A CHAOTIC-DYNAMICAL CONCEPTUAL MODEL TO DESCRIBE FLUID FLOW AND CONTAMINANT TRANSPORT IN A FRACTURED VADOSE ZONE

Project 55359

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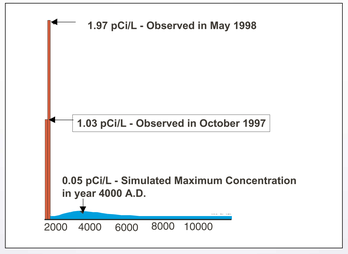
I. STATEMENT OF PROBLEM

Fractured Rock Research Needs

- To protect human health and the environment, numerous INEEL sites require remediation and long-term monitoring
- Contaminants in fractured rock include radionuclides (Cs, Sr, U, Tc) and volatile organic compounds
- Available characterization and monitoring technologies for fractured rocks are often expensive or inadequate to detect preferential flow and transport phenomena

Comparison of Actual and Simulated Americium-241 Concentrations in Groundwater at the Radioactive Waste Management Complex of INEEL

from Magnuson and Sondrup, 1998

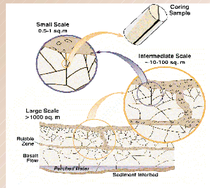


II. OBJECTIVES

- Determine if dynamical chaos theory better describes and predicts infiltration of fluid and contaminant transport in heterogeneous fractured rocks than deterministic and stochastic methods
- Apply multiscale, hierarchical characterization of flow and transport in fractured basalt vadose zones

III. METHODS AND RESULTS

Hierarchy of Scales of Investigations in Fractured Basalt

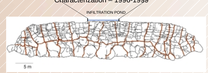


Radioactive Waste Management Complex – Spring Flooding 1962

Large Scale Infiltration Test - 1994

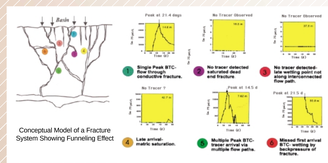
Analog Site for Fractured Rock Characterization – 1996-1999

Hell's Half Acre Chaos Research Site - 1997-1999



IIIa. LARGE-SCALE INFILTRATION TEST

Typical Multimodel Breakthrough Curves for Se-75 Observed During the Test

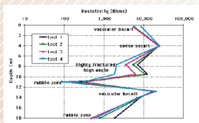


IIIb. INTERMEDIATE-SCALE PONDED INFILTRATION TESTS IN FRACTURED BASALT AT BOX CANYON SITE

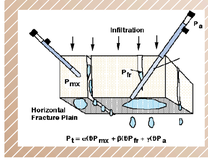
Intermediate-Scale Investigations at the Box Canyon Site

Fractured Basalt:

- Is highly heterogeneous with localized fast flow paths
- Has nonconductive fractures and matrix where contaminants are accumulated



Depth profiles of time averaged resistivity in well II-5 during pulsed infiltration tests showing that the tracer appeared mostly within the fractured zones



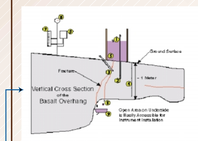
The tensiometer gauge pressure is primarily affected by the water-conducting component that transmits water into or out of the ceramic cup of the tensiometer:

During drying—by matrix pressure, and

During wetting—by fracture pressure

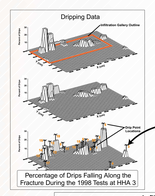
IIIc. SMALL-SCALE INFILTRATION TESTS AT HELL'S HALF ACRE SITE

Test Design

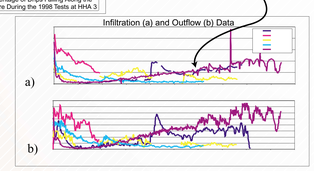


1. HEAD AND INFILTRATION RATE AND/OR INFLOW RATES — Mass balance of the system, Boundary conditions for modeling efforts, determining temporary variations in flow/infiltration.
2. BASALT MATRIX WATER PRESSURE — Examine wetting front propagation and volume of water imbibed into matrix, aid in determination of mass balance, examine drain-out of matrix following testing.
3. FRACTURE WATER PRESSURE — Define head field around matrix blocks, examine pressure propagation through system, aid in mass balance calculations, compare with laboratory experiments.
4. BASALT TEMPERATURES — Determine flue viscosities, examine thermal gradients in basalt matrix, examine any thermal effects of flowpaths.
5. AIR AND WATER TEMPERATURES — Determine fluid viscosities, use as background for instrument corrections, examine thermal effects on flow.
6. BAROMETRIC PRESSURE — Determine boundary conditions, examine pressure relationships between the air phase and liquid phase, calculate instrument efficiency.
7. PRECIPITATION — Provide background values for mass balance calculations, determine larger scale head/moisture fields at the research site.
8. OUTFLOW DRIP INTERVALS — Examine with high resolution the temporal and spatial variability of fracture outflow, provide detailed time series data for chaotic analysis, compare with laboratory experiments.
9. OUTFLOW RATES ALONG FRACTURE — Examine temporal and spatial variation of outflow, determine mass balance of the system.

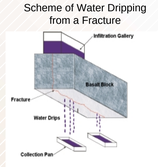
Typical Results of Observations



- Tests Not Repeatable Under Same Ponding Conditions
- Flowpaths Highly Variable in Time and Space
- Infiltration and Outflow Highly Unstable in Time and Space



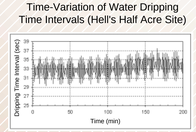
Scheme of Water Dripping from a Fracture



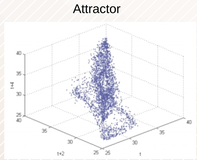
Water dripping from a single location can be described using a chaotic model with some random component

Steady state was never achieved for any appreciable length of time.

Time-Variation of Water Dripping Time Intervals (Hell's Half Acre Site)



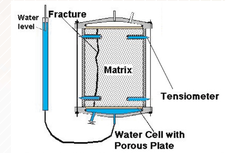
Attractor

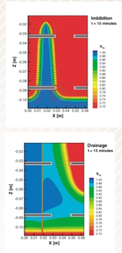


Podgorney, Wood, Faybishenko, and Stoops, 2000

IV. LABORATORY INVESTIGATIONS

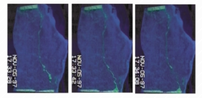
IVa. LABORATORY CORE EXPERIMENT: What Tensiometers Measure?





IVb. WATER SEEPAGE IN A FRACTURED BASALT REPLICA

We investigate dripping water between parallel plates as a model of water seepage through fractured rock and look for the existence of a chaotic component of such flow. This can be viewed as an extension of the classic chaos experiments with the "dripping faucet" (Shaw, 1984) to drips in the presence of capillary forces as they are affected by the surface properties and the small aperture of the parallel plates.

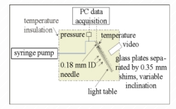


Water seepage through a dense basalt fracture is visualized by mating the fracture with a transparent replica of the other fracture half, dyeing the water with a fluorescent dye and illuminating with near-UV light.

Time-varying water seepage in fractures undergoes channeling during a cycle of filling and draining.

While deterministic numerical models with stochastically distributed soil properties can describe the general spatial features of liquid distribution, they do not describe intermittent flow, which can significantly affect predictions of solute travel-time and solute-solid interaction.

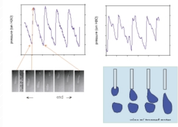
IVc. DESIGN OF WATER DRIPPING EXPERIMENTS



A constant flow rate of water to a needle emplaced between parallel glass plates of sub-millimeter separation.

Pressure responds to the formation and release of drips from the needle, verified by video photography.

The time-trend of the pressure is measured for a range of flow rates and surface texture of the glass plates.

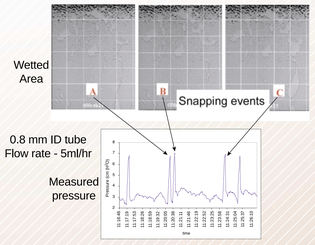


Effect of Glass Plate Texture on Water Drips

The water thread snaps in the smooth plates when the weight of the water drop overcomes the capillary forces due to the presence of the small aperture.

In the rough plates, the drop merges with residual water in the region of the needle, generating a longer drop that overcomes the capillary forces and flows down the plates, as shown in the cartoon.

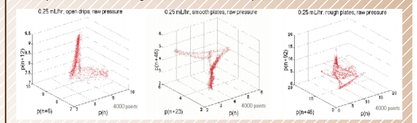
Constant Flow Rate Water Injection in a Transparent, Variable Aperture Fracture



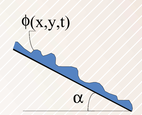
Effect of Capillarity on Attractor

The presence of chaos in the dripping data is characterized with phase-space plots for the raw pressure measurements, and the times between drips.

Pressure data. Attractors using the pressure data for the open drip , smooth plates, and rough plate conditions for 0.25 mL/hr show an increased deterministic-chaotic component as the flow regime becomes more complex.



V. 1D SPATIAL-TEMPORAL EVOLUTION EQUATION FOR FILM FLOW DOWN AN INCLINED PLANE

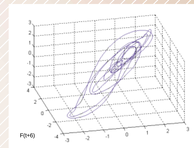


Inclined plane with a disturbed film

$$\phi_t + \phi\phi_z + \phi_{zz} + \phi_{zzzz} = 0$$

Nonlinear advection — Destabilizing dispersion and viscosity — Stabilizing hydrostatic and capillary pressure

3D attractor of film thickness



The magnitude of deterministic-chaotic and stochastic components in the data was analyzed using a set of nonlinear dynamical parameters such as Hurst exponent, Lyapunov exponent, capacity dimension, correlation dimension, information dimension, correlation time, and constructed and three-dimensional attractors in phase-space.

VI. CONCLUSIONS

- The System is Chaotic if the System Processes are:
  - Nonlinear
  - Dissipative
    - dissipates energy in space and time
    - contains elements that exhibit temporal fluctuations
  - Sensitive to initial conditions and oscillate because of intrinsic properties of the system, but not random external factors
  - Irreversible
- A new discovery coming from the field ponded infiltration tests conducted at two fractured rock field sites, the Hell's Half Acre (the scale of 1 x 0.5 m) and the Box Canyon (scale of 7 x 8 m) sites, is the temporary and spatial instability of water flow affecting rock permeability.
- Several new technologies have been developed including piezoelectric probes, a leak detection system, a laser surveying system, and a 3D Electrical Resistivity Tomography system.
- TOUGH2 numerical modeling with a hierarchical pattern of column-bounding and column-normal fractures confirmed the presence of complex, irregular flow paths for liquid-phase tracer, as well as air trapping and escaping in the vadose zone.
- Laboratory experiments showed the presence of chaotic behavior in water seepage through fracture models, and the pervasiveness of highly localized and extremely nonuniform flow paths in the plane of the fracture.
- Ongoing theoretical studies have shown that as a fluid film flows on an inclined fracture surface, it is inherently unstable and exhibits chaotic behavior, even for low Reynold's numbers. Chaotic film flow may enhance the fracture-matrix interaction and accelerate contaminant transport.

The Scientific Significance of the Vadose Zone Research for DOE

- The development of a unique nonlinear-dynamics method for data sets such as fracture and matrix flow rates, pressure, and tracer concentrations.
- The results of this project are expected to change the current approach used by industry to predict flow and transport in environmental systems.
- Because the nonlinearity of environmental systems limits their predictability, we aim to determine how far into the future it is realistic to predict the state of the environmental system, and determine the bounds for contaminant transport. This information will be used to design remediation efforts.
- The significance of the research for the DOE will be in the form of technology developed for vadose zone monitoring and in improved vadose zone site characterization and predictability.

Application of New Methods for Characterization, Monitoring, and Predictions of Environmental Sites

- Geologic Characterization using fractal models of the fracture pattern
- Hydrogeologic settings using deterministic chaotic models of permeability distribution
- Predictions of the movement and fate of contaminants using models of deterministic and stochastic chaotic spatial and temporal evolution of unsaturated, preferential flow

New Experimental Tools and Methods are Ready to be Deployed at DOE Sites

- Remotely operated:
  - deep tensiometers
  - suction lysimeters
  - unsaturated zone fluxmeter
- Miniature electrical resistivity probes for point and cross-borehole measurements
- Water dripping sensors
- New design of monitoring of infiltration tests

R & D Transition Strategy

Conduct Theoretical, Experimental, and Modeling Investigations

- Develop algorithms for predicting 3D preferential flow and transport based on chaos theory
- Prove the concept that in situ chaotic mixing can be used for accelerated remediation of NAPLs and VOCs in fractured rocks and heterogeneous soils

Provide Recommendations for Regulators

- Conduct field demonstration infiltration tests with tracers using developed tools and methods
- Recommend improvements to soil cleanup and segregation technologies for dispersed radionuclides at existing DOE sites.
- Alleviate stockholder concerns over mismatches between transport models and observations
- Risk assessment under CERCLA, and performance assessment per NRC regulations.
- Enhanced decontamination of soils using vacuum extraction and groundwater treatment using a modified pump-and-treat approach.
- Ongoing and potential applications at INEEL, LBNL, Yucca Mountain, Hanford, and Apache Leap Site.

WEB SITES:
http://www-esd.lbl.gov/ERT/esp.html
http://www.osti.gov/em52/1997projsum/55359.pdf
http://www.osti.gov/em52/1998projsum/55359.pdf
http://www.osti.gov/em52/1999projsum/55359.pdf

Main Publications

Benito, P.H., P. J. Cook, B. Faybishenko, B. Freifeld, and C. Doughty. "Cross-Well Air-Injection Packer Tests for the Assessment of Pneumatic Connectivity In Fractured, Unsaturated Basalt", Rock Mechanics for Industry, Amadei, Kranz, Scott & Smeallie (eds), Balkema, Rotterdam, 843-851. 1999.

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Pruess, K., B. Faybishenko, and G. S. Bodvarsson, Alternative concepts and approaches for modeling flow and transport in thick unsaturated zones of fractured rocks, Journal of Contaminant Hydrology - Special Issue, 38, 281-322, 1999.

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Acknowledgments

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