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U.S. Nuclear Regulatory Commission
ATTN: Mrs. Deborah A. DeMarco
Two White Flint North
11545 Rockville Pike
Mail Stop T8A23
Washington, DC 20555

Subject: Programmatic Review of Poster

Dear Mrs. DeMarco:

The enclosed poster components are being submitted for programmatic review. These poster components will be assembled as a poster and will be presented at the American Geophysical Union Fall Meeting to be held December 10–14, 2001, in San Francisco, California. The title of this poster is:

> "Monte Carlo Analyses of Unsaturated Flow in Thick Vadose Zones of Layered, Fractured Rocks" by W. Illman and D. Hughson

Please note that this poster is based on an abstract previously submitted to NRC on September 7, 2001. Please advise me of the results of your programmatic review. Your cooperation in this matter is appreciated.

Sincerely,

Budhi Sagar
Technical Director

/ph
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Monte Carlo Analyses of Unsaturated Flow in Thick Vadose Zones of Layered, Fractured Rocks

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- This work is an independent product of the CNWRA and does not necessarily reflect the views or regulatory position of the U.S. Nuclear Regulatory Commission.

Abstract

We conducted Monte Carlo simulations of flow in unsaturated fractured rocks using a two-phase, non-isothermal, flow simulator. In this simulator the fractured rock is idealized as a dual-continuum porous media, in which the matrix and fracture constitute two distinct continua represented by two overlapping, interacting numerical grids. Darcy's law and the area of the matrix-fracture interface open to flow govern the exchange of fluids between the two continua. To investigate the applicability of the dual-continuum approach for modeling unsaturated flow in a thick vadose zone of fractured rocks, we applied the model to site data collected from Yucca Mountain. We used grid blocks with dimensions of 1 *m* that is commensurate with the support volume of fracture permeabilities estimated from single-hole pneumatic injection tests. We investigated the consequences of simplifying fracture permeability on unsaturated flow by comparing the model results using uniform formation properties to a stochastic model that represents spatial variability of the fracture permeability within the layers as a multivariate lognormal random field. In both models, the water flux boundary condition was varied to simulate the effects of variable recharge rates.

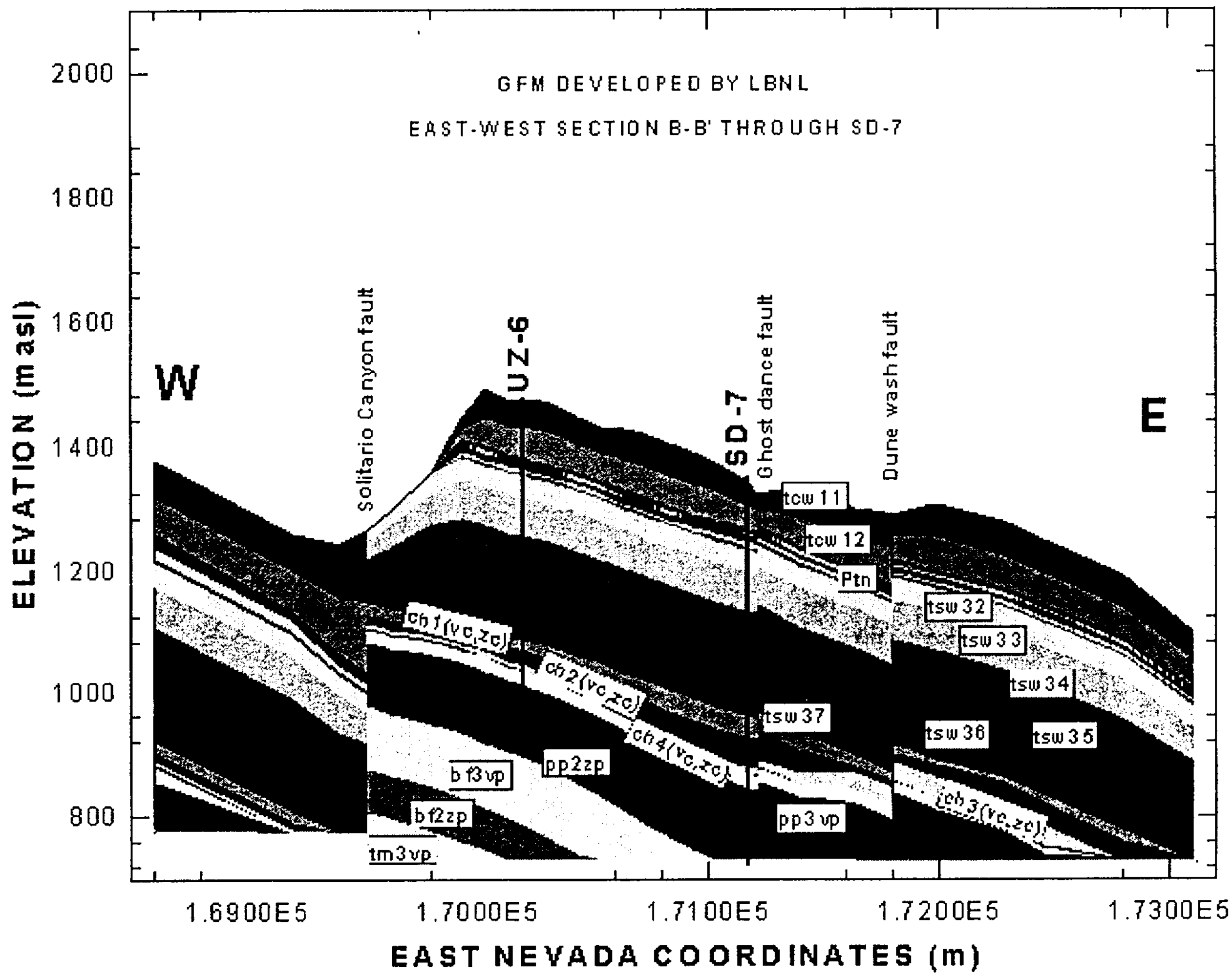
We found that the variability in fracture permeability causes the development of preferential flow paths in the fracture continuum for the welded tuff units and in the matrix continuum for the nonwelded unit. The magnitude of variance in fracture permeability correlates well with the degree of flow focusing. Water flow rates in preferential flow pathways have been found to be locally very high (more than ten times the input flow rate). Flow focusing due to the development of preferential pathways increases saturation locally. This local increase in saturation causes an increase in relative permeability to water along the pathway and may reduce the wetted surface area for fracture-matrix interaction.

Comparison of results obtained from the homogeneous and heterogeneous models of unsaturated flow through thick vadose zones shows that deep percolation can take place rapidly through persistent, preferential flow paths. These pathways are hard to detect and may carry large volumes of water. Simplification of site hydrogeology [illegible] lead to erroneous conclusions on the spatial and temporal distribution of unsaturated flow through [illegible] fractured vadose zones.

Study Objectives

- To compare deterministic and stochastic continuum analyses of water flow in thick vadose zones of fractured rocks.
- To investigate the effect of flow focusing on deep percolation in layered, heterogeneous media.
- To investigate the effects of varying σ^2 on flow focusing.
- To investigate the effects of varying water flow rate (q) on flow focusing.
- To investigate the consequences of simplifying model structure and parameters on deep percolation.

Current DOE conceptualization of Yucca Mountain

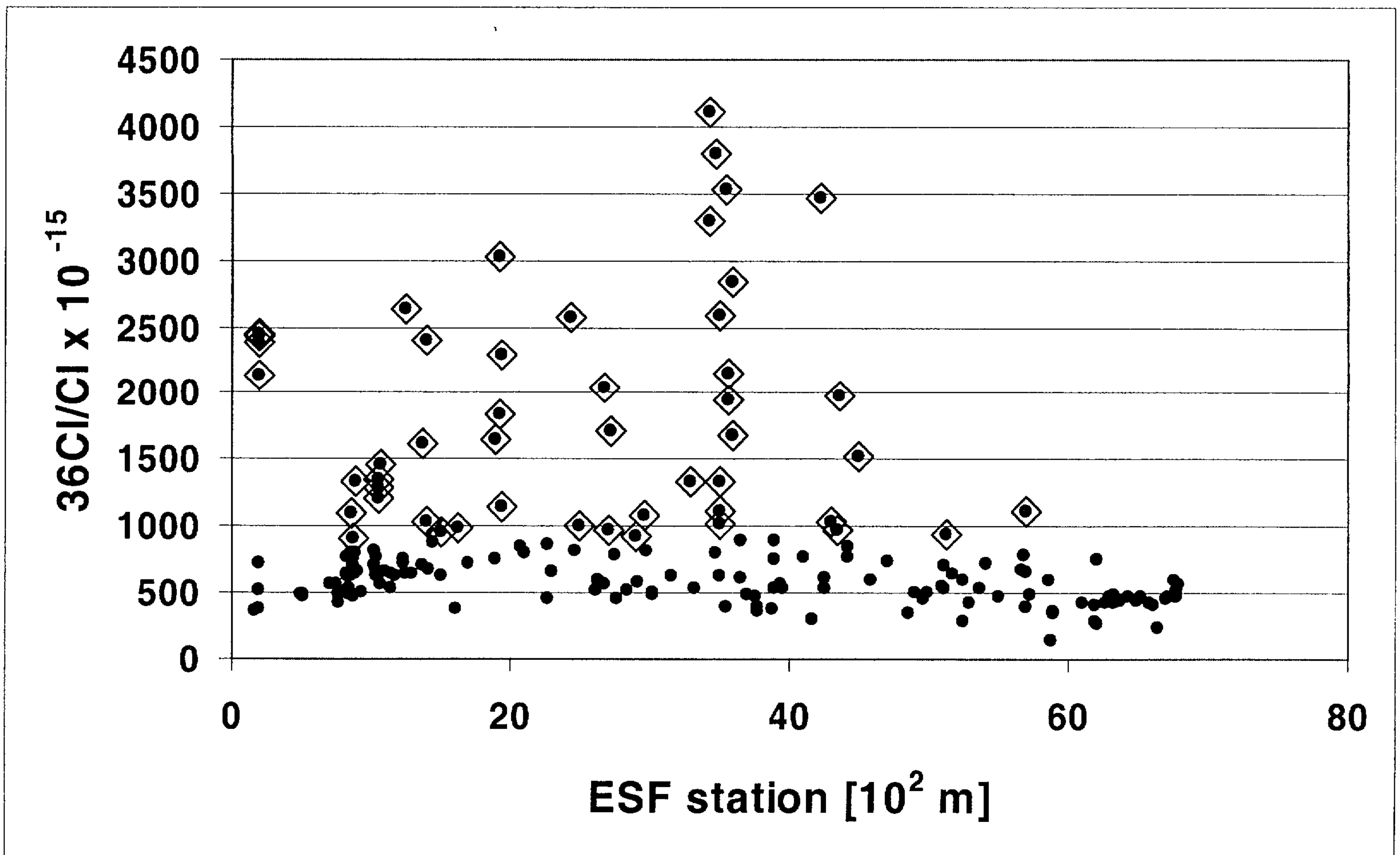


Adapted ... RWMS M&O, 1998

Complexity of Unsaturated Flow in Thick Vadose Zones of Fractured Rocks

- Episodic nature of precipitation events
- Localization of infiltration
- Poorly understood transport of water, air, and heat in the shallow subsurface
- Poorly understood constitutive relationships for unsaturated fractured rock.
- Spatial and temporal variability of water and air flow resulting from heterogeneity in rock properties at multiple scales
- Difficulty in measuring ambient percolation rates in situ

Cl-36 Data in the ESF
Evidence for fast flow?



Simulation of permeability fields

- Permeability fields - direct Fourier Transform Method developed by A. Gutjahr and his coworkers (Robin et al., 1996).
- 10 unconditional simulations were conducted to generate permeability fields with isotropic correlation scales for the TCw, PTn, and TSw units.
- Lack of information at Yucca Mountain precludes rigorous geostatistical analysis of data.

Exponential model

$$\gamma(h) = \sigma^2 \left[1 - \exp\left(\frac{-h}{\lambda} \right) \right]$$

h = separation vector magnitude

? = correlation length (2 *m*)

σ^2 = variance (0.5 - 2.0)

Mass and Energy TRAnsport (METRA)

Lichtner et al., (2000)

- Two-phases (fluid and vapor), non-isothermal flow
- Computations in 1-, 2-, or 3-D
- Block-centered structured / unstructured grids: Integrated Finite Volume (IFV)
- Single, dual, or equivalent continuum
- Flexibility in incorporating various empirical relations to describe two-phase flow properties (van Genuchten, Brooks-Corey, linear, or user-defined)
- Three primary equations solved:
  - Total mass balance
  - Air mass balance
  - Energy balance
- Primary field variables for two-phase problems:
  - Total gas pressure (p_g)
  - Partial pressure (p_a)
  - Gas saturation (s_g).
- Solution based on a fully implicit formulation using a variable substitution approach
- Spatial heterogeneity in rock flow and thermal parameters

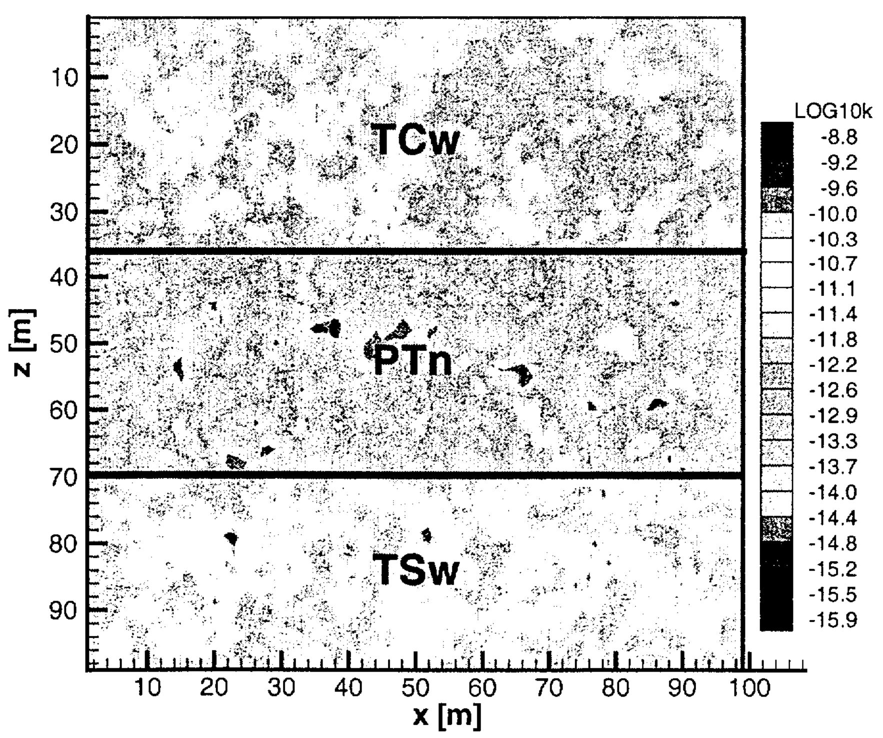
Model Assumptions

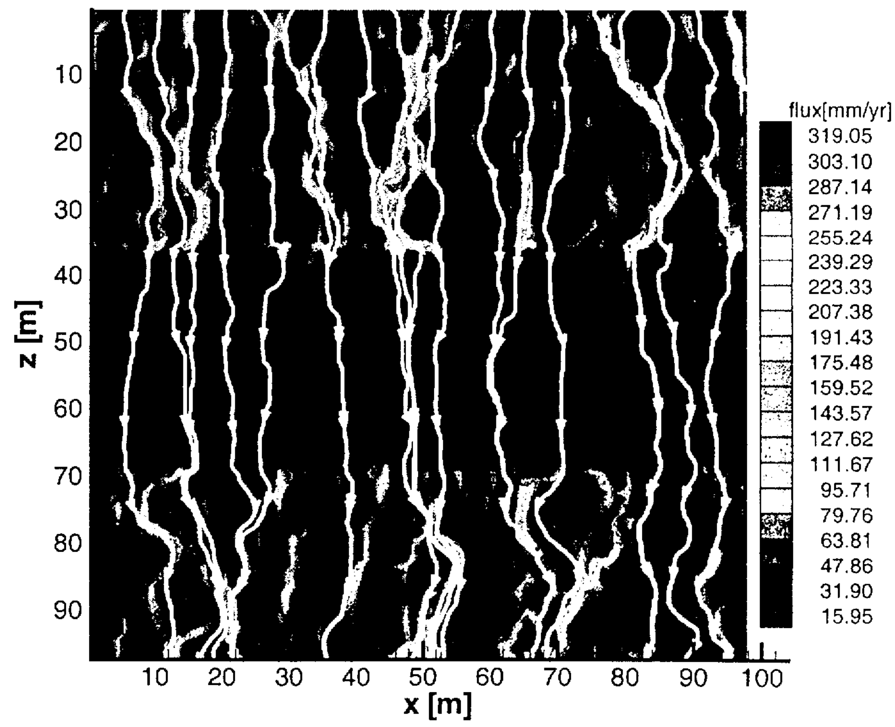
- 2D, isothermal simulation
- Dual continuum model with fractures treated as stochastic continuum; matrix treated as homogeneous continuum.
- 1 m^3 grid blocks
- 2 phase flow (air and water)
- Mixed BC at the top; no-flow BC at the sides and constant head BC at bottom.

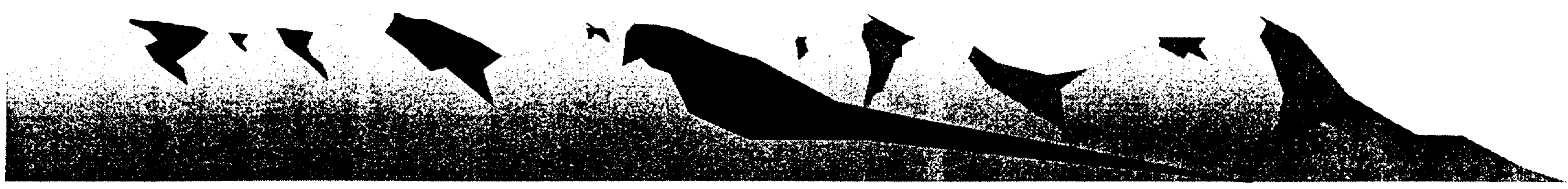
Numerical Simulation Parameters

- DCM parameters from TSPA-VA
- Fracture permeability statistical parameters:
  - Mean values from single-hole pneumatic injection tests at Yucca Mountain.
  - Variance and correlation lengths chosen arbitrarily.
  - Variance also derived from geostatistical analysis of air injection tests at the Apache Leap Research Site (ALRS).

Case 1
$\sigma^2 = 0.5$; $q = 42.5$ mm/yr

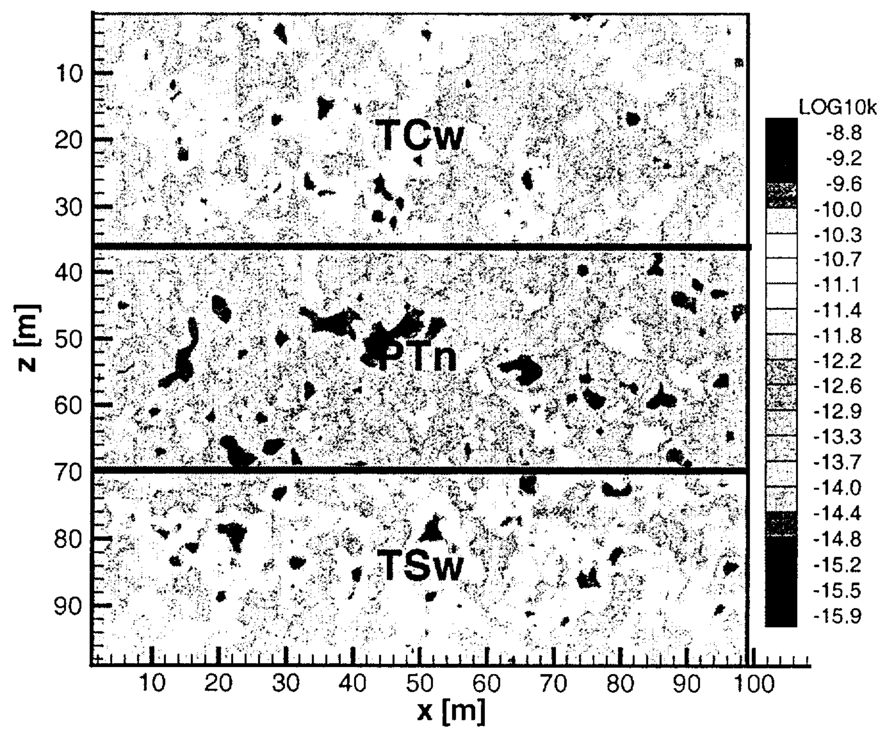




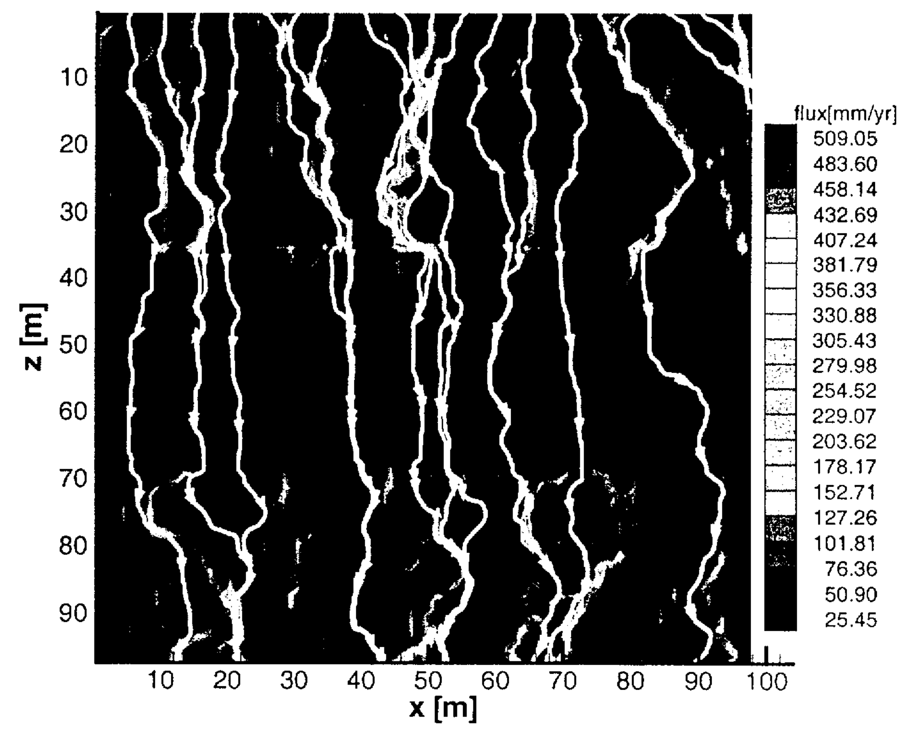


Case 2
$\sigma^2 = 1.0$; $q = 42.5$ mm/yr

Fracture continuum

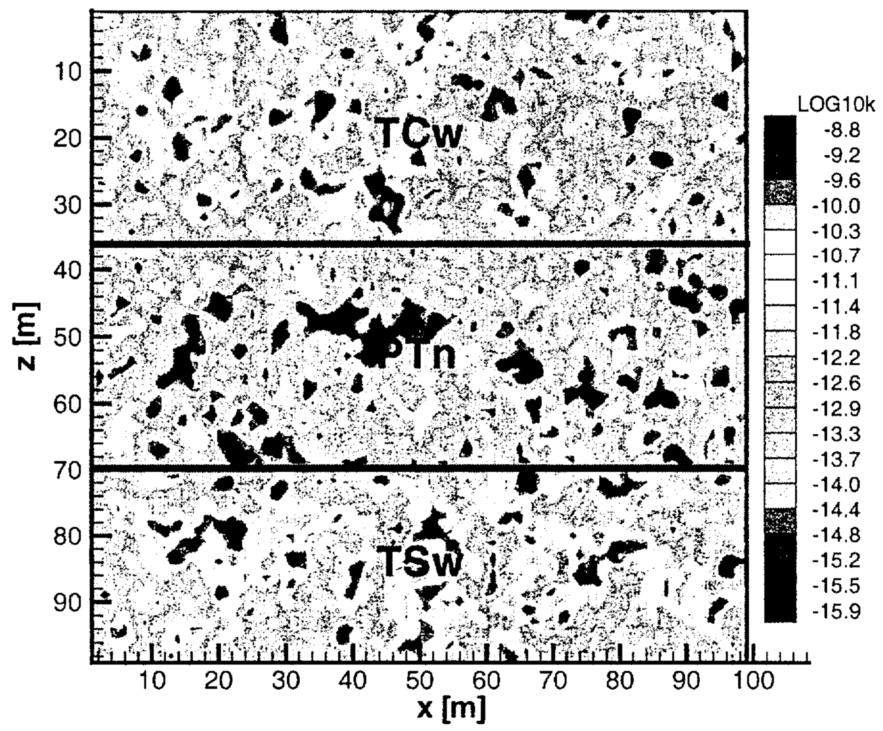


Water Flux in Fracture Continuum

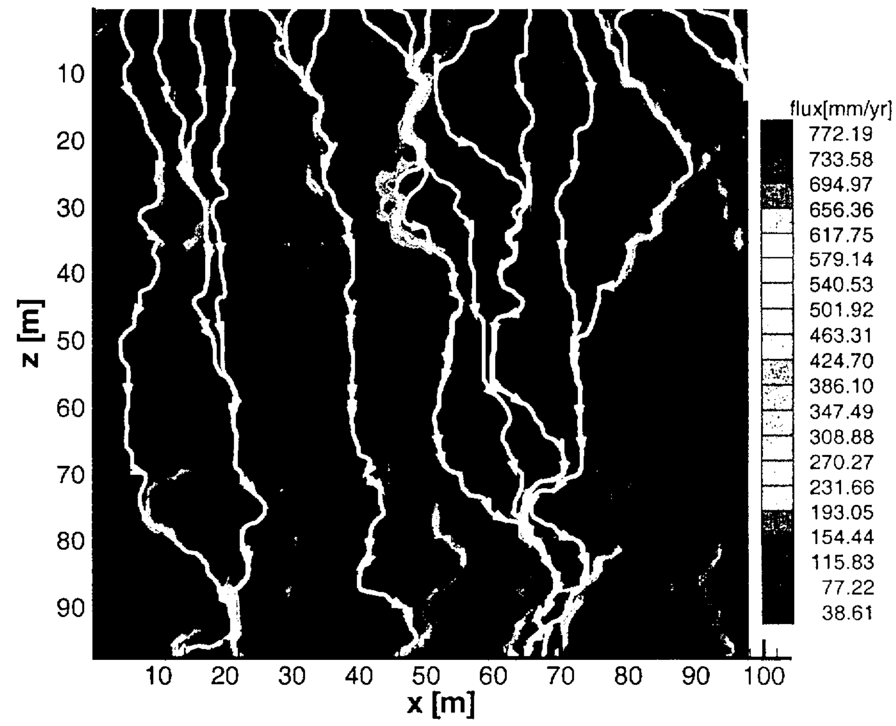


Case 3
$\sigma^2 = 2.0$; $q = 42.5$ mm/yr

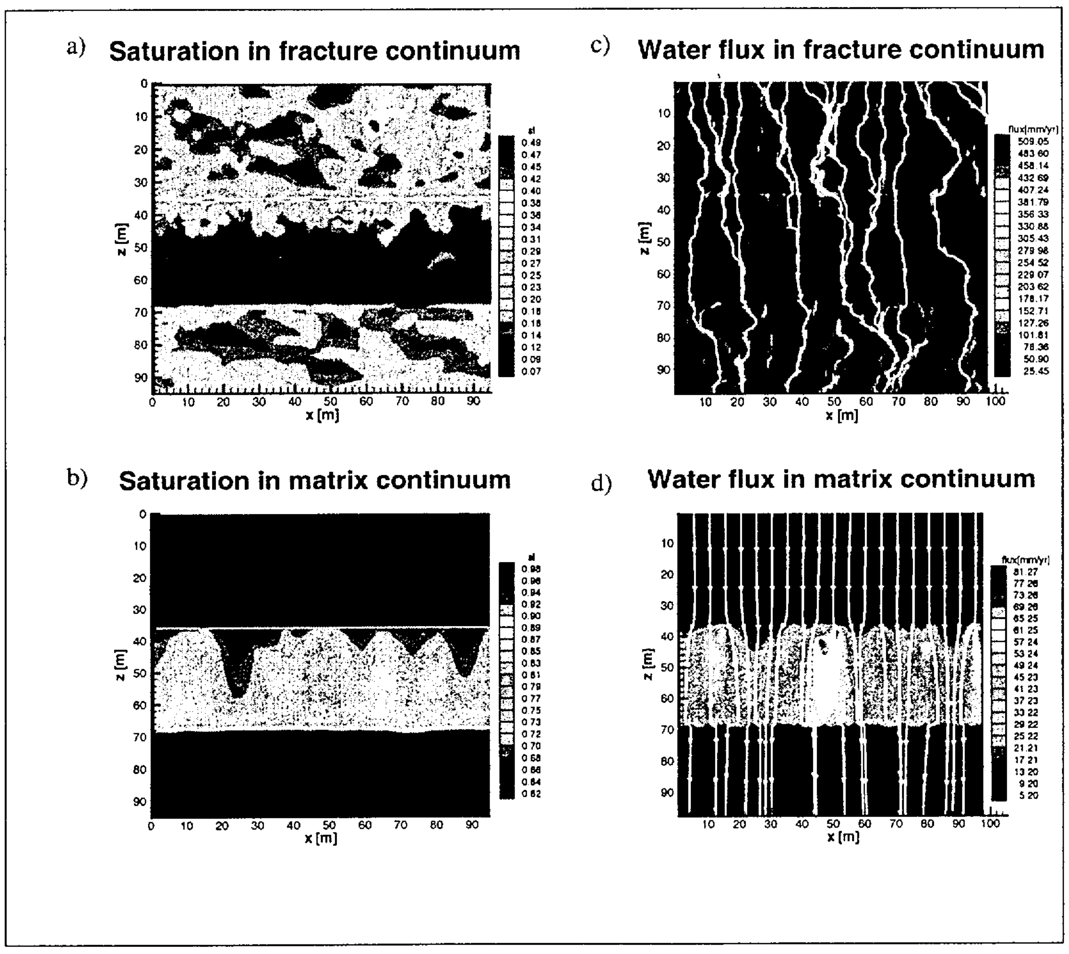
Fracture continuum



Water Flux in Fracture Continuum



Case 1
$\sigma^2 = 1.0$; $q = 42.5$ mm/yr

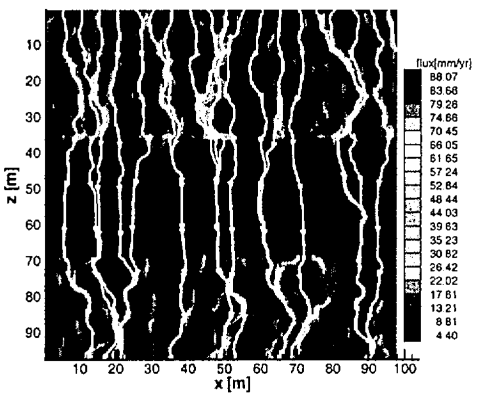


Observations

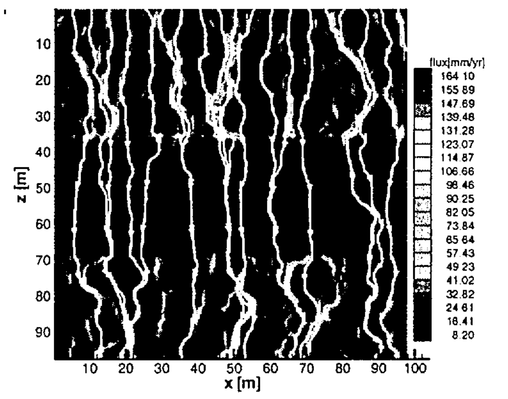
- High variability in saturation of fracture continuum in welded units (TCw, TSw).
- Variability in saturation of matrix continuum in the nonwelded unit (PTn).
- Flow focusing in fracture continuum of TCw and TSw
- Flow focusing in matrix continuum of PTn.

Variation in flow rate at top boundary

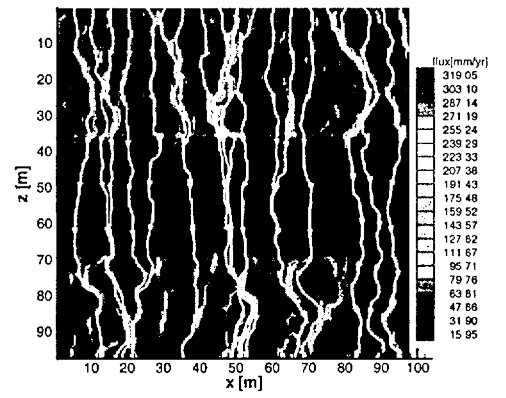
$\sigma^2 = 0.5$; $q = 12.5$mm/yr



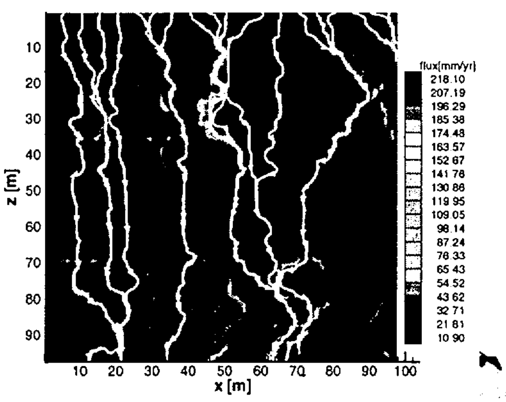
$\sigma^2 = 0.5$; $q = 22.5$mm/yr



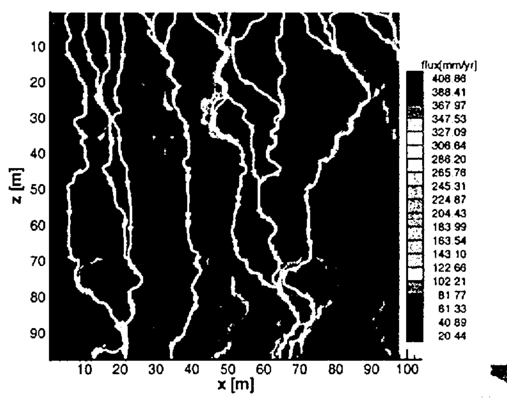
$\sigma^2 = 0.5$; $q = 42.5$mm/yr



$\sigma^2 = 2.0$; $q = 12.5$mm/yr



$\sigma^2 = 2.0$; $q = 22.5$mm/yr



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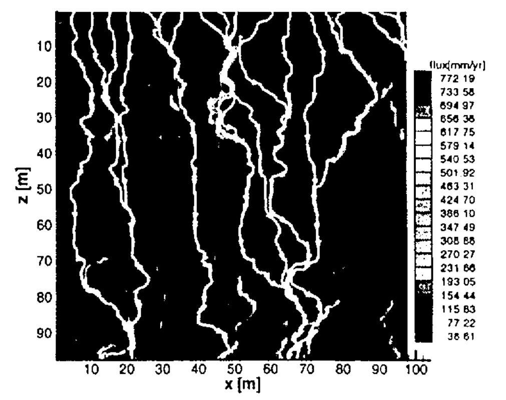

Conclusions

- Preferential flow paths develop in the fracture and matrix despite the uniform application of water at the top boundary and without explicitly building in high permeability pathways or discrete features that represent fractures.

- The development of preferential pathways in the fracture continuum increases the relative permeability to water along these pathways and reduces the wetted surface area for fracture-matrix interaction.

- Water flow rates in preferential flow pathways can be locally very high (more than ten times the input flow rate).

Conclusions (cont.)

- The presence of the nonwelded PTn in the UZ led to the past conceptualization that deep percolation at Yucca Mountain becomes attenuated and laterally diverted once it reaches the PTn unit. Our model shows that:
  - (a) rapid flow takes place through persistent, preferential flow paths in the TCw and TSw units;
  - (b) the focusing of flow at the TCw/PTn contact causes localized increases in matrix saturation that can extend from the TCw/PTn contact to the PTn/TSw contact;
  - (c) increase in saturation causes the development of preferential pathways in the PTn matrix continuum; and
  - (d) the preferential pathways allow for the rapid, predominantly downward movement of water through the unit.

Conclusions (cont.)

- Comparison of results obtained from the homogeneous and heterogeneous models of unsaturated flow through thick vadose zones shows that deep percolation can take place rapidly through persistent, preferential flow paths.

- These pathways are hard to detect and may carry large volumes of water. Simplification of site hydrogeology may lead to erroneous conclusions on the spatial and temporal distribution of unsaturated flow through thick, fractured vadose zones.

- The effect of episodic infiltration on unsaturated flow through thick, layered vadose zone is currently under investigation.

References

- Civilian Radioactive Waste Management System Management and Operating Contractor, Chapter 2 *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document, Unsaturated Zone Hydrology Model*, B00000000-01717-4301-00002 REV 00, Las Vegas, NV, Civilian Radioactive Waste Management System Management and Operating Contractor, 1998.

- Flint, L. E., 1998, Characterization of hydrogeologic units using matrix properties, Yucca Mountain, Nevada, US Geological Survey Water Resources Investigation Report 98-4243, US Geological Survey, Denver, CO.

- Lichtner, P. C., M. S. Seth, and S. Painter, 2000, MULTIFLO User's Manual, MULTIFLO Version 1.2, Two-phase Nonisothermal Coupled Thermal-Hydrologic-Chemical Flow Simulator, Center for Nuclear Waste Regulatory Analyses, San Antonio, Texas, Rev. 2 Change 0, January 2000.

- Robin, M. J. L., A. L. Gutjahr, E. A. Sudicky, and J. L. Wilson, 1993, Cross-correlated random field generation with the direct Fourier Transform Method, Water Resources Research, Vol. 29, No. 7, 2385-2397.