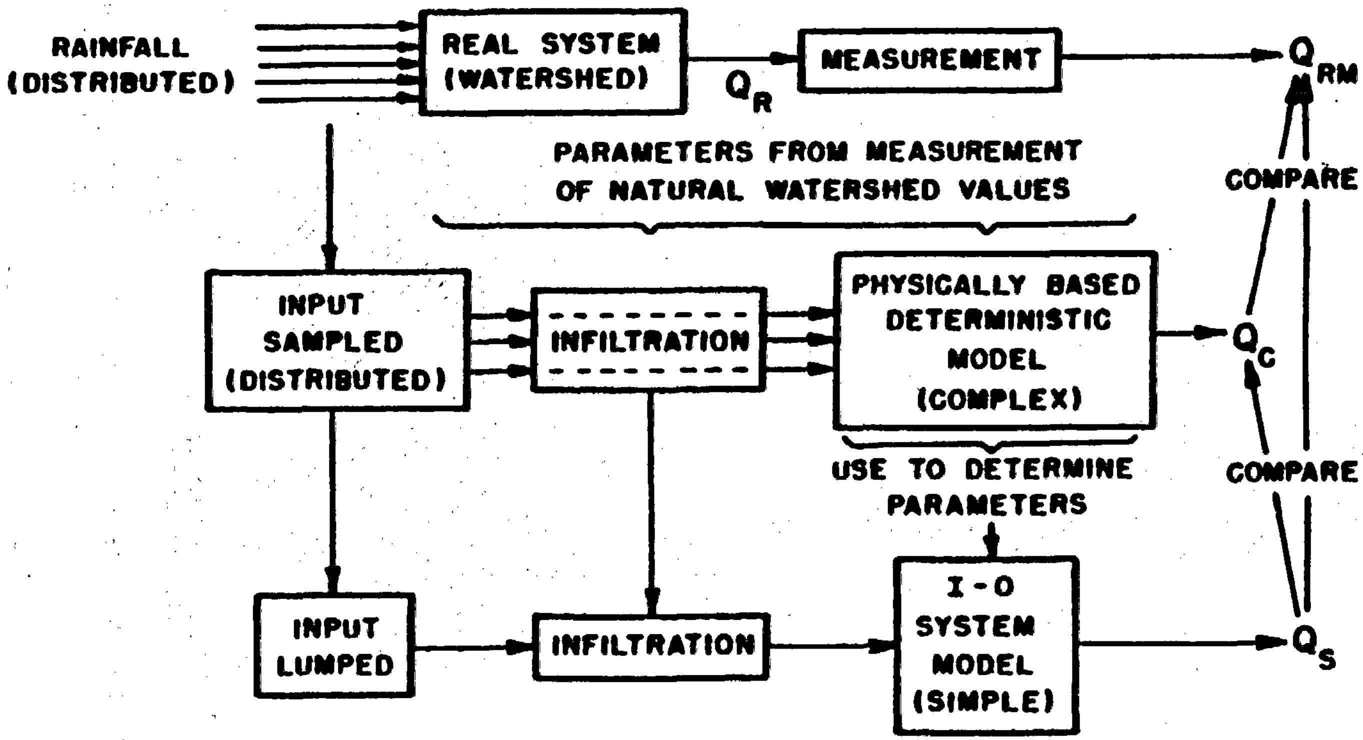
1) Natural Analog Studies
2) Groundwater Chemistry Evolution
3) Valence Effects Radionuclide Transport [Unsaturated Flow & Transport]
4) Backfill (EBS) Mineralogy
5) Repository Response to Strong Ground Motion
6) Effects of Spatial Variability on Groundwater Flow and Radionuclide Transport

EARTH SCIENCES — NEW RESEARCH TOPICS

1) Model Validation
2) Climatology
3) Expert System Assisted Evaluation of Tremendously Large Files of Site Data
4) Decision Making Procedures
5) Tectonic Effects on Hydrogeology



Known inputs
Reference inputs
REFERENCE SYSTEM (Distributed)
Reference output
SAMPLING PROCESS
Sampling strategy
Sampling errors
Modeling strategy
Prediction error
Measurements
INPUT ESTIMATION PROCESS
Estimated inputs
MODEL (Discretized)
Predicted output
Prior information
Estimation strategy


RAINFALL (DISTRIBUTED)
REAL SYSTEM (WATERSHED)
Q_R
MEASUREMENT
Q_{RM}
PARAMETERS FROM MEASUREMENT OF NATURAL WATERSHED VALUES
COMPARE
INPUT SAMPLED (DISTRIBUTED)
INFILTRATION
PHYSICALLY BASED DETERMINISTIC MODEL (COMPLEX)
Q_C
USE TO DETERMINE PARAMETERS
COMPARE
INPUT LUMPED
INFILTRATION
I - O SYSTEM MODEL (SIMPLE)
Q_S

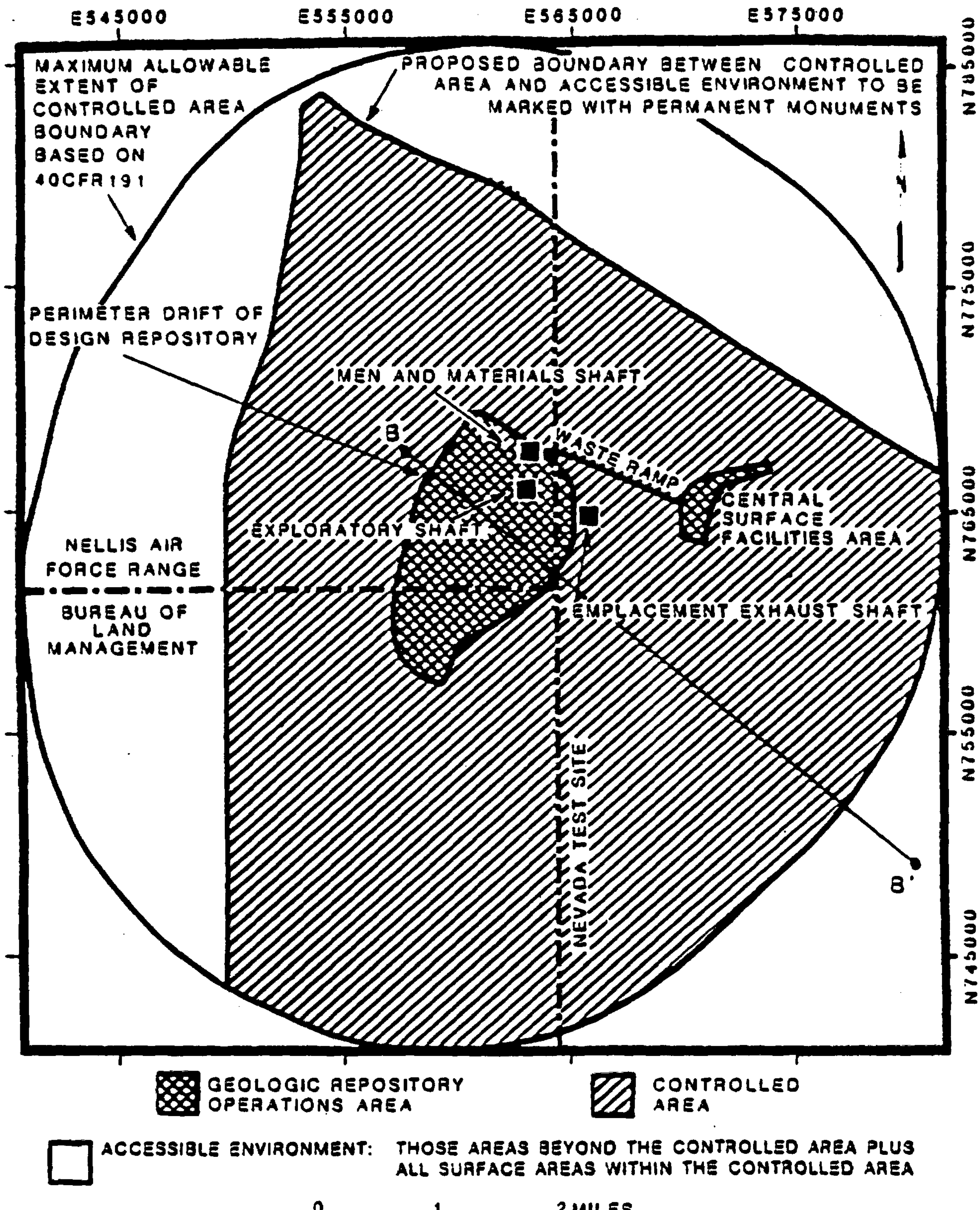
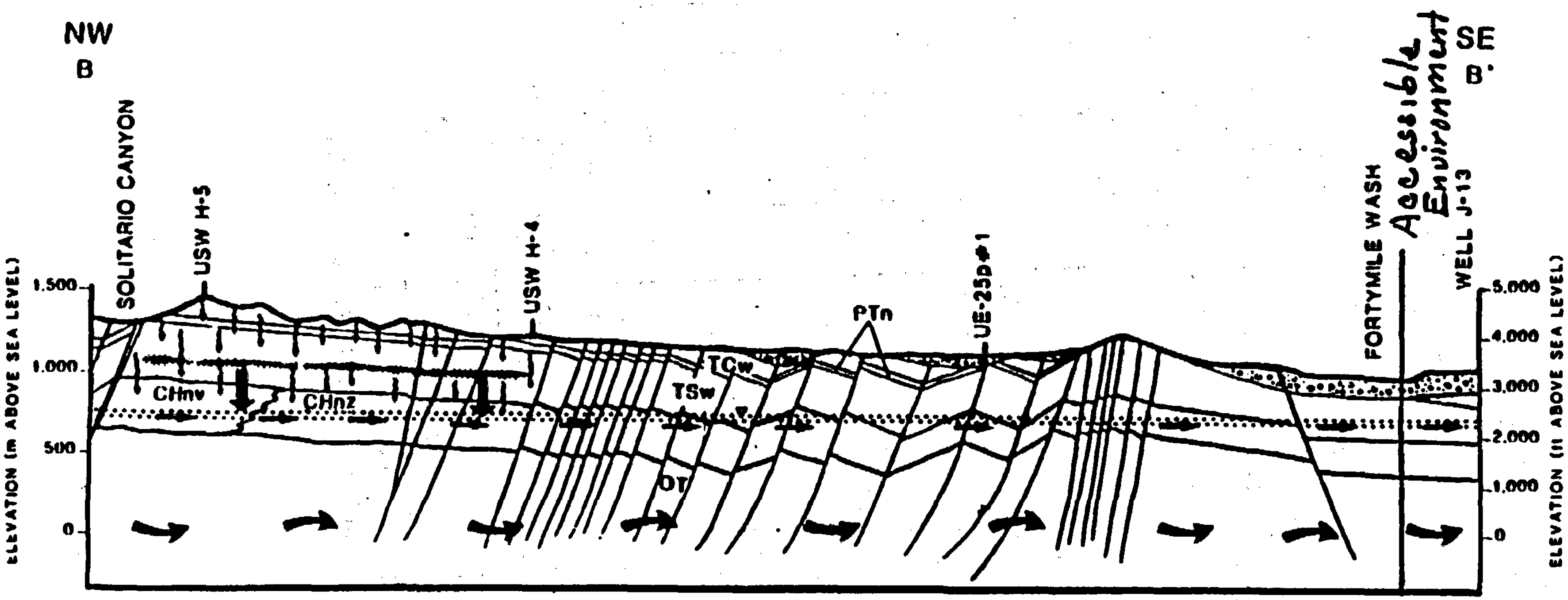


Figure 8.3.5.12-1. Preliminary definition of the boundary of the accessible environment (Rautman et al., 1987) and the location of section B-B'. Figure 8.3.5.12-2.



ALLUVIUM AND TIMBER MOUNTAIN TUFF

REPOSITORY (THICKNESS EXAGGERATED)

WATER TABLE

FLUX THROUGH THE UNSATURATED ZONE

UNSATURATED FLOW PATHS USED FOR TRAVEL TIME CALCULATIONS

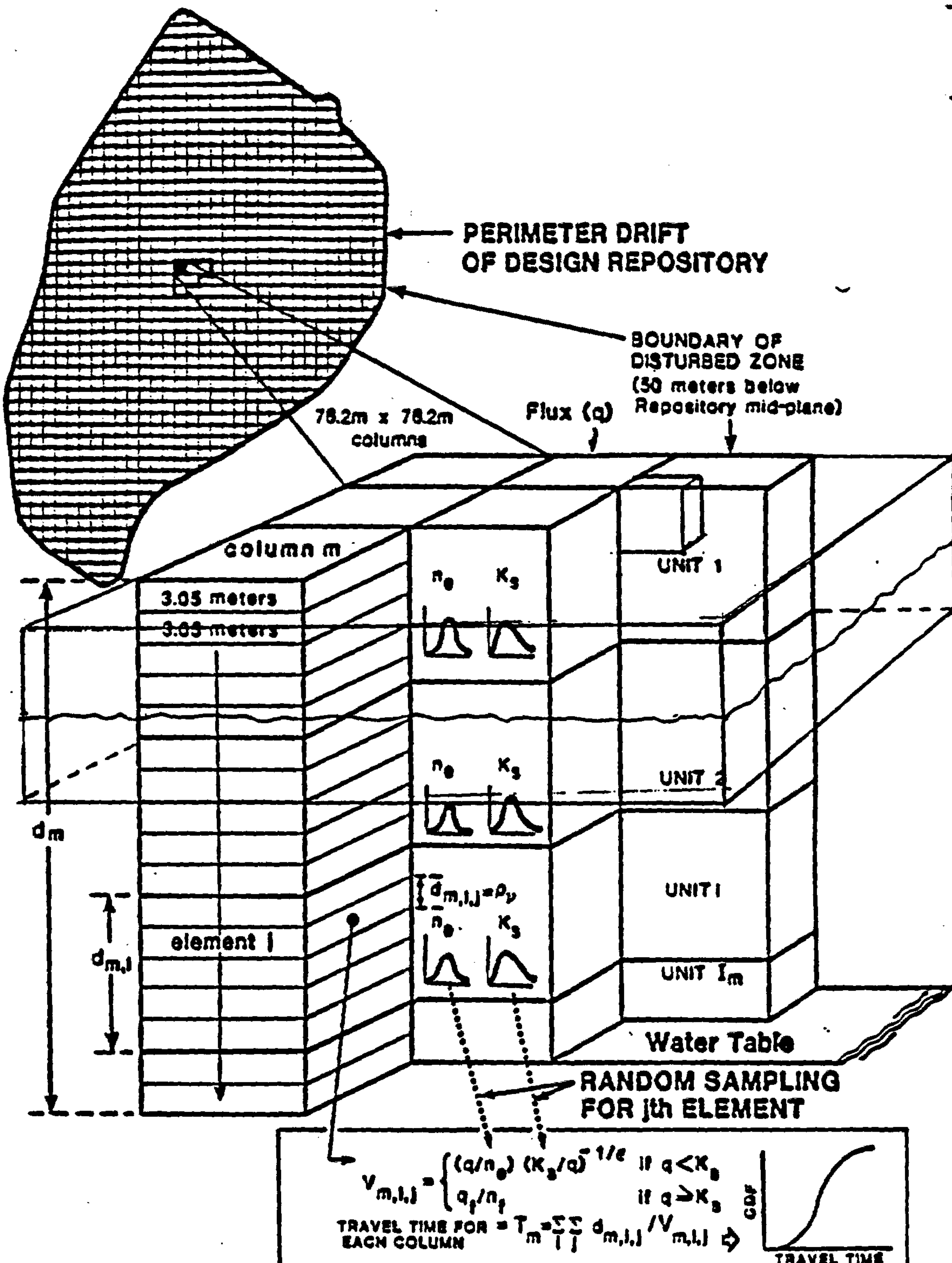
SATURATED FLOW PATH USED FOR TRAVEL TIME CALCULATIONS (WATER THAT HAS PASSED THROUGH THE REPOSITORY LEVEL)

DEEP SATURATED FLOW PATHS FOR WATER THAT HAS NOT PASSED THROUGH THE REPOSITORY LEVEL

TCw	TIVA CANYON WELDED UNIT
PTn	PAINTBRUSH NONWELDED UNIT
TSw	TOPOPAH SPRING WELDED UNIT
CHnv	CALICO HILLS VITRIC UNIT
CHnz	CALICO HILLS ZEOLITIC UNIT
OT	OLDER TUFF UNIT

0 0.5 1 MILE
0 0.5 1 KILOMETER

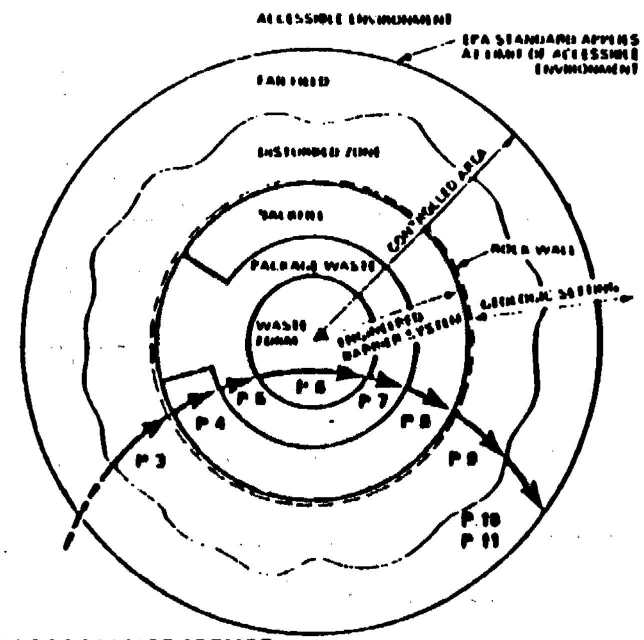
Figure 8.3.5.12-2. Conceptual hydrogeologic section from Solitario Canyon to well J 13 Section location shown in Figure 8 3 5 12 1 (modified from Scott and Bonk, 1984)



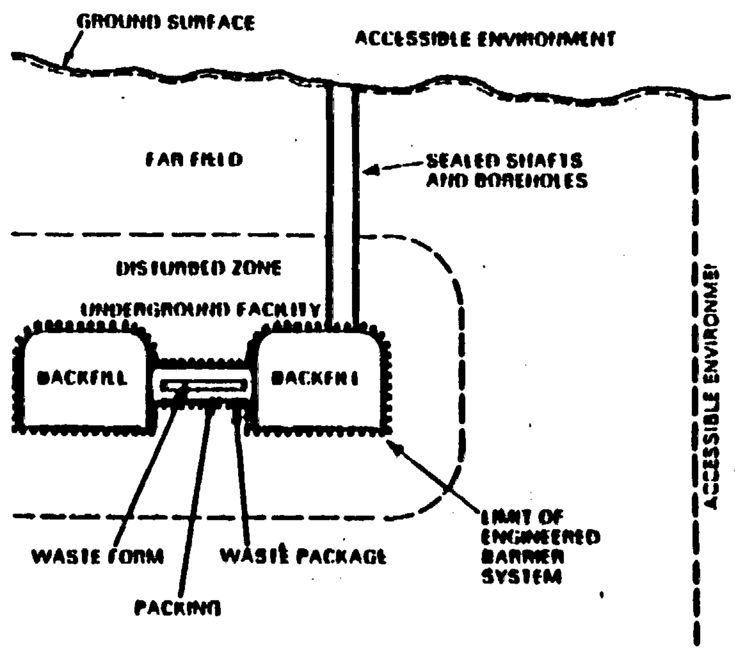
$n_s = 10^{-4}$

SOURCE: GE/CALMA PRODUCT NO. 0116

DIAGRAMMATIC PLAN VIEW (not to scale)



DIAGRAMMATIC CROSS SECTION VIEW (not to scale)



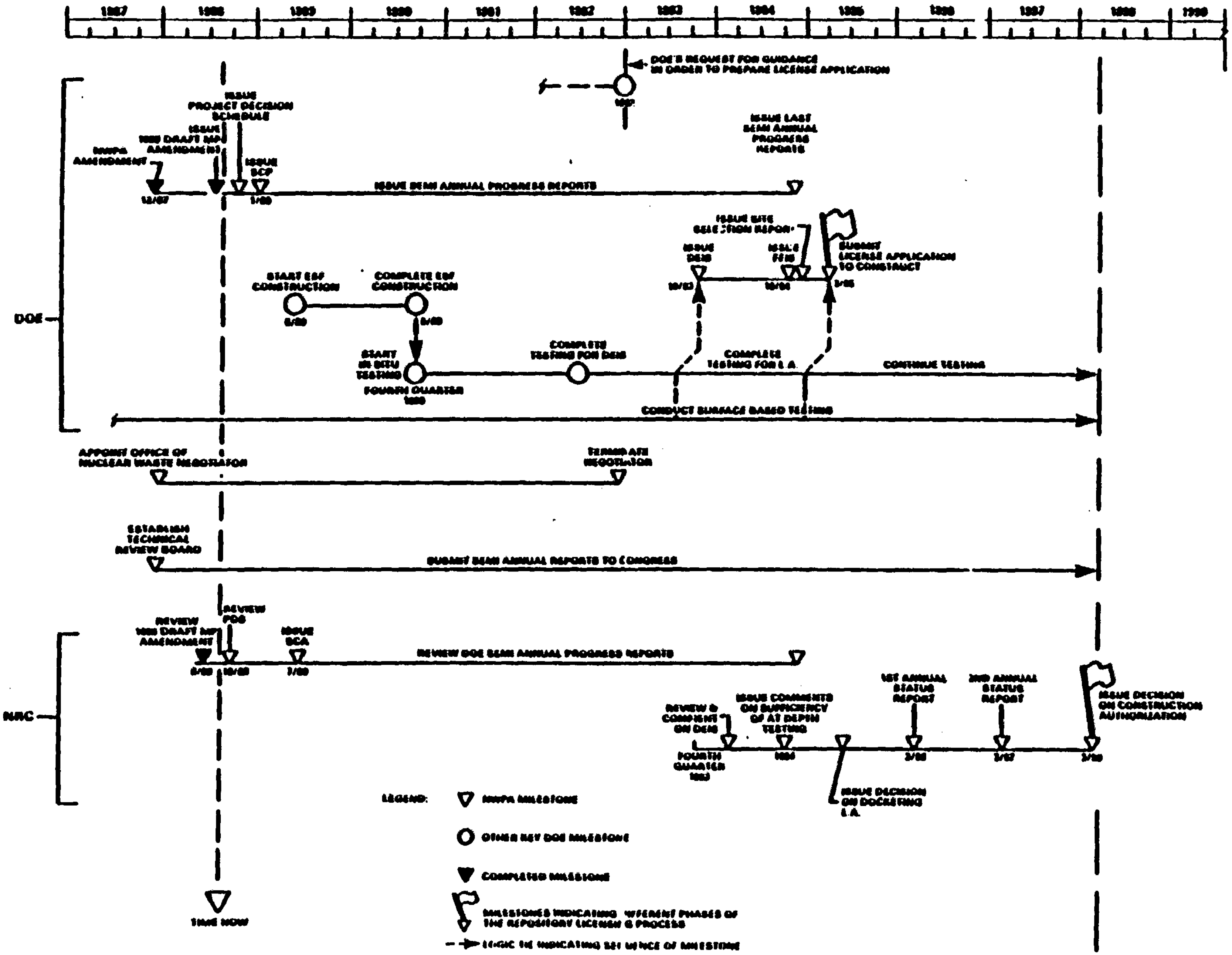
PERFORMANCE ISSUES

- P 3 When and how does water contact the underground facility?
- P 4 When and how does water contact the waste package?
- P 5 When and how does water contact the waste form?
- P 6 When, how, and at what rate are radionuclides released from the waste form?
- P 7 When, how, and at what rate are radionuclides released from the waste package?
- P 8 When, how, and at what rate are radionuclides released from the underground facility?
- P 9 When, how, and at what rate are radionuclides released from the disturbed zone?
- P 10 When, how, and at what rate are radionuclides released from the far field to the accessible environment?
- P 11 What is the pre waste emplacement groundwater travel time along the fastest path of radionuclide travel from the disturbed zone to the accessible environment?

FIGURE 2 REPOSITORY SYSTEM ELEMENTS AND PERFORMANCE ISSUES RELATED TO LONG-TERM PERFORMANCE AFTER PERMANENT CLOSURE

TIMELINE OF LEVEL I NRC & DOE NWPA MAJOR REPOSITORY MILESTONES

ENCLOSURE 3



WORKSHOP IV ON FLOW AND TRANSPORT THROUGH UNSATURATED FRACTURED ROCK AS RELATED TO A HIGH-LEVEL WASTE REPOSITORY

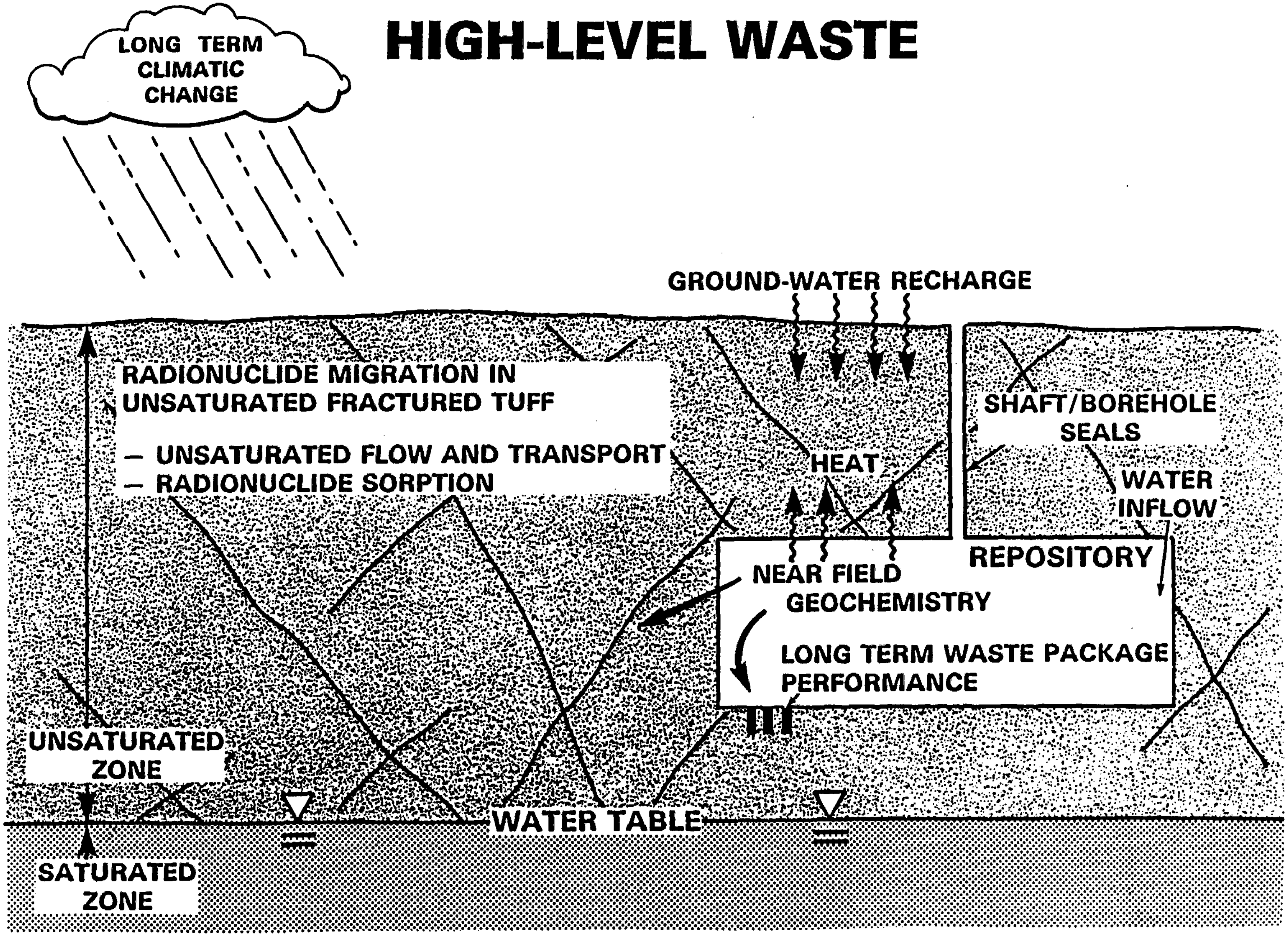
ABSTRACT

RESEARCH QUESTIONS

Thomas J. Nicholson
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, DC 20555

The U.S. Nuclear Regulatory Commission (NRC) staff has been actively formulating and executing a confirmatory research program in support of licensing activities for high-level waste (HLW) repositories. Based upon contractor's research results and NRC staff analyses, the NRC has promulgated regulatory criteria (10 CFR Part 60) for licensing a HLW site. Technical criteria include those for site characterization, performance assessment, and monitoring. In order for the NRC staff to adequately review technical investigations and reports submitted by the applicant to address these licensing issues, additional research studies are being supported to provide detailed technical information and analytical techniques (e.g. unsaturated flow and transport models). To accomplish this mission, the NRC staff needs to have in place a well formulated and integrated strategy for identifying the relevant research subject areas; what is known, what is not known; and where research work is needed. As a means of revisiting and possibly revising the present strategy for research in unsaturated flow and transport phenomena, the following flow chart on "Processes Affecting the Unsaturated Zone (Rasmussen, 1988)", and generic "Research Questions" will be presented to obtain information, ideas and comments from the workshop attendees.

HIGH-LEVEL WASTE



PROCESSES AFFECTING THE UNSATURATED ZONE

PRECIPITATION
-Frequency
-Duration
-Intensity
-Particulate loads
-Dissolved loads

SOLAR RADIATION
-Day length
-Solar angle
-Cloud cover

SURFACE STORAGE
-Interception losses
-Depression volume
-Surface area

SURFACE RUNOFF
-Peak Flow
-Total volume
-Dissolved and Suspended sediments

-----------------------------Ground Surface-----------------------------

INFILTRATION
-Matrix permeability
-Fracture density
-Fracture permeability
-Surface sealing
-Surface dissolution

EVAPOTRANSPIRATION
-Humidity
-Surface temperatures
-Wind Velocity
-Root depth
-Salt accumulation

DEEP PERCOLATION
-Areal extent
-Rate
-Duration
-Ion exchange
-Dissolution/Precipitation

VAPOR LOSS
-Geothermal gradient
-Subsurface heat sources
-Topographic relief

+ +Capillary Fringe+ + + + +

-----------------------------Water Table-----------------------------

RECHARGE
-Location
-Rate
-Duration
-Chemical composition

INPUTS

OUTPUTS

* * * * * * * * * * * * * *Regional Ground-Water System* * * * * * * * * * * *

GEOTHERMAL HEAT AND FLUID FLUX
-Location
-Rate
-Duration
-Chemical composition

TECTONIC
-Faulting
-Dilation and compression of voids
-Elevation changes to recharge and hydrogeologic boundaries

(After Rasmussen, 1988)

RESEARCH QUESTIONS

PREMISE: After examining the various processes affecting the unsaturated zone (Rasmussen, 1988), what are the fundamental questions for understanding the regional and local ground-water flow systems that influence solute transport ?

The following questions from the NRC staff are meant to provoke discussion:

1. What are the mechanisms and conditions that will enable ground-water to come into contact with the waste containers and may cause release of contaminants ?

2. Can sampled ground-water from either the underlying water table or nearby-perched zones be used to conduct leach tests ?

3. What are the mechanisms for release and transport of radionuclides in the gaseous phase during the period of HLW's significant heat output ?

4. What are the most appropriate performance measures for calibrating and validating unsaturated flow codes ? For example, is moisture content and its variation with depth, the most reliable measure ?

5. What are the most appropriate performance measures for calibrating and validating unsaturated transport codes ? For example, are concentrations distributions from breakthrough curves using core samples, the most reliable measure ?

6. Are there reliable geochemical indicators (e.g., stable isotopes) for either determining or confirming ground-water recharge, flow path delineation, mixing zones, and sorption/desorption mechanisms for the unsaturated zone ?

7. What are the important geochemical retardation processes in unsaturated media ? Why are they ?

8. What are the crucial field data for determining under what conditions a pressure continuum (both liquid and vapor) exists in unsaturated fractured media ? (On what scale ?)

9. Under what conditions does liquid water in the unsaturated zone move ;
   a. across fractures during matrix to matrix flow (Flow Regime 1) ?
   b. past porous blocks along fractures (Flow Regime 2) ?
   c. What are the physical criteria for transitions from Flow Regime 1 to Flow Regime 2 ?

10. How would site performance predictions change if the specified ground-recharge were intermittent rather than an average constant value ?

11. Can vertical and horizontal fluxes be determined at various hydrogeologic unit interfaces ? What field methods are available to determine them ?

RESEARCH QUESTIONS

PREMISE: After examining the various processes affecting the unsaturated zone, what are the fundamental questions for understanding the regional and local ground-water flow systems that influence solute transport ?

(Continued)

12. Can large-scale air flow tests including air tracer tests (e.g., dipole injection/withdrawl tests) be used to determine effective mean field pneumatic and hydraulic properties ?

13. Can pneumatic flow properties (e.g. air permeability) and fracture geometry data (e.g. fracture connectivity) derived from air flow tests be related to hydraulic flow parameters and mechanisms ?

14. Is there sufficient sampling methods for collecting transient data for modeling flow across hydrogeologic interfaces ?

15. Which regional geothermal and tectonic processes need to analyzed for significantly affecting either vertical or horizontal thermal and hydraulic fluxes to the regional water table and subsequently affecting the unsaturated zone ?

16. What role can stochastic methods and models play in characterizing and modeling unsaturated flow and transport in fractured media particularly on a regional basis ?

17. Given that one needs to validate unsaturated flow and transport models, what is the proper mix of laboratory and field experiments, and natural analogue studies to cover the entire range of temporal and spatial scales non-isothermal conditions, heterogeneous media, and coupled liquid/vapor systems relevant to a HLW repository's performance?

Response to Research Questions
Roger R. Eaton, Polly Hopkins and Nate E. Bixler
Sandia National Laboratories

In response to your January 6th letter regarding the 17 NRC research questions, Polly Hopkins, Nate Bixler and I offer the following combined response. We have addressed only the areas in which we have been participating; consequently we do not respond to questions in the areas of geochemistry and tectonic processes. We have tried to keep our answers relatively brief.

We appreciate the considerable amount of work done by you and your organizing committee to assure that the workshop was a success. Our interaction with many of the participants during the week exceeded that during the rest of the year.

RESPONSES TO QUESTIONS

1.) What may cause groundwater to come into contact with the waste canisters?

Significant increases in precipitation could conceivably result in a rise in the water table to the point where it interferes with the repository. In addition, such increases could cause the larger fractures or faults in the vicinity of the repository to saturate and channel groundwater into the drift areas, which could then reach the waste canisters.

4.) What are the most appropriate performance measures for calibrating and validating unsaturated flow codes?

Even though the verification programs such as COVE and HYDROCOIN receive criticism, we believe that they serve a role in the verification and to some extent validation of the codes. These code-code comparisons along with results from properly instrumented laboratory and field experiments appear to be the appropriate approach. Field data is necessary to assure ourselves that we are developing codes which are applicable in the appropriate flow regimes. For example, are the *in-situ* water flux magnitudes appropriate for Darcy's model and is the local-pressure-equilibrium assumption appropriate?

For validation purposes experimentally obtained moisture profiles would be helpful. Even more helpful would be velocity profiles since they are considerably more sensitivity to computational techniques. However, we realize that it is probably impossible to measure velocities directly in the field.

8.) What field data will show that pressure continuum exists in unsaturated fractured media?

In order to use pressure equilibrium in the computational models it will be necessary to show that the mountain is near equilibrium state. Currently we believe this to be true except very near the mountain surface.

Since time scales would be extremely long for field experiments. laboratory experiments could be used to determine relaxation times for water in tuff. These times could then be extrapolated to large scales using numerical codes. The computed time scales could then be compared with our best estimates of historical weather conditions.

9.) Under what conditions does liquid water in the unsaturated zone move?

Water can travel from matrix to matrix across fractures via means of contact areas between the fracture surfaces and possibly by vapor transport. Along fractures the water will most likely travel through the adjacent matrix blocks because of the relative magnitude of the unsaturated permeabilities, provided that the matrix does not become saturated. The flow will always follow the path of least resistance which varies with the relative size of the saturation dependent permeabilities.

10.) Would intermittent groundwater recharge alter performance predictions?

Previous calculations by Mario Martinez, of Sandia National Laboratories, Bryan Travis of Los Alamos and Wang *et. al.* of LBL have each shown that normal variations in surface recharge dampens out within a few meters of the ground surface. Therefore, we believe that only very slow transients, such as a gradual change in precipitation over thousands of years, would be felt at the repository level.

16.) What role can stochastic methods and models play in characterizing flow in fractured media.

Currently the modeling on the regional scale is severely hindered by excessively large computer time requirements. These large time requirements result from the nonlinearities in the material characteristic curves. Permeability curves calculated using a composite of fracture and matrix materials and the Mualem theory generate expressions which are extremely sensitive in the flow regions where fracture flow is present. If stochastic methods could be used to smooth the material curves and reduce the nonlinearities, a considerable savings in computer time could be realized. We believe that further work is needed to develop faster ways to solve the regional problem so that stochastic methods can be employed.

17.) What is the proper mix of laboratory, field, and natural analogue studies?

As model developers, we believe that there has always been a deficiency in the number of experimental results that are available to validate and verify the host of codes that have been developed. Laboratory scale experiments are particularly useful because they can be carefully controlled. Field experiments will be necessary in order to verify that spatial scaling is properly understood. The natural analogue studies are important in establishing temporal scaling.

Responses to Research Questions

Natalie Olague, Alva Parsons, David Gallegos, and Paul Davis
Sandia National Laboratories

1. What are the mechanisms and conditions that will enable ground-water to come into contact with the waste containers and may cause release of contaminants?

We feel that this question is answered in a report being written for the NRC by SNLA concerning different scenarios related to a HLW repository located in unsaturated, fractured tuff (NREG/CR-4770).

2. Can sampled ground water from either the underlying water table or nearby perched zones be used to conduct leach tests?

The important properties of the ground water that are necessary to conduct a leach test are composition and pH. Using water from the underlying water table may not be representative of unsaturated zone in situ water due to the presence of carbonate aquifers which may affect the composition and pH of the water. Perched zones located in the unsaturated zone may or may not be representative water samples. Before using water from a perched zone, the chemistry should be compared to in-situ water samples from the unsaturated zone. Another aspect to consider is, if leaching occurs, it may be under conditions of extreme climatic changes. Consequently, the water reaching the canister at that time may be of significantly different composition from both the saturated and unsaturated zone water.

3. What are the mechanisms for release and transport of radionuclides in the gaseous phase during the period of HLW's significant heat output?

The period for significant heat output from HLW has been estimated to reach maximum temperatures at approximately 100 years (NUREG/CR-4759). According to the regulations (NRC 10 CFR 60) for a HLW repository, the canister must last at least 300 years. Therefore, during the period of HLW's significant heat output, there will be no mechanisms for release and transport of radionuclides in the gas or liquid phase. After 300 years, gas phase radionuclides such as carbon-14 and iodine-129 may be released to the accessible environment along a continuous path to the land surface through fractures and/or matrix. However, if there is a continuous path for the gas phase, there must also be a continuous path for water infiltration, and this water transport may be more significant than vapor phase transport.

4. What are the most appropriate performance measures for calibrating and validating unsaturated flow codes? For example, is moisture content and its variation with depth, the most reliable measure?

It is not appropriate to validate a code, but rather the validation process must be performed on a model applied to a specific site. The only important performance measures for a flow model are ground-water flux and ground-water velocity, since these are the only measures used in regulating a HLW repository. The method for calculating the performance measures may vary according to the model. For instance, in a stratified profile where moisture content may be discontinuous across textural boundaries, pressure head gradients should be used rather than moisture content distributions.

5. What are the most appropriate performance measures for calibrating and validating unsaturated transport codes? For example, are concentration distributions from breakthrough curves using core samples the most reliable?

Again, the performance measures for validation refer to a model for a specific site. The performance measure for transport is integrated discharge because it is the relevant measure used in regulating a HLW repository at Yucca Mountain. Other performance measures that are related to regulations are concentration and dose. Breakthrough curves from core samples are not appropriate performance measures due to scale differences and spatial variability between the cores and the actual repository setting.

6. Are there reliable geochemical indicators (e.g., stable isotopes) for either determining or confirming ground-water recharge, flow path delineation, mixing zones, and sorption/desorption mechanisms for the unsaturated zone?

Carbon-14 and tritium have been used to delineate flow paths in the saturated zone. Ground-water composition has been used to determine ground water mixing on a regional scale. Chlorine-36 studies have been conducted in the vadose zone to determine the infiltration rate. However, the reliability of these methods is in question.

7. What are the important geochemical retardation processes in unsaturated media? Why are they?

The important geochemical retardation processes are the same for the saturated and unsaturated zones. The main difference is how these processes are modeled. The processes are discussed in a short report, "Important Physical and Chemical Processes for Unsaturated Zone Transport", submitted to the NRC with the November 1988 FIN A1266 monthly progress report.

8. What are the crucial field data for determining under what conditions a pressure continuum (both liquid and vapor) exists in unsaturated fractured media? (On what scale?)
The question of treating a medium as a continuum hinges on our ability to define a representative elementary volume (REV) which is applicable to a repository scale problem. To date, no one has proven that an REV exists for unsaturated, fractured rocks. However, if it was shown that most water moves large distances along discrete fractures, then the continuum approach could be disproved.

9. Under what conditions does liquid water in the unsaturated zone move:

a. across fractures during matrix to matrix flow (Flow Regime 1)?
b. past porous blocks along fractures (Flow Regime 2) ?
c. what are the physical criteria for transitions from Flow Regime 1 to Flow Regime 2?

There is no experimental evidence which answers these questions under field conditions. It is known, through laboratory experimental results, that if a fractured media is under high suction the flow is matrix dominated and, if a large flux of water infiltrates, fracture dominated flow occurs.

10. How would site performance predictions change if the specified ground-water recharge were intermittent rather than an average constant value?

We cannot answer this question until the fracture versus matrix flow question has been addressed with experimental field evidence.

11. Can vertical and horizontal fluxes be determined at various hydrogeologic unit interfaces? What field methods are available to determine them?

Yes, vertical and horizontal fluxes across interfaces can be measured in the field. Pressure head must be measured on both sides of the interface to determine the vertical gradient, and laterally along both sides of the interface to measure the horizontal gradient. With this information, vertical and horizontal fluxes can be calculated. Pressure head can be measured with psychrometers, heat dissipation probes, or tensiometers. Unfortunately, direct pressure head measurements are limited to certain ranges. If pressure head can not be directly measured due to adverse conditions, associated moisture content profiles can be measured using neutron logging or TDR techniques. The pressure head can then be determined from the associated moisture retention curve. These tests can only be performed in a near surface environment, or in tunnels at depth. If these experiments were run, the flux rate in the field may be so slow that actual changes in pressure are indistinguishable from instrumentation error.

12. Can large-scale air flow tests, including air tracer tests (e.g. dipole injection/withdrawal tests), be used to determine effective mean field pneumatic and hydraulic properties?

Effective mean values should not be important for regulation purposes.

13. Can pneumatic flow properties (e.g. air permeability) and fracture geometry data (e.g. fracture connectivity) derived from air flow tests be related to hydraulic flow parameters and mechanisms?

For hydraulic flow parameters in the saturated zone, pneumatic flow properties can be used, but for the unsaturated zone the flow paths for water and air may be different.

14. Are there sufficient sampling methods for collecting transient data for modeling flow across hydrogeologic interfaces?

See question 11.

15. Which regional geothermal and tectonic processes need to be analyzed for significantly affecting either vertical or horizontal thermal and hydraulic fluxes to the regional water table and subsequently affecting the unsaturated zone?

We feel that this question is answered in a report being written for the NRC by SNLA concerning different scenarios related to a HLW repository located in unsaturated, fractured tuff (NUREG/CR-4770).

16. What role can stochastic methods and models play in characterizing and modeling unsaturated flow and transport in fractured media particularly on a regional basis?

The continuum question needs to be answered first before the applicability of stochastic methods and models can be addressed. In addition, however, the inability to prove stationarity and to determine correlation scales may preclude their use.

17. Given that one needs to validate unsaturated flow and transport models, what is the proper mix of laboratory and field experiments, and natural analogue studies to cover the entire range of temporal and spatial scales, non-isothermal conditions, heterogeneous media, and coupled liquid/vapor systems relevant to a HLW repository's performance?

Given the current technical knowledge of unsaturated, fractured media, it is unlikely that there will be an overabundance of validation experiments; therefore, all available information should be utilized.

Response to Research Questions
John Smoot
Battell PNL

1. What are the mechanisms and conditions that will enable ground water to come into contact with the waste containers and may cause release of contaminants?

Probably will have contact as vapor, given the high temperatures of the waste containers. This could aid corrosion of the waste containers, although corrosion of the containers could occur from the inside out. The nature of any convection cells that might form around the canisters should be investigated.

2. Can sampled ground water from either the underlying water table or nearby perched zones be used to conduct leach tests?

Seems like there might be problems obtaining sufficient volumes for leach tests- the water chemistry might be replicated for large volumes, however.

3. What are the mechanisms for release and transport of radionuclides in the gaseous phase during the period of HLW's significant heat output?

Canister failure prerequisite for release. Assume repository in unsaturated zone. Probably have some gas and some dissolved in water vapor. Would expect some adsorption onto fractures or matrix. May reach accessible environment as gas through continuous fractures.

4. What are the most appropriate performance measures for calibrating and validating unsaturated flow codes?

There are several appropriate performance measures for calibrating and validating unsaturated flow models. For flow, moisture content with depth is a good measure- compare to neutron probe measurements if available. However, some codes output tension rather than moisture contents. Therefore, need good characteristic curves to validate.

5. What are the most appropriate performance measures for calibrating and validating unsaturated transport codes?

Moving to unsaturated transport performance measured, core experiments are an important first step. Validation of these types of experiments should provide some confidence in our approach. Calibrating and validating to the breakthrough curves would be appropriate for these types of experiments. Next- expand to larger scale, perhaps some of the U. of Arizona block experiments. Larger scale experiments such as Apache Leap and the Las Cruces Trench will be helpful in examining the affects of increasingly larger scale.

6. Are there reliable geochemical indicators (e.g., stable isotopes) for either determining or confirming ground-water recharge, flow path delineation, mixing zones, and sorption/desorption mechanisms for the unsaturated zone?

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7. What are the important geochemical retardation processes in unsaturated media? Why are they?

It seems that many geochemical retardation processes would be the same for both saturated and unsaturated media.

8. What are the crucial field data for determining under what conditions a pressure continuum (both liquid and vapor) exists in unsaturated fractured media? (On what scale?)

I'm not sure that I understand this question. Strictly speaking, it seems that some continuum of pressure would always exist in unsaturated, fractured media.

9. Under what conditions does liquid water in the unsaturated zone move: a) across fractures during matrix to matrix flow (regime 1), b) past porous blocks along fractures (regime 2), and c) what are the physical criteria for transitions from regime 1 to 2?

For low water contents, liquid water should move across a fracture or joint in those places where the aperture is approximately less than or equal to the average intergranular space. Otherwise, the fracture should act as a capillary barrier until the water content increases sufficiently to overcome this. For Flow Regime 2, seems that porous matrix would tend to "wick off" flow in the fractures.

10. How would site performance predictions change if the specified water recharge were intermittent rather than an average constant value?

A more natural or intermittent recharge vs. an average constant value might affect site performance predictions.. Would begin to see the influence of extreme precipitation events. This could increase ground-water travel times. Note: should also investigate the time scale on which recharge measurements are made (e.g., monthly, weekly, daily) vs. total recharge- some evidence that total measure of recharge will increase with increasing frequency of measurements.

11. Can vertical and horizontal fluxes be determined at various hydrogeologic unit interfaces? What field methods are available to determine them?

Vertical and horizontal fluxes are commonly determined through computer modeling exercises for hydrologic unit interfaces and other points of interest using some form of Darcy's Law. I don't know of any field methods that could determine these fluxes for the unsaturated zone.

12. Can large scale air flow tests including air tracer tests (e.g., dipole injection/withdrawal tests) be used to determine effective mean field pneumatic and hydraulic properties?

Large-scale air flow tests should be able to determine field pneumatic properties. I'm not sure how effectively these numbers could be translated into hydraulic properties (Would it be a linear or nonlinear function of viscosity?, etc.).

13. Can pneumatic flow properties (e.g. air permeability) and fracture geometry data (e.g. fracture connectivity) derived from air flow tests be related to hydraulic flow parameters and mechanisms?

As noted under number 12, it seems that there would be some problems relating pneumatic to hydraulic data. However, for problems such as fracture connectivity, pneumatic methods might prove very useful.

14. Are there sufficient sampling methods for collecting transient data for modeling flow across hydrogeologic interfaces?

I'm not sure that I understand this question. Wouldn't we still be interested in tensions and moisture contents on either side of an interface.

15. Which regional geothermal and tectonic processes need to be analyzed for significantly affecting either vertical or horizontal thermal and hydraulic fluxes to the regional water table and subsequently affecting the unsaturated zone?

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16. What role can stochastic methods and models play in characterizing and modeling unsaturated flow and transport in fractured media, particularly on a regional basis?

Role of stochastic methods- provide an estimate of the variability of predictions about performance based upon limited knowledge. Hopefully, they will promote the procurement of more data. Problem: how to deal with multiple spatial realizations of coefficient distributions vs. the one "true" but unknown distribution.

17. Given that one needs to validate unsaturated flow and transport models, what is the proper mix of laboratory and field experiments, and natural analogue studies to cover the entire range of temporal and spatial scales, non-isothermal conditions, heterogeneous media, and coupled liquid/vapor systems relevant to a HLW repository's performance?

Laboratory, field, and natural analogue experiments should be able to provide much information about repository performance assessment. A good mix should include all three types of experiments and perhaps even synthetic experiments. Budget and time constraints will probably limit the extent to which the "entire range" can be covered.

RESPONSES TO TOM NICHOLSON'S PRESENTATION

Scott Tyler
Desert Research Institute
Reno, Nevada

Before responding to some of the points raised by Tom's presentation, I would like to offer my praise for his(and the NRC staff) insight and originality in his presentation. Tom Nicholson is a shining star amongst a sea of bureaucracy in the high level waste program. Such praise may go well beyond Tom to such others such as Dick Codell however, I am not familiar with too much more of the NRC staff. Such discussion–style presentations are a valuable part of the workshop and the overall HLW program. I am very sorry that I was not able to stay for the entire discussion period.

RESPONSES TO SELECTED QUESTIONS:

1. The question of ground water processes affecting transport from the canisters is obviously a difficult one. Only very limited field testing (Climax Stock experiments) have been conducted with actual waste in the ground and unfortunately, I do not anticipate much more work to be accomplished on field scalewaste experiments prior to licensing of the repository. In addition, the Climax experiments were primarily designed to test emplacement technology and rock mechanical properties during heating. Little attention was paid to hydrologic processes occurring during heating and cooling phases. With this in mind, it appears that the HLW program will be sorely lacking in knowledge of processes controlling flow during the short time that the heat load is highest. It is interesting to note that during this heating phase will be the only time that the repository will be monitored to any degree. Once the waste has cooled, the repository will be out of sight and out of mind. What will happen to the entire program if radionuclide migration occurs due to unforeseen processes occurring during the waste emplacement/heating phase. Will the program come to a screaching halt as we try to redesign engineering barriers when it may be too late?

   There appears to be a logical experimental approach (although politically unpalatable) to solve the heating phase uncertainty. The DOE and NRC should design a field scale experiment (much like the WIPP site) and emplace actual waste in tuffaceous rocks and study all processes of potential transport. Multiple experimental sites within the tuff horizon may be needed to study geomechanical, vapor and liquid transport, but the money is certainly available to conduct such experiments. Since we have never disposed of HLW in tuffaceous rocks in the unsaturated zone, it appears foolhardy to assume that we know all of the processes controlling fluid/vapor movement around the canisters. Such experiments will undoubtedly slow the repository program as they will take many years to complete, but then again we have 10,000 years to wait.

Although important processes may occur during the heating phase which may be apparent during the monitoring phase, I think the post-heating phase in which water will flow through the repository under gravitational affects must be looked at in greater detail. It is during this phase that little or no monitoring will be possible. How are we to know that the repository is not leaking until it is much too late to do anything about it? For this phase, very simple models should be used with large factors of safety. For instance, assume a worst case of several centimeters of recharge passing through the repository. Using data on the solubility of the various radionuclides, let this recharge reach the water table in very short times. By short time, I mean in relation to the number of 10,000 years. Short may be 5–10 years (based upon data from Rainier Mesa) or perhaps 100–500 years. Since we poorly know the flow processes, we must be conservative. For instance, are we convinced that fluid flow in the zeolitic horizons will be matrix dominated and therefore radionuclides will be sorbed in these horizons? Based on data from various radionuclide migration experiments conducted on the NTS (Buddemeier and Isherwood, 1984), migration through fractured zeolitic tuff is rather poorly understood. As a result, performance models must be very conservative and incorporate large factors of safety similar to those used in reactor design.

2. What type of ground water do we use?

Since we have very limited chemistry from the unsaturated zone at Yucca Mt., this is a very difficult question. With this uncertainty, we must be conservative in our estimates. The geochemists and radiochemists must tell us: Under what aqueous chemistries are the radionuclides most mobile?. The soil physicists and hydrogeologists must then look at these chemistries and determine if they are likely chemistries to be found at the repository horizon both during the heating phase and during the cooling phase. We need to look in other tuffaceous environments such as the perched springs on NTS and vicinity for some fingerprints on geochemistry of typical waters. Some of this work has already started (see Raker, 1987) but much more work is needed in this area.

3. Gaseous transport?

This is an area that we had very little knowledge about up until several years ago and we have not progressed very far from the stage of discovering where else it may occur. I also feel that this may be one of most important release mechanisms for the repository in the short term. With this in mind, work should concentrate in two areas: phenomonology and modeling. In the first area, lets go back to areas where vapor transport of radionuclides may be already occurring. Significant data is available (although it may have some security aspects associated with it) on the venting and seeping of noble gases from nuclear testing in tuffaceous rocks. Although pressure conditions may be radically different than those encountered in the repository, I believe some analogies can be made and our data base on this relatively new process may be expanded. Other areas to obtain phenomological data are from uranium mill tailings cover programs, and low level disposal sites such as Hanford or Savannah River.

Modeling will play a major role in estimating the magnitude of the various forces (buoyancy, thermal, and barometric) affecting vapor and gas transport from the repository. Modeling efforts should be aimed at the development of experimental designs to test the gas mobility in the unsaturated zone.

4+5. Validation of flow and transport codes.

Validation should be based upon the variables of interest, fluid or vapor flux and radionuclide concentration. Validation on other variables assumes that we know the relationship between, for example, water content and fluid flux, which we may not. Codes validated for performance assessment (which I equate with leak rate to the environment) must be validated using flow and transport behavior. Using water content or capillary pressure as code validation parameters are fine if we are using them for agronomic purposes, but not for radionuclide migration.

6. Geochemical indicators.

I'll defer my comments to the geochemists.

7. Geochemical processes.

I'd suggest that the geochemists look to the soil chemists and the hard rock geochemists to begin their analysis of geochemical processes in the unsaturated zone. Besides this suggestion, I'll defer my comments to the geochemists.

8. Crucial field data for pressure continuum.

I strongly believe the work underway at the University of Arizona, both in the lab and in the field, represents excellent progress in the study of the validity of Richards' equation for fluid flow in soils and rock. We also must design simple lab experiments where we may measure the movement of water in fractures. At the DRI, we have gone back to basics in some of our experimental procedures and gained significant insight into the behavior of transient flow in fractures. For example, we are studying the behavior of water in parallel glass plates to simulate fracture flow. These simple visual experiments clearly show that fluid continuum is a transient phenomenon in unsaturated fracture flow. We will need to rethink our continuum approaches and perhaps apply new theories such as chaos to our modeling of fluid flow.

We must therefore continue and intensify our laboratory scale simulations and experiments on fracture flow to better quantify the affects of transient water flow. In the field, we must design experiments which also look at the transient, high frequency behavior of fluid flow. The transient aspects must be included since an unsaturated zone composed of fractured tuff may not act as a damper on the transient input (rainfall) and, in fact, may intensify the high frequency components.

9. Under what conditions does liquid water move?

We do not know the answer to this question. The rock block infiltration experiments underway in the lab at the University of Arizona will provide some insight into this question, but more experiments are clearly needed. We clearly need to look at the affects of wetting front instability and viscous fingering as potentially dominant processes in the transition from matrix to fracture flow. These processes are also transient phenomenon and will take carefully designed lab experiments to study. We must also go into the field (or more appropriately under it) and look for analog sites such as mine shafts and tunnels to inspect the type of flow occurring in these environments. From my experience, there are very few mines and tunnel both above and below the regional water table which do not show saturated fracture flow at some times of the year. Such behavior in tunnels above the water table suggest that matrix block tensions are not sufficient to eliminate fracture flow. Several other explanations such as fracture skins which reduce the flow of water from the fracture to the matrix or the transient nature of fracture flow which may overwhelm the diffusion into the matrix.

10. Transient conditions.

It is imperative that transient input be used in modeling efforts until it is proven (experimentally and in the field) that steady flow conditions occur both in the matrix and fractures. We have no data that I am aware of that suggests that the upper units of Yucca Mt. diffuse the highly transient rainfall over all areas of the repository block and produce steady flow in the repository horizon. Data from many other underground workings (for example see Russell et al., 1987) show variability in discharge deep within unsaturated fractured rock. The transient recharge will have a major impact on the affects of water diffusion from the fractures into the matrix. Under steady flow assumptions, we may be given false confidence in the ability of the matrix to reduce fracture flow. Under actual conditions in which infiltration has been occurring for millennium, fracture channeling and fracture skin development may completely negate the impacts of high tensions in the matrix blocks and matrix diffusion may be an insignificant process in deep fluid flow.

11. Can fluid fluxes be measured at interfaces?

It is important to recognize that we generally do not measure fluid flux directly but infer it from pressure and conductivity measurements. We must therefore employ methods whereby we use tracers to determine water flux and direction or utilize large scale weighing lysimeters. It is also important to include transient effects in our studies of flow at boundaries since it will be likely that these processes will show sensitive dependence to initial conditions.

12. Mean properties from air flow tests.

Large scale airflow tests will prove useful to estimate pneumatic properties over the scale of the test. It is important to remember however that these properties, much like hydraulic properties, are likely to be scale-dependent and be dominated by spatial variability. For example, hydraulic conductivity often increases (and its variance decreases) as the scale of experiment moves from the core size to the aquifer test scale. Such behavior is easily explained by accounting for spatial variability and the existence of long range correlation in conductivity. Similar behavior is likely in pneumatic properties. The scales of our experiments must match the scale of our modeling or performance assessment. In conjunction with experiments, theoretical efforts must be devoted to developing techniques to extend our small scale measurements to larger scales. Traditional techniques such as kriging will have to be modified and improved in light of long range correlations such as those predicted by fractal scaling.

13. Relation between pneumatic and hydraulic properties.

Given the impacts of channeling and fracture skins, I do not believe that pneumatic and hydraulic properties will be easily relatable. We must design our experiments around performance measures, i.e., if we are interested in gaseous transport of radionuclides then we must conduct pneumatic tests to determine air transport parameters. If, on the other hand, we are concerned with liquid transport, we must conduct experiments which stress the hydraulics of the system to determine their properties.

In hydrology and soil physics, we seldom deal with the air or gas phase in a realistic manner. Perhaps it is time we opened the lines of communication with our colleagues in the petroleum fields to investigate their treatment and successes in three-phase flow and transport in reservoir rock. We may be surprised to find that there has been significant progress made in this field.

14. Are methods available to measure transient flow?

Yes and no. We most likely can measure fluid behavior under transient conditions in porous media. It has been done for many years with success based upon performance measures consistent with well hydraulics and agronomic practices. We have not developed techniques to predict response in transient fracture flow and it is not clear to me that we will in the near future. To demonstrate this, I suggest perusing F. Schwille's text entitled "Dense Chlorinated Solvents in Porous and Fractured Media" for a very graphic display of the chaotic nature of fracture flow under ideal laboratory conditions. Prediction of transient behavior in fractures and interfaces will go far beyond the application of Richard's or Darcy's equations of slow fluid movement.

15. What regional and tectonic processes are critical to HLW?

In the last year, the concepts of regional tectonic and geothermal interactions in the repository performance have been brought to the scientific as well as public attention. It appears to me, at this time, that these processes will have a significant impact on the saturated zone and a much less important role in the unsaturated zone when compared to the impacts of spatial variability in hydraulic properties. The geothermal gradient in the unsaturated zone may become a dominant process long after the thermal load of the repository is diminished however, during the heating cycle, the waste heat load will likely dominate the hydrologic processes. As a result, we should be focusing some attention on the thermal regime in the unsaturated zone and estimating its affects on ground-water recharge. More attention will need to be paid to thermal regime produced by the heat load of the waste, however.

With regard to regional tectonic stress and its impact on the unsaturated zone, I believe our uncertainty in the present distribution of hydraulic properties will easily encompass any changes in these properties brought about by tectonic stress changes. As a result, tectonics in the unsaturated zone is likely to be an area of little importance. Tectonic activity such as major uplift or volcanology will, of course, have significant impact on water flow however, research in the probability of such occurrences is best left to the tectonophysicists and volcanologists. If such events are deemed probable, their affects on performance will manifest themselves in the area of repository integrity and not hydrology.

16. The role of stochastic methods.

Probabalistic or stochastic methods are only as good as the data base from which the distributions and correlations of such properties as hydraulic conductivity are drawn. Given the level of complexity of the flow system at Yucca Mt. it appears unlikely to me that the density functions will be estimated within reasonable levels of certainty. As a result, large scale stochastic flow or transport models may give false security in their estimates of travel times, etc. Stochastic models may be applicable in areas of dense data collection such as in the near field environment but care must be used in developing models with sparse data. To overcome this lack of data, research efforts should be devoted to developing integration technology whereby data from such fields as geophysics, basic geology and geochemistry may be incorporated to estimate, for example, hydraulic conductivity. If these technologies cannot be integrated to "fill in the holes", it may be most appropriate to apply very simple "back of the envelope" models with inflated factors of safety. Such models would provide a more valid worst case scenario of repository performance and would allow more resources to be devoted to data collection and interpretation.

17. Validation of models.

At this point, I believe we need to validate our assumptions of processes controlling transport for the designed repository. Given the fact that the scientific community has been studying flow in partially saturated fractured tuff for less than a decade, it is clear that we have a long way to go. As a result of this short time, we have no long-term experiments or data to base our perceptions of which processes are dominant in transport of radionuclides from waste canisters. Without such experiments, assessing the performance of the repository is of questionable scientific judgment.

It is clear from this lack of a sound data base that field scale experiments must be conducted in fractured partially saturated tuff similar to that found at the proposed repository site. Such experiments must be conducted over reasonable time frames since many of the processes of concern may take years to develop into dominant processes. Such large scale experiments will give the scientific community the time and data needed to develop new theoretical models needed to couple fluid and thermal properties and to incorporate the impacts of spatial variability on flow and transport. Just as Rome was not built in a day, a repository designed to last a minimum of 10,000 years cannot be designed and built in a decade.

Rainfall/Runoff Considerations at Yucca Mountain and Apache Leap

Roger E. Smith
Agricultural Research Service

I very much enjoyed the opportunity to participate in the subject workshop, and I wish to thank you for your support for my visit. I found the discussions interesting, and I learned mech of the questions being posed and attacked concerning the Yucca Mountain project. I also appreciated the opportunity to visit your field research site.

In response to the inquiry in your Jan. 6 memo, the main comment I have is an elaboration on the one I made at the workshop. This relates to Question nos. 1, 10, and 16 on Tom Nicholsen's list. I am concerned that one important part of the problem is not being adequately addressed in the focus on the problems of characterizing the fractured flow mechanics. That is the upper boundary condition for the period of design.

It may be that for a porous matrix of whatever properties, the flow at the storage site resulting from surface inputs may be properly assumed to be some long term mean of 1 mm. per year or less (I forget the figure I heard.). Nevertheless it seems prudent to me to look more carefully at the expected sequence of upper boundary inputs to the fractured rock mass. It seems to me significant that there is apparently a soil mantle covering the rock at the Yucca site, as opposed to what I saw at Apache Leap. This can and surely would make a significant difference in inputs from rainfall.

It is very feasible to simulate with current tools a reasonable time sequence of the occurence of soil saturation at the soil mantle/rock interface at whatever depth the soil covers. Rainfall records can be extended with very sound stochastic models now available, and an extremely long record used. We have a relatively fast unsaturated soil water flow simulator which includes the natural pattern of root extraction and surface evaporation driven by weather data. The result would be a picture of the number, length, and spacing of the occurrence of saturation at the top of the fractured rock (bottom of soil profile).

The assumption I would make is that there would be insignificant input to the fractured rock unless the soil above it became saturated, and I would want to know, as a designer, what the probability of this occurrence would be, assuming an extrapolated (or other trends, even) weather and plant cover condition over the design life. Soil properties necessary can be measured. I understand that infiltration tests are planned.

This is the research need that I see. If the NRC agrees with this need, and is interested in my cooperation, let me know.

Research Considerations
Rien van Genuchten
Agricultural Research Service

At the workshop in Tucson last week I promised you to document some of my reactions to the discussions. Unfortunately, somehow I lost your list of questions (research needs?), so I shall not address the specific questions on that list. However, since Dan Evans and others also provoked some thoughts, I will write down a few items which I believe are pertinent to the problem of nuclear waste disposal in unsaturated fractured rock. Perhaps you could mail me a copy of the list later.

1. In my opinion, by far the most challenging problem is how to estimate the amounts, rates and directions of water flow through the rock fractures. Roger Smith gave some well-founded theoretical arguments that flow in the fractures at Yucca Mountain may be less that expected because of the presence of a top soil. Still, the natural system there will likely exhibit enough noise and soil heterogeneity to still cause flow into the subsurface fractures. The presence of limited bare spots at or close to the soil surface, and the usual presence of soil macropores, may by itself also lead to significant flow in the fractures. Finally, high intensity rains can easily saturate the lower parts of the top soil, especially in depressions, and still provoke gravity flow into the rock fractures.

2. Unsaturated water flow in rock fractures is probably a highly unstable process subject to gravity flow, wettability problems, and a lack of macroscopic flow equilibration between the fractures and the rock matrix (the latter caused by, among other things, fracture wall coatings and resultant lower hydraulic conductivities at the interfaces). These processes likely also contribute to significant channeling phenomena within the fracture network. All this suggests that it will be very difficult to predict the <u>flow</u> network (as opposed to the <u>fracture</u> network) using established approaches based on the Richards or Navier-Stokes differential equations. It is my guess that ultimately indeed selected tracer tests are needed to fully define fluxes and directions of unsaturated water flow in the fractures (notably the channeling process). While experimentally elaborate and hence costly, payoffs from such tracer experiments may be very large. A test of this type could, among other things, involve different tracers applied to different parts of the soil surface so that the origin of the flow paths can be optimally identified with a single experiment. Note that a similar tracer test would be immensely useful also for Jane Long's research involving the Template (?) model and her "annealing" functions. Inverse procedures restricted only to water flow generally exhibit too many problems with parameter non-uniqueness and identifiability. The key issue here is that water during its movement through a soil/aquifer will not reveal its origin in the system, nor does it leave "traces". Recent work by Jack Parker and others also suggests that simultaneous inversion of water and solute transport data gives much more information than when water flow and solute transport data are analyzed independently (e.g., consecutively).

3. Experimental validation of numerical predictions should involve flow and transport fluxes through the system (notably through the fractures if occurring). Because flow rates can change orders of magnitude with small changes in water contents, validations using water content measurement alone are incomplete and probably must be considered inadequate (i.e., water content measurements may suggest accurate predictions while in reality the maximum flow rate in especially the fractures may be orders of magnitude underpredicted). Instead, it would be better to focus on concentrations, volumetric solute fluxes and directions of tracers moving through the system. [Wasn't this one of your questions?].

4. There must be equal attention to conceptual considerations including physico-chemical experimentation, as to numerical modeling. For example, I believe that one relatively weak area of research is the lack of improved methods and procedures for estimating the unsaturated hydraulic properties of soils, including unsaturated fractured rock. On Tuesday we had a session on standardization of sampling of soil water, solutes and gases. A similar standardization is sorely needed for unsaturated hydraulic conductivity measurements. Attached is a paper summarizing the "state of the art" as I see it. As stated in the paper, current measurement techniques are still largely those that were introduced several decades ago. Very few methods have been proposed that take advantage of modern tools, including improved computational support (and computers). An added problem is that people in different countries (or even states) often prefer different (and always imperfect) measurement methods, leading to different hydraulic estimates for the same soils. Another good example is the correlation of soil texture (particle-size distributions) with soil water retention and unsaturated hydraulic conductivity data. Such exercises have been carried out in different countries (USA, Canada, The Netherlands, Germany, Australia, South Africa). The accuracy of soil texture correlations is generally limited unless also some index of soil structure (or the fracture network) can be included in the analysis (e.g., organic matter, clay mineralogy, bulk density and other parameters). Work by different authors in different countries has resulted in different correlations, not because soils are necessarily that different in different parts of the world but, again, because users often use radically different measurement methods, instrumentation, and mathematical analyses once the field data are collected. Joe Wang in his summary had some good points about this also.

5. Closely related to point 4 is a need to verify current theoretical approaches for predicting the unsaturated hydraulic conductivity from observed soil water retention data. Too often these predictions are taken too seriously, or are adopted too eagerly, because of a near complete lack of reliable data. No wonder that theoretical pore-size distribution models are being applied nearly universally with little or no experimental validation. While predictive approaches can be very useful and have shown to fill an enormous data gap, it is to me unthinkable that - as far as I know - few if any people in the world are trying to improve/validate the theoretical methods. Mualem 10 years ago was about the last one to seriously work on these types of models. His research has since been re-directed, in part because of a lack of support for this "unpractical theoretical" work. Still, many people are forced to resort to his predictive equations because of a lack of experimental data; the equations are even being applied to unsaturated flow in fractures without having any indication to suggest that such an extrapolation is acceptable. All this shows that additional or continued work in this particular area of research in extremely important.

I hope that these limited comments are useful to your project; much more undoubtedly can be said (I may do so at a later time). In any case, I appreciate having been able to participate in the workshop. Clearly, NRC and DOE are sponsoring some excellent and highly innovative research; research that is also very relevant to the mission of the Agricultural Research Service, including our own U.S. Salinity Laboratory. We need to continue or increase this type of interdisciplinary communication. We actually may benefit from each other's work!

SUMMARY OF RESEARCH NEEDS

from Technical Sessions in
Workshop IV - Flow and Transport
through Unsaturated Fractured Rock
as Related to a High-Level
Radioactive Disposal

Tucson, Arizona
December 12-15, 1988

transcribed from
the presentation
by

Joseph S. Y. Wang

Lawrence Berkeley Laboratory

1. INTRODUCTION (viewgraphs 1 and 2)

Dan Evans has asked Glendon Gee, Linda Kovach, Robert Baca, and myself to report on the research needs discussed in this workshop. I met yesterday with Glendon Gee to have his input on the hydrology session, and today over lunch with Linda Kovach on the geochemistry session and Robert Baca on the modeling session. I will try to outline the research needs identified and discussed by the speakers and participants, incorporate the comments by the reporters, and summarize what I have learned from the technical sessions in the past two days, from the interesting laboratory and field trip on Tuesday, and from the exciting presentations on University of Arizona experiments and USGS studies on Monday. If I miss or misrepresent some important points, please correct my mistakes.

Tom Nicholson has just presented a number of comprehensive research questions. From the enthusiastic responses and comments, it is clear that many important issues require further research. I will also start by listing some simple questions before discussing the research needs. It is important to address *simple* questions which are likely to be asked by people not working in a specific research field, including the general public. To answer a simple question, we usually start with a simple analysis, and follow with more complex analyses. It is essential that results of analyses, both the initial simple ones and the follow-up complex ones, are convincing. If complex analyses are convincing, we may want to reproduce these results again with simple analyses to formulate a simple answer to the simple question. It is very important that we have simple answers for simple questions. If there is no answer, or the answer is too complicated, we need to do more research. *(Tom Nicholson comment: Remember that !)*

After the general issues, I will describe the research needs discussed in this workshop in three categories. The first category is on the processes and mechanisms for flow and transport in unsaturated fractured rocks. The second category is on parameters and measurements we need to characterize the system. The third category is on the research needs in modeling to predict the system performance. Hopefully this summary will be useful to the development of a systematic list of research needs for high-level radioactive disposal in unsaturated fractured rock from this workshop.

2. ISSUES (viewgraphs 3 to 5)

Ambient Liquid Flow at Depth: Our first focus is on the determination of the ambient conditions of liquid flow. It is generally assumed that liquid water is moving downward driven by gravity. The possibility of lateral movement induced by stratigraphic dipping and heterogeneity has also been raised. The possibility of net upward movement, however, should be investigated. Karsten Pruess has shown this morning that other mechanisms (barometric pumping, surface drying, ...) may remove water from the formation at the ground surface. After we determine flow directions and flow patterns, we then need to address the questions on quantity and speed (how large ? how fast ? how long it will take to have water flow from one point to another ?).

Infiltration Distribution: A more detailed set of questions concerns the distribution of flow. A key issue in the study of unsaturated fractured rock is the question whether flow is in the tuff matrix or in the fractures. If water is moving along the fractures near the ground surface, will the infiltration be averaged out spatially at depth by the suction of the unsaturated tuff matrix or remain concentrated along a few channels through the fractures or through the fault zones ? The groundwater travel time (GWTT), an important issue for performance assessment, is very sensitive to presence or absence of fracture/fault flow and the GWTT distribution will be determined by the flow distribution in a heterogeneous medium.

Long Term Evolution of Vadose Zone: Since we need to model the system behavior over thousands of years, it is important to understand the long term evolution of the unsaturated formation. Has the system already reached steady state and we expect no change in the ambient conditions over time ? Or is the system still changing with time ? Another issue related to GWTT through the unsaturated zone relates to the change of the water table boundary location. If the water table is moving downward, the length of flow path may increase. If the water table is rising, the shortening of flow paths and the onset of fast fracture flow may be of concern. One can ask these temporal questions, but one may not get simple answers due to the long time scales involved.

Vapor Transport: In addition to liquid flow, the vapor movement has received more attention recently. Is the direction of vapor flow mainly upward and can it effectively remove a large amount of moisture from the formation ? Or does the vapor movement follow the circular pattern of convection cells ? Is fast vapor movement mainly a near surface phenomenon or can vapor flow also be fast at depth ? How important are the topographic and barometric variations as driving mechanisms for vapor flow ? We also need to know if the coupling between vapor flow and liquid flow is important.

Responses to Extreme Precipitation: In addition to the ambient conditions, we need to analyze the responses of the system to outbursts of heavy rainfalls and other extreme transient events. How effective are the near surface layers in damping out the transient precipitations ? Can local ponding and fracture flow be induced ? Does flow through fractures occur in a few fast channels ? We also need to know if lateral flows can effectively divert the dispersed infiltration in the unsaturated units into concentrated flow through the fault zones.

Responses to Thermal Loading: The repository is a thermal source with radioactive decaying waste releasing heat for a long period of time. We need to determine whether the canisters are in wet or dry conditions and whether heat pipe effects are important to enhance heat transfer from canisters to the surrounding rocks. The thermohydrologic conditions in the near field can affect the performance of canisters to contain wastes. On a much larger spatial scale, we need to assess the potential of buoyancy flow and gas convection effects for inducing fast flow from the repository to the ground surface. The extent of the disturbed zone will depend on whether near field or far field criteria on thermally induced alterations and perturbations are used in its determination.

Radionuclide Transport: In nuclear waste isolation studies, the transport of radionuclides, not the transport of water, is the ultimate concern. The travel time of radionuclides is different from the travel time of water due to many geochemical factors. I am not familiar with many geochemical issues and will just list some of the mechanisms which may be important: such as retardation, sorption, precipitation, matrix diffusion, and solid diffusion. For the unsaturated environment, the oxidation process due to deep circulation of air may also affect the geochemical environment.

Spatial Variability: To answer many issues we just discussed, especially in performing complex analyses, we need to have many parameter distributions measured and parameter correlations determined. To characterize a heterogeneous medium, we need to determine spatial distributions, spatial correlations, and scaling properties (eg. fractal dimensions) of the formations. Once we have the statistical and geostatistical properties of parameters determined, we then need to use different approaches, such as Monte Carlo simulations and other stochastic models to incorporate and quantify the uncertainties associated with parameter distributions and correlations. Also important in modeling analyses are the issues associated with efficiency and accuracy. We need to feel that we have carried out sufficient analyses with computationally efficient models which are verified and validated to our satisfication.

3. PROCESSES AND MECHANISMS (viewgraphs 6 and 7)

Precipitation - Infiltration Relationship: On Monday, Dan Evans and Todd Rasmussen showed us that for the Apache Leap Tuff site 80% of precipitation stays within a watershed, and only 20% of rainfall leaves the watershed as runoff. Some of the water in the watershed will remain near the ground surface and evaporate after the rainfall or transpire through vegetations, and the remaining water moves down to the water table. In Yucca Mountain, only a few percent of the precipitation, much less than 80%, is estimated to go down and become net infiltration through the mountain. We need to analyze the difference in site characteristics and/or mechanisms to understand and resolve this issue on the ratio of infiltration to precipitation to determine what percentage of precipitation is really moving down from the surface to the deep water table.

Fracture Flow versus Matrix Flow: This question about fracture flow or matrix flow is going to stay with us during the course of this unsaturated repository project, regardless of which model we use and believe in. I will just summarize some of the findings discussed during this workshop that support both sides of argument. The 80% retention of water within the watershed suggests that fracture flow can be fast near the ground surface to absorb large amounts of precipitation in a short time. The question is whether the fracture flow is fast only near the surface or fast all the way down through the repository to the water table. One field evidence showing that the fractures near the ground surface are entrances of water flow is the growth of vegetations along fracture traces in the watershed. Since a fracture is likely open near the ground surface and closed by stress at depth, water may fill a V-shape fracture and stay near the ground surface to supply water to the plants. If water disappears very quickly, a dry fracture will not support the vegetation growth. This is just a conjecture concerning the flow and distribution of water near the ground surface based on one field observation.

We have different experimental evidences on the connectivity of fractures. Some of the z-holes at the Apache Leap Tuff Site blow out air, indicating that fractures are connected and air can easily circulate through the fractures. On the other hand, some of the helium injection tests in near-by boreholes do not show sensitive responses in cross-hole testings. How can we model flows through fractures if it is difficult to characterize the fracture connectivity and other fracture properties ?

The large block experiments in the lab we saw on Tuesday do show that matrix flow is the mechanism, at least for low infiltration rates applied to the top of the fractured block. It will be interesting to increase the infiltration rates to determine the transition from matrix flow to fracture flow. We expect that fracture flow dominates in saturated condition and that fracture flow occurs along a few channels, as shown in the chemical analyses on the fracture planes in the saturated solute transport experiment. It will be interesting to study how the channel flow characteristics change when the fracture system becomes unsaturated.

Tracer Breakthrough Curve: Glendon Gee commented that there is a need to better evaluate lumped parameters in lumped models for dual porosity system with both fractures and porous matrix. This is related to Rien van Genuchten's lumped parameter models. Lumped parameter models are very attractive and simple. The question is how to determine the parameters without explicitly using flow geometry characterisitcs. Related to this, Glendon Gee also asks the question whether lumped parameters can be obtained without elaborate tracer experiments. Rien van Genuchten showed us this morning that lumped parameters, without using geometry, can be obtained most reliably by fitting the model to the whole tracer breakthrough curve.

Paul Kaplan and others have voiced the following concern about breakthrough curves in this workshop. Due to GWTT criteria in regulation, we are interested mainly in the portion of the first arrival of fast moving particles, not the whole breakthrough curve of a tracer. In soil studies with high permeability media in saturated or near saturated conditions with plenty of mobile water in the system, we can carry out a tracer experiment in a relatively short time and with less effort than similiar experiments in tuff formation. If we can use information on the first arrival of a breakthrough curve to determine the parameters instead of the whole breakthrough curve, we can collect more data and focus on the portion of primary concern in performance assessment.

Flow Path Changes with Saturation: Rien van Genuchten has shown us that flow paths can change with saturation. In saturated conditions, flow in a heterogeneous soil is mainly through macropores. Under unsaturated conditions, flow is through preferential paths in the soil matrix. In fractured tuff systems, we need to carry out similiar experiments to assess the change of flow paths with saturation to see if fractures in tuff, in analogy to macropores in soil, will change from active flow paths in saturated condition to passive dry pores under unsaturated conditions.

Coupled Processes: Jane Long has discussed the benefit and stressed the need to have better interactions among geophysics, geomechanics, geology, and hydrology. Better understanding of geophysical testing, rock mechanical deformation, and geological description of a site can help us to construct a better hydrological model. I also add geochemistry to the list. The next few bullets are from the Linda Kovach's input concerning the coupling of geochemistry with hydrology.

Geochemical Reactions: Don Langmuir has emphasized the need for a better understanding of different retardation and adsorption mechanisms so that we can model the transport more accurately. Bill Murphy has discussed the importance of surface reactions and diffusion mechanisms to understand the gas, water, and rock interactions. Randy Bassett has discussed the supersaturation phenomena and mechanisms in the evaporation-precipitation of minerals in unsaturated conditions. Linda Kovach also emphasizes that the vapor phase transport, in addition to liquid phase transport, deserves more attention. For geochemical modeling, we need more information on spatial heterogeneity and temporal distribution for both the fluid phases and the chemical reactions.

Field Site and Natural Analog Studies: Field observations and natural analog studies, as the example discussed by James Kumhansl, can give us a lot of information on the geochemical evolution of a system. After geochemical observations and studies, we should continue to perform infiltration experiments with man-made or natural tracers. We need not only observe a system, but also actively test it to understand geochemical and hydrological behavior of a site.

Fracture Coatings: On a much smaller spatial scale within a fracture plane, geochemists, hydrologists, and rock mechanists can interact to have a better understanding of the fracture coatings. It is known from availbale core samples that tuff fracture surfaces have a small fraction of area coated with calcite, zeolite, and other secondary minerals. Most of these secondary minerals are probably deposited by liquid water which transports these minerals to the fracture surfaces in the region with small apertures around surface contact areas. The rest of the fracture surfaces are clean, suggesting that regions with large open aperture in the fracture may be dry with no liquid flow to transport these secondary coating minerals. According to rock mechanical analyses, the fraction of contact areas between two fracture surfaces are likely to be less than 50%, in the same range as the fracture coating fraction. Geochemical, hydrological, and rock mechanical studies can be used to analyze this and other hypotheses. This is an example where multi-disciplinary analyses can be used to answer the simple question: is liquid water in the fractures ?

Thermally Induced Effects: Bryan Travis has shown us this morning that the saturation outside the heated zone can increase due to condensation of vapor. If some of the region outside the heated zone approaches full saturation, this may induce fast fracture flows. Karsten Pruess has shown us that gas velocity induced by buoyancy forces associated with repository heat can be very high. Fast gas velocity is certainly of concern for the transport of volatile radionuclides. We can also use the fast gas velocity in remote monitoring of repository induced changes. In addition to experiments for determining the ambient conditions, we should start to design experiments to measure parameters useful for modeling of thermally induced processes. For example, large scale helium (or other light gas) injection tests, in addition to nitrogen or air injection tests, can be useful to study the gravity or buoyancy effects if a full scale, long term thermal study is not feasible.

4. PARAMETERS AND MEASUREMENTS (viewgraphs 8 and 9)

Relative Permeabilities: Todd Rasmussen has shown that the sum of liquid relative permeability and gas relative permeability may be larger than one in some range of saturation for the tuff matrix. Karsten Pruess has discussed the constraint and interference of flows within a two-dimensional fracture plane which can reduce the sum of relative permeabilities to a value less than one in partially saturated conditions. These two examples strongly suggest that we need to study the relative permeabilities in more detail. We have essentially no published data, and relatively few known ongoing efforts, to measure relative permeabilities even for the tuff matrix, and none, to my knowledge, for the fractures. Without relative permeability measurements, we can not determine the infiltration fluxes. Our current estimate of infiltration flux, 0.1 mm/yr or so, is really convoluted out from theoretical models of relative permeabilities, and can not be regarded as a measured value. The applicability of theoretical models developed for soils to tuff matrix and fractures also needs to be assessed. Karsten Pruess has shown that relative permeability in fractures can determine if a waste canister is in a dry environment with temperature reaching several hundred °C or in a two-phase environment with maximum temperature around 100 °C.

Long Tails in Distributions: Some of the permeability distributions presented by Todd Rasmussen have long tails toward large permeability values. Long tails in distributions exist not only in permeability but also in many other parameters. The effects of long tails in parameter distributions in modeling predictions can be significant. For example, again in the issue of GWTT, a large permeability tail may control the early arrival portion of GWTT distribution.

Wet versus Dry Drilling: Alan Flint discussed some of the effects of wet versus dry drilling in the prototype experiments in G-Tunnel. It is generally assumed that dry drilling will have less adverse effects in disturbing the unsaturated environment. However, we should be aware of some problems associated with dry drilling. Al Yang wants to collect ambient gas samples and requires as little contamination and perturbation as possible in the drilling operation with air. The ongoing experiments in G-Tunnel in comparing neutron log variograms after wet and dry drilling hopefully will help us to understand better the drilling effects in unsaturated systems.

Characteristic Curves: Todd Rasmussen has shown that the tuff matrix has a bimodal pore size distribution based on mercury intrusion measurement of the characteristic curve. David Galliegos, representing Douglas Smith, has presented results of tuff characteristic curves showing multi-modal pore size distribution with nitrogen condensation technique, and nearly uniform distribution with water adsorption method. We need to resolve the differences among different measuring techniques to determine the pore size distribution of the same material, tuff. We also need to address the network, ink bottle and other effects to have a better understanding of the characteristic curve of saturation change with suction pressure. Related to this issue of characteristic curve, we should explore the relationship between saturation characteristics and texture of the medium. We have texture data on the degree of welding and other alterations. We have not used this texture information to a great extent to improve our description of hydrological characteristic curves. It is also interesting to hear David Galliegos presenting the data on the wetting characteristic of water on tuff rock. We have assumed that tuff is hydrophilic and it is good that data support this assumption.

Unsaturated Sampling and Testing Equipments: On Tuesday night, we heard L. G. Wilson describing the development of guidelines in an ASTM project for sampling unsaturated media. The development of guidelines, or even standards, for unsaturated sampling and testing can be beneficial to our unsaturated repository project.

Tomographic Imaging: Silvio Crestana has shown us that Computer Assisted Tomography with X-ray or other imaging sources is a very interesting and promising technique for unsaturated soil studies. We should try to apply similiar techniques to unsaturated, fractured tuff to generate two-dimensional or even three-dimensional images for the distribution of fluid phases in heterogeneous media. On a much larger scale, we can use seismic tomography, described by Jane Long, to detect fractured zones. One attractive feature of the tomographic imaging approach is its noninvasive nature to study the interior of a flow system without breaking it apart. A picture is worth a thousand words. We should explore the use of these tomographic techniques more in our studies.

Unsaturated Testing Techniques: Glendon Gee has commented that the existing techniques for unsaturated testing, such as the use of tensiometer, psychrometer, and other instruments for measuring hydraulic heads and tensions, are not good enough to characterize the unsaturated state in the field. We need more work to measure the unsaturated flow field in fractured, unsaturated media.

Scaling of Characteristic Curves: Art Warrick has described some interesting scaling relationships in saturation functions and permeability functions. We need to understand more the meaning and implication of the scaling properties. Fractal dimensions and other measures have been related to scaling. Hopefully scaling laws can help us to relate laboratory measurements with field scale predictions.

Fractal Analyses: Glendon Gee has commented that we need more work on water retention prediction on aggregated soils with fractal analyses. Scott Tyler has presented an interesting fractal analysis to relate particle size distribution to pore size distribution for soil characteristic curve. Since tuff is a consolidated material, we can not readily measure the particle size distribution when the solid phase is cemented together. We need to use some other measures in texture, morphology, or mineralogy to replace particle size distribution if we want to use fractal geometry of solid phase to relate to flow path geometry. Fractal analyses have received more attention by many investigators lately. In addition to Scott Tyler's work, Bryan Travis has discussed some of their fractal work and we are also working on the use of fractals for fracture studies. Glendon Gee has voiced his concern about whether we can determine fractal dimensions unequivocally. Scott Tyler has some success in using log-log analysis in his study. He also commented that it is easier to get a straight line in log-log data plots than linear or semi-log plots. However, log-log analyses should be added to supplement the conventional data analyses. For example the variograms for spatial correlation analyses are usually presented in linear plots and fitted with spherical or other empirical models for the variance as a function of spatial separation. If the same data is plotted in log-log scale, the spherical and most empirical models have a unit slope. The field data may have a log-log slope different than one, which can be interpreted by fractal models in terms of fractal dimensions but not by the spherical and most empirical models. Also in a log-log plot, we emphasize the range of small spatial separation over which the variance is determined more accurately with more pairs of data included in the averaging. I suggest that both traditional linear analyses and log-log analyses should be used in geostatistical spatial correlation studies.

Thermodynamic Data on Secondary Minerals: To understand the fracture coatings and alterations as discussed by Randy Bassett, we need thermodynamic data on secondary minerals, such as zeolite and clay. Information on solid-solute surface reactions, reaction rates, and kinetics of relevant phases can then be used to model the geochemical evolution of these secondary minerals and hopefully yield information on the flow and transport of fluid phases in fractures.

Phase Compositions: Linda Kovach indicated that there is a need to have baseline information on compositions of all phases. The phases include the liquid fluid phase in pores and fractures, gas fluid phase, and solid phases of fracture coatings and tuff matrix mineralogy. Al Yang has described the experimental difficulties and challenges to squeeze pore water out of tuff matrix cores. I presume that it will be even more difficult to collect water in the fractures for chemical analyses. We need to study if very sophisticated spectroscopic techniques are available to analyze chemical compositions of small amounts of fluid in fractures. This is one area where advanced technologies need to be explored to help us get the data we need to model transport in fractured tuff formations.

Tracer Selection: Don Langmuir has discussed the selection criteria and development needs for conservative tracers in hydrologic testing and in monitoring potential contamination related to construction activities. The possibilities of tracer losses due to adsorption (eg. lithium, borate), volatilization (eg. iodine), and biodegradation (eg. nitrate, halogenated hydrocarbons) need to be evaluated for different tracers in tuff. Hopefully further tests with stable isotopes, anions, organics, and other compounds can identify an adequate number of suitable and inexpensive tracers for site characterization.

Data Extrapolation: Many geochemical studies use crushed samples in laboratory batch experiments to determine chemical properties, as discussed by Don Langmuir. We need to address this issue on how to extrapolate laboratory data on small samples to field scale predictions with large chunks of rocks. This is not only limited to geochemical studies but perhaps also to hydrological studies. How do we relate the permeability values measured in centimeter-size cores to modeling blocks with dimensions of meters to hundreds of meters ?

Correlation Lengths: Scott Sinnock has shown this morning that the modeling results on GWTT predictions can be very sensitive to the correlation lengths which characterize the heterogeneity of the system. This example again emphasizes one of the key issue in parameter measurements. We must address the scale dependence of parameters to properly use the measured values in modeling predictions.

Parameter Distributions: Robert Baca felt that we did not discuss much in this workshop on how to define parameters from limited data and how to determine if we have sufficient data. Right now, we have very little data on most parameters at Yucca Mountain and we try to collect as much data as we can. Eventually, we need to address this issue concerning the number of data points required to define parameters. Hopefully we can have a convergent understanding of the system as more data are collected and used in the models.

5. MODELS (viewgraphs 10 and 11)

Experimental Design: We have used models more in prediction exercises and less in experimental design. Close interactions between modelers and experimentalists during the course of design, measurement, and interpretation can really help us to understand the processes and mechanisms and generate useful parameters for predicting the system behavior. Modelers usually are eager to get reliable data, not trying to interpret the experimental results, but more due to concern about the credibility of their predictions. Hopefully we will see more modeling results tied to experiments in the near future with experimental activities shifting to higher gears.

Percolation Experiments: Ed Kwicklis has described some interesting results in the design of a percolation experiment with numerical simulations. It seems that a sand layer coupled to the in-flow boundary with the fractured tuff block is very important in controlling the distribution of flow into the block. We hope that the experiments can be carried out soon to study the percolation of flow through fractured tuff systems.

Analytic Models: Nora Okusu has described some of the recent development in simple analytic solutions and comparison with numerical solutions. I have discussed at the begining of this summary that we need to go through this route of first doing simple analysis, then complex analyses, then back to simple analysis to provide simple answer for a simple issue. I believe that more efforts are needed in this direction to develop simple solutions to reproduce numerical predictions. Another example by Karsten Pruess will be discussed later.

Matrix to Matrix Cross Flow: Tom Nicholson has listed this matrix-to-matrix flow as one of the research questions to be addressed. If matrix flow is the mechanism under ambient conditions, we need to model the matrix to matrix flow in a fractured medium with fractures separating the tuff matrix into blocks. We can model a small system with a few fractures and a few matrix blocks in a discrete fashion taking fractures and matrix blocks explicitly into account. If we try to model a large system, we need to develope double-porosity, double-continuum models. The traditional double-porosity model is not quite adequate for an unsaturated, fractured system. The double-porosity model assumes that the global flow is through the fracture network only, and the matrix blocks act as source/sink terms. As a result of this assumption, flow from one matrix block can end up only in the neighboring fractures but not across the fracture into the next matrix block. More work is needed to evaluate and generalize double-porosity and multiple-continuum models to handle matrix-to-matrix cross flows in large grid domains containing many fractures and matrix blocks and to quantify the macro-tortuosity associated with flow line distortions around drained fractures.

Coupled Hydro-chemical Transport Codes: We need to evaluate and develop more coupled hydrochemical codes for modeling dissolution, precipitation, and transport. Hydrologists usually use very simple dissolution and precipitation equations in the flow codes to model the change of permeability and porosity with mineral redistribution, as described in the examples by Karsten Pruess and Bryan Travis. Geochemists usually start with a sophisticated geochemical model and add simple flow equations with either constant velocity or a given flow velocity field along an one-dimensional flow path, as in the example described by Bill Murphy. The effects of mineral redistribution may be important in coupling the hydrological flow field and the geochemical processes, especially in nonisothermal conditions in the vicinity of waste repository.

Adsorption Models: Don Langmuir discussed the need to study and model adsorption on whole rocks taking into account fundamental controls on adsorption. These include the relative abundances and surface properties of specific sorbent minerals in rock pores and fractures. Adsorption models which consider such fundamentals include the constant capacitance, and the surface ionization and complexation models. At the other extreme, the simple K_d model ignores adsorption fundamentals and treats the water rock system as a black box, and so can lead to serious errors if used to predict adsorption for conditions that differ from these of the experiments used to evaluate K_d. The more complex adsorption experiments and models need to be considered if we are to develop confidence in our ability to predice adsorption in a variety of natural water-rock systems.

Code Verification: Karsten Pruess has presented a similarity solution for multiphase flow which can be useful for code verification in nonisothermal process with heat-pipe contributing to heat transfer. Both Karsten Pruess and Bryan Travis have compared the numerical solutions of their codes with semi-analytic solutions. Code verification is the first essential step to gain confidence in the performance of a given code. Following code verification, we then move on to code validation.

Equivalent Medium Models: Karsten Pruess has discussed the development of an equivalent medium model to approximate the complex multi-phase processes in a fractured, porous medium. If we can establish the range of validity for simple equivalent medium models, we can model multi-phase processes in large regions.

Micro Models: Bryan Travis has shown some interesting results with a pore-size lattice-gas cellular-automaton model. Micro models are important for us to gain insight in fundamental processes and mechanisms. Many fundamental assumptions we use in macroscopic models can be tested with microscopic models.

Stochastic and Fractal Models: Rachid Ababou has presented some interesting results with large scale stochastic simulations. Certainly more work is needed in this area. Stochastic models focus mainly on the proper treatment of spatial heterogeneity, taking the spatial correlation into account. We can also tackle the spatial correlation using fractal considerations. Monte Carlo simulations have been used to generate flow field distributions and to check other stochastic models. For example, Scott Sinnock has shown this morning an interesting plot on GWTT distributions. The GWTT along vertical columns was first calculated with mean values for hydrological parameters for the different layers. Then Monte Carlo simulations were carried out allowing parameters to sample different values according to given distributions. All the Monte Carlo results have shorter GWTT than that calculated by mean values. One possible explanation for such a shift to shorter GWTT is the constraint of one-dimensional flow used in the model. On the other hand, we have other one-dimensional results presented by

Rachid Ababou and Jim Yeh showing that the stochastic results fluctuate around the mean profile. I do not know enough about all these calculations to understand the conditions which are responsible for the shift or lack of shift. I just want to point out that the conceptually simple Monte Carlo simulations can generate results which are, at least to me, not necessarily obvious and easy to interpret without in-depth studies.

One-dimensional versus Multi-dimensional Results: After Scott Sinnock's presentation, we had some interesting discussions on the difference between one-dimensional results and two-dimensional results, especially in relation to the effects of spatial correaltion scales. We see a lot of one-dimensional results and very few two- or three-dimensional results. We need to assess the limitations of one-dimensional results and develope more efficient multi-dimensional modeling capabilities.

Model-Experiment Integration: We can carry out many modeling predictions. However, if we do not compare the modeling results with experiments, modeling predictions are just academic exercises. Todd Rasmussen has shown us a good example on how to use simple models to understand experimental results. The Apache Leap Tuff study directed by Dan Evans, combining numerical modeling, laboratory measurements, and field testings, has really helped us a lot to understand unsaturated flow in fractured systems.

6. CONCLUDING REMARK (viewgraphs 12 and 13)

Uncertainties: Scott Sinnock has developed an approach to address and quantify uncertainties. I have listed his four categories: parameter, scale, temporal, and process uncertainty to focus on the key research needs in our unsaturated repository study. We need to quantify all these uncertainties to understand and predict the system performance over large space and long time.

Model Validations: We need modeling tools to predict the system performance. To have confidence in our modeling capabilities, our models need to be validated. Tom Nicholson has described one validation exercise: the INTRAVAL international model validation project. We are glad to learn that the Apache Leap Tuff data set by the Dan Evans group at University of Arizona, together with the NRC-New Mexico State University Las Cruces trench soil experiments by Pete Wierenga's group, and the DOE-USGS NTS G-Tunnel Tuff Prototype experiments described by Alan Flint, will be included in the unsaturated test cases in the INTRAVAL project. I am sure this validation project, together with other validation efforts, will be beneficial for the model predictions.

Go Underground: To answer many questions and to resolve many issues in unsaturated repository project, we really need to carry out testings in the field and in in situ conditions. Let us move ahead and go underground !

7. DISCUSSIONS

Parvis Montazer: I like to commend you on the excellent summary of the whole session. There is one point I felt that was missed in the whole workshop. We are assuming that we know how we are able to measure potential field (i.e. the metric potential, the vapor pressure, etc.). I don't think we know, and I don't think there is enough research emphasis in place, on this issue as it should be. Potential field is the driving mechanism. We can measure all the parameters until the earth ends. If we don't have the driving mechanism, the potential field, it's not going to do us any good.

Joe Wang: Glendon Gee has expressed the same concern. He is not happy with the tools we have been using in hydrological testings. I agree with you and Glendon Gee that this is an important issue.

Al Yang: I want to clarify one point. We like to use air in coring. If we use water in drilling, we can not collect anything useful. In UZ-1 hole, they did not pump long enough to get the contaminated gas out. We can do that in the new holes so that we don't have the problems like those in UZ-1. In UZ-1, they did not pump enough before they stemmed it. Now it takes a long time to pump the contaminated gas out. In the future, we can pump the contaminated gas out right after drilling before sealing the wall. It may only take two days.

Joe Wang: I am responding to the concern you have about contaminated gas from drilling air, stemming materials, or other sources. We typically are more concerned about the liquid we use in experiments, like the use of J-13 water in geochemical tests. We are not usually worried about the composition of air we use in drilling or testing.

Al Yang: There is only two ways to drill a hole, either by liquid or by air. You got to cool the bits. We insist that we always use air drilling. There is no way out of that.

Rachid Ababou: I have a short point about the tail and the regulation which formulates the problem in terms of first arrival of breakthrough curve. I really have a problem with this. I think for either measurements or numerical simulations, to really say something about the first arrival or the tail, we need to look at the whole distributions of either travel time, or concentration in space, or concentration in time. You really need to look at the whole thing. You have fluctuations due to heterogeneity, uncertainties due to measurement noise, so you really want to know whether you have a tail by looking at the whole thing.

Joe Wang: For our problem, we are concerned with the first arrival part of the distribution because the ground water travel time regulation, as we understand it now, allows us to have a percentage of travel time shorter than a given time. So the portion of short travel times is of primary concern. I think from soil physics studies, as Rien van Genuchten has shown us, we do need the whole curve to get the parameter fitting right. This is an inverse problem, and we may need the whole curve to do it. For prediction purpose, we focus on the first arrival portion of travel time distribution and like to have that portion of curve determined better.

Karsten Pruess: I want to strongly endorse your final call to go underground. I think that in all the research needs that were talked about here it comes through loud and clear, to me anyway, that we need a much stronger emphasis on field observations and field experiments in DOE's program. To be able to do this, I think, we need convenient access to the subsurface on a scale on which we can do meaningful experiments. I don't see how we can do this without an underground research laboratory.

Joe Wang: I agree with you. We have a lot of experience in mining and tunneling in the mining industry, as the examples we observed on Tuesday in the field trip. Drilling and mining out an underground facility should not be a difficult job. The problem is, right now, we are very cautious. This repository is going to be a custom-made, one of a kind, facility. We need to go ahead and go down there to eventually build such a facility. Once we go underground, we may have a very different picture than the one we envision now.

Summary of Research Needs from Previous Sessions

reported by

Glendon Gee

Linda Kovach

Robert Baca

summarized by

Joe Wang

Unsaturated, Fractured Workshop IV

Tucson, 12/15/88

Simple Questions

Simple
Complex Analyses
Convincing

Simple Answers

No Answer/Complex Answer → Research Need

Processes/Mechanisms

Parameters/Measurements

Models

ISSUES

- **Ambient Liquid Flow at Depth:**
  downward ? lateral ? upward ? how large ? how fast ?

- **Infiltration Distribution:**
  in tuff matrix ? in fractures ? dispersed through the welded - nonwelded layers ? concentrated in a few faults ? how to define and calculate GWTT in heterogeneous medium ?

- **Long Term Evolution of Vadose Zone:**
  ambient conditions steady ? transient ? time scale ? water table rising or falling ?

ISSUES (Continued)

- **Vapor Transport:**
  vertically upward ? convective cells ? depth of penetration ? topographic and barometric effects important ? coupled to liquid flow ?

- **Responses to Extreme Precipitation:**
  depth of damping ? local ponding ? fracture flow ? channeling ? lateral diversion ?

- **Responses to Thermal Loading:**
  wet- or dry near-canister environment ? heat-pipe effect ? buoyancy flow ? gas convection ? extent of disturbed zone ?

ISSUES (Continued)

- **Radionuclide Transport:**
  geochemical retardation ? sorption ? precipitation ? matrix diffusion ? solid diffusion ? oxidation due to deep air circulation ?

- **Spatial Variability:**
  parameter distributions ? parameter correlations ? spatial correlations ? fractal scaling ? Monte Carlo approach ? stochastic models ? computational efficiency ? verifiability ? validation ?

PROCESSES/MECHANISMS

- **Understand Precipitation - Infiltration Relationship**
  80% in Apache Leap watershed ? (Dan Evans/Todd Rasmussen)
  less in Yucca Mountain ?

- **Resolve Fracture Flow vs. Matrix Flow**
  fast fracture flow near surface ? at depth ?
  ponded/perched water in fractures supporting vegetation ?
  fractures connected ? not connected ?
  matrix flow in low infiltration rate (block expt.) ?
  channel flow in unsaturated fracture ? (yes for saturated fracture ?)

- **Need to Better Evaluate Lumped Parameters in Lumped Models for Dual Porosity** *(Rien van Genuchten, Glendon Gee)*
  can we obtain parameters without elaborate tracer testing ? (first arrival vs. whole breakthrough curve)

- **Assess Change of Flow Paths with Saturation**

- **Need Better Understanding/Interaction Among Geophysics, Geomechanics, Geology, Hydrology** *(Jane Long)* **(+ Geochemistry)**

PROCESSES/MECHANISMS (Continued)

- **Coupled Gas, Water, Rock Reactions**
  (surface reaction, diffusion, supersaturation)

- **Vapor Phase Transport**

- **Spatial Distribution of Phases and Reactions**
  Temporal Distribution of Phases and Reactions

- **Need More Studies on Field Sites and Natural Analogs**
  infiltration studies - natural/man-made tracers
  mineral coating on fractures

- **Understand Retardation Mechanisms**

- **Thermally Induced Nearly Saturated Zone** *(Bryan Travis)*
  Thermally Induced Fast Gas Velocity *(Karsten Pruess)*

PARAMETERS/MEASUREMENTS

- **Need to Measure Relative Permeabilities for Matrix and Fracture**
  $k_l + k_g > 1$ *for matrix ?* *(Todd Rasmussen)*
  $k_l + k_g < 1$ *for fracture ?* *(Karsten Pruess)*

- **Quantify Long Tails in Permeability Distributions**

- **Assess Influence of Wet vs. Dry Drilling** *(Alan Flint)*

- **Compare Mercury Intrusion, Nitrogen Condensation, Water Adsorption Methods** *(David Galliegos/Doug Smith)*
  bimodal ? multi-modal ? network effects ? ink bottle ? relation to welding & other texture ? hydrophillic ?

- **Develope Guideline/Standard for Unsaturated Sampling/Testing** *(L. G. Wilson)*

- **Apply CAT Scan Tomography to Unsaturated Fractured Rock** *(Silvio Crestana)*
  Seismic Tomography *(Jane Long)*

- **Need More Work to Measure Tensions in Fractured, Unsaturated Medium** *(Glendon Gee)*

- **Assess the Scaling of S(h), K(h) Functions** *(Art Warrick)* $h_1/h_2 = \lambda_2/\lambda_1$ $k_1/k_2 = \lambda_1^2/\lambda_2^2$
  (αh) *and* $(k/\alpha^{1/2})$ *function of* S ?

PARAMETERS/MEASUREMENTS (Continued)

- **Need Work on Water Retention Prediction on Aggregated Soils (and Fractured Rock) with Fractal Analyses** *(Glendon Gee, Scott Tyler)*
  can fractal dimension be determined uneqivocally ?
  with log-log analyses ?

- **Need Thermodynamic Data on Secondary Minerals** *(Randy Bassett)*
  zeolite, clay
  solid - solution surface reactions
  reaction rates, kinetics of relevant phases

- **Need Baseline Information on Compositions of All Phases** *(Linda Kovach)*
  liquid phase - pores, fractures
  gas phase
  solids - fracture coatings, matrix mineralogy

- **Identify Useful Tracers** *(Don Langmuir)*
  bromide, borate, nitrate, stable isotopes, halogenated hydrocarbons ?

- **Extrapolate Lab Data to Field Scale**
  crushed sample

- **Determine Correlation Length** *(Scott Sinnock)*

- **Determine Number of Data Points Needed to Define Distribution** *(Robert Baca)*

MODELS

- **Use Models More in Experimental Design, in Addition to Predictions**

- **Assess the Influence of Sand Layer near Boundary in Percolation Experiments** *(Ed Kwicklis)*

- **Compare Numerical Solutions with Analytic Solutions** *(Nora Okusu)*

- **Evaluate Double-Porosity Models to Handle Matrix to Matrix Cross Flow and Matrix to Fracture Flow**

- **Need Coupled Hydrochemical Transport Codes** *(Bill Murphy, Karsten Pruess, Bryan Travis)*
  dissolution, precipitation
  effects of mineral redistribution on flow paths, temperature, and pressure around repository

- **Develop More Sophisticated Adsorption Models** *(Don Langmuir)*
  surface ionization/complexation and constant capacitance models
  compare with K_d *model*

- **Code Verification** *(Karsten Pruess, Bryan Travis)*

MODELS (Continued)

- **Develop Simple Models to Approximate Complex Models** *(Karsten Pruess)*
- **Develop Micro Models to Understand Processes/Mechanisms** *(Bryan Travis)*
- **Develop Stochastic (and Fractal) Models to Handle Spatial Heterogeneity** *(Rachid Ababou, Jim Yeh)*
  mean $\pm\sigma$ *vs.* *tail*
- **Check Modeling Results with Experiments** *(Todd Rasmussen)*
- **Evaluate 1D Results with 2D, 3D Results**

- **Uncertainty Quantification** *(Scott Sinnock)*

  - *parameter*
  - *scale*
  - *temporal*
  - *process*

- **Model Validation** *(Tom Nicholson)*

  - *INTRAVAL*

Go Underground

RESEARCH NEEDS FOR PERFORMANCE ASSESSMENT OF A HLW REPOSITORY

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The performance assessment methodology developed for the U.S. Nuclear Regulatory Commission by Sandia National Laboratories in Albuquerque is currently being updated for the unique problem of ground-water flow and radionuclide transport in unsaturated, fractured tuff adjacent to a high-level nuclear waste (HLW) repository. Conducting this excercise provides a basis to identify certain areas needed for a performance assessment which may be critical in evaluating the suitability of a candidate repository site, and consequently, can indicate the direction in which additional research efforts need to focus.

One area identified is that of decreasing uncertainty in the conceptual models for both ground-water flow and contaminant transport. This could be accomplished primarily by increasing the amount of data to support and/or refute proposed models. For performance assessment, the efficiency of the models as implemented in computer codes would need to be increased. An area related to the use and application of conceptual models in a performance assessment is that of improving scenario probability estimates and the techniques used to make those estimates, as both the conceptual model and scenario probability will be applied in the consequence analysis.

Although current uncertainty analysis techniques may remain applicable, the efficiency of these needs to be increased.

Currently, available sensitivity analysis techniques, on the other hand, do not appear to be adequate for highly the non-linear problems associated with unsaturated flow and transport, warranting the need to develop alternative techniques.

Several areas have been identified as to where experiments need to be conducted to assist in a performance assessment. These include experiments to identify important and/or dominant flow and transport processes, experiments to assist in the development of models and codes, and experiments to validate or invalidate proposed models. It should be noted that site characterization is not needed at this time. That is, the gathering of data should be directed toward developing a conceptual model and not be based on a presumed model.

Specific examples and summary may be found in the attached figures.

Research Needs For Performance Assessment Of A HLW Repository

David P. Gallegos
Sandia National Laboratories

NEED FOR PERFORMANCE ASSESSMENTS

EPA - "DISPOSAL SYSTEMS ... SHALL BE DISIGNED TO PROVIDE A REASONABLE EXPECTATION, BASED UPON *PERFORMANCE ASSESSMENT,* THAT THE CUMULATIVE RELEASE TO THE ACCESSIBLE ENVIRONMENT FOR 10,000 YEARS AFTER DISPOSAL ...SHALL:

1. HAVE A LIKELIHOOD OF LESS THAN ONE CHANCE IN 10 OF EXCEEDING THE QUANTITIES CALCULATED ACCORDING TO TABLE 1; AND
2. HAVE A LIKELIHOOD OF LESS THAN ONE CHANCE IN 1000 OF EXCEEDING TEN TIMES THE QUANTITIES CALCULATED ACCORDING TO TABLE 1."

NRC - "THE COMMISSION WILL EVALUATE COMPLIANCE WITH THE CONTAINMENT REQUIREMENTS BASED ON A *PERFORMANCE ASSESSMENT*."

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DEFINITION OF PERFORMANCE ASSESSMENT

NRC - AN ASSESSMENT THAT:

1. IDENTIFIES ALL SIGNIFICANT PROCESSES AND EVENTS WHICH COULD AFFECT THE REPOSITORY;
2. EVALUATES THE LIKELIHOOD OF EACH PROCESS OR EVENT AND THE EFFECTS OF EACH ON RELEASE OF RADIONUCLIDES TO THE ENVIRONMENT; AND
3. TO THE EXTENT PRACTICABLE, COMBINES THESE ESTIMATES INTO AN OVERALL PROBABILITY DISTRIBUTION DISPLAYING THE LIKELIHOOD THAT THE AMOUNT OF RADIOACTIVE MATERIAL RELEASED TO THE ENVIRONMENT WILL EXCEED SPECIFIED VALUES

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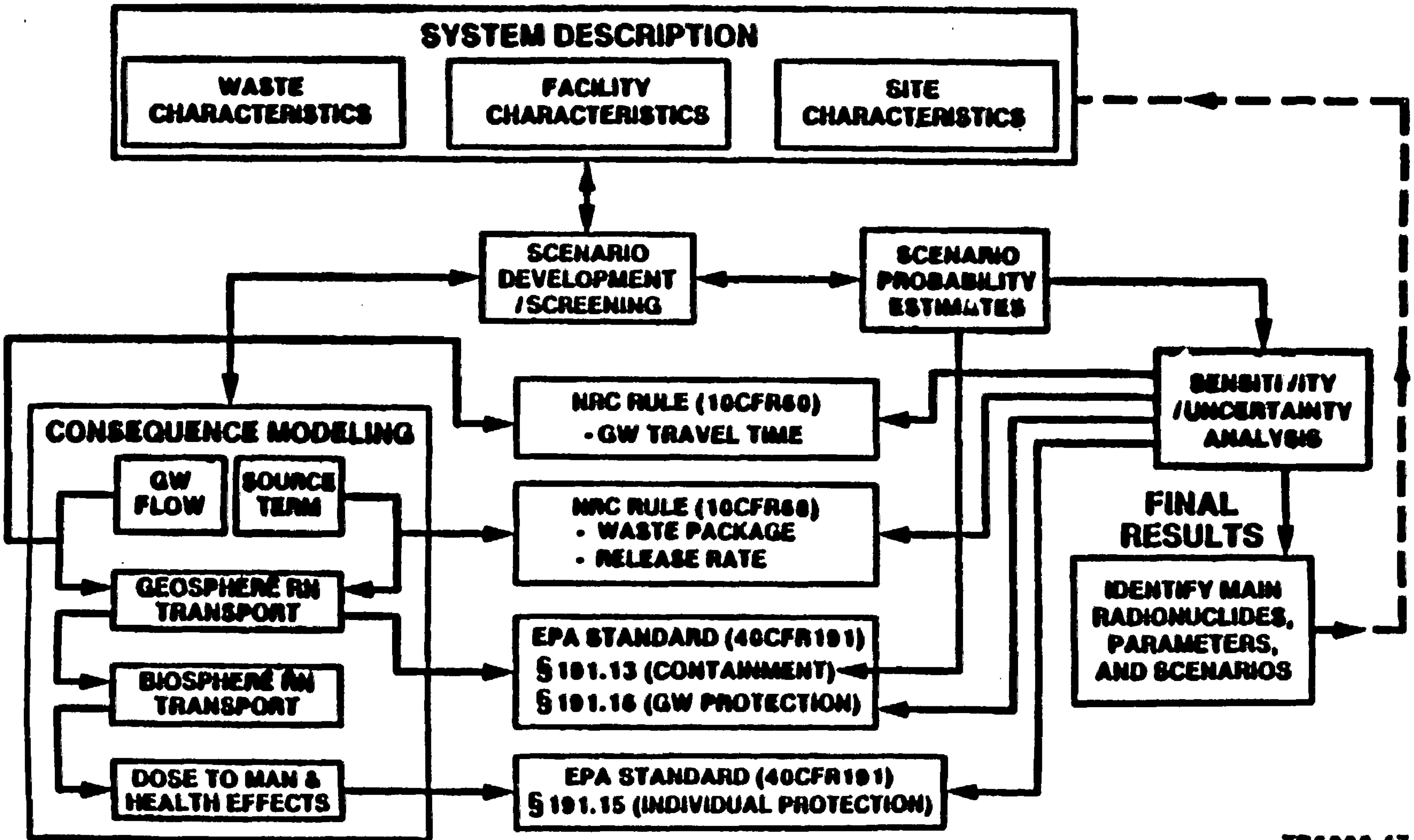
Sandia National Laboratories

METHODOLOGY FOR PERFORMANCE ASSESSMENT OF HLW REPOSITORIES



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CONCEPTUAL MODEL FOR A HLW REPOSITORY SITE

- GROUND-WATER FLOW
- RADIONUCLIDE TRANSPORT
- SCENARIOS

GROUND-WATER FLOW

- FRACTURE/MATRIX FLOW
- VALIDITY OF DARCY'S LAW
- INFILTRATION / RECHARGE
- APPROPRIATE MODELS

RADIONUCLIDE TRANSPORT

- IMPORTANT PROCESSES

- EFFECT OF VARIABLE SATURATION
  - Saturated vs. unsaturated
  - Linearity of processes

- DETERMINATION OF PROPERTIES

- APPROPRIATE MODELS

UNCERTAINTY AND SENSITIVITY OF PARAMETERS AND PROCESSES

- SPATIAL AND TEMPORAL VARIABILITY IN THE UNSATURATED ZONE
- TECHNIQUES TO QUANTIFY/ PROPAGATE UNCERTAINTY
- APPLICABILITY OF CURRENT SENSITIVITY ANALYSIS TECHNIQUES

UNCERTAINTY ANALYSIS

- EFFICIENCY
- EASE OF USE
- CODE COUPLING
- CONSISTENT PROPAGATION OF UNCERTAINTY

SENSITIVITY ANALYSIS

- CURRENT TECHNIQUE INADEQUATE FOR UNSATURATED ZONE
- ALTERNATIVE TECHNIQUES
  - Adjoint Technique
  - Combination of Current and Adjoint Techniques

PERFORMANCE ASSESSMENT EXPERIMENTAL NEEDS

NEEDED:

- Experiments to Identify Processes
- Experiments to Help Develop Models/Codes
- Experiments to Validate Models

NOT NEEDED:

- Numerical Values for Parameters
  (i.e., Site Characterization)

OUTSTANDING TECHNICAL ISSUES

- VALIDITY OF CONTINUUM APPROACH FOR FLOW AND TRANSPORT
- APPLICABILITY OF CONVECTIVE/DISPERSION EQUATION TO TRANSPORT IN UNSATURATED, FRACTURED TUFF
- EFFICIENT NUMERICAL TECHNIQUES FOR FLOW AND TRANSPORT
- TREATMENT OF SPATIAL CORRELATION IN UNCERTAINTY ANALYSIS
- SENSITIVITY ANALYSIS OF HIGHLY NON-LINEAR PROBLEMS