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Project Title: **Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone**

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A Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone

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RESEARCH OBJECTIVE:

DOE faces the remediation of numerous contaminated sites, such as those at Hanford, INEEL, LLNL, and LBNL, where organic and/or radioactive wastes were intentionally or accidentally released to the vadose zone from surface spills, underground tanks, cribs, shallow ponds, and deep wells. Migration of these contaminants through the vadose zone has led to the contamination of (or threatens to contaminate) underlying groundwater. A key issue in choosing a corrective action plan to clean up contaminated sites is the determination of the location, total mass, mobility and travel time to receptors for contaminants moving in the vadose zone. These problems are difficult to solve in a technically defensible and accurate manner because contaminants travel downward intermittently, through narrow pathways, driven by variations in environmental conditions. These preferential flow pathways can be difficult to find and predict.

The primary objective of this project is to determine if and when dynamical chaos theory can be used to investigate infiltration of fluid and contaminant transport in heterogeneous soils and fractured rocks. The objective of this project is being achieved through the following activities:

- Development of multi scale conceptual models and mathematical and numerical algorithms for flow and transport, which incorporate both (a) the spatial variability of heterogeneous porous and fractured media and (b) the temporal dynamics of flow and transport

- Development of appropriate experimental field and laboratory techniques needed to detect diagnostic parameters for chaotic behavior of flow

- Evaluation of chaotic behavior of flow in laboratory and field experiments using methods from non-linear dynamics

- Evaluation of the impact these dynamics may have on contaminant transport through heterogeneous fractured rocks and soils and remediation efforts.

This approach is based on the consideration of multi scale spatial heterogeneity and flow phenomena that are affected by nonlinear dynamics, and in particular, chaotic processes. The scientific and practical value of this approach is that we can predict the range within, which the parameters of flow and transport change with time, which allows us to design and manage the remediation even when we cannot predict the behavior at any point or time.

RESEARCH PROGRESS AND IMPLICATIONS:

This progress report summarizes work after two years and eight months of a three-year project.

A series of ponded infiltration tests with tracers was conducted in Idaho at two fractured rock field sites: the Hell's Half Acre (a pond scale of 1 by 0.5 m) and the Box Canyon (a pond scale of 7 by 8 m). Field investigations included monitoring of water movement at drip points, geophysical (radar and electrical resistivity) imaging, measurements of the moisture content, water flow rate, water pressure in the rock matrix and fractures, subsurface tracer distribution, and temperature. Several new technologies have been developed specifically for this project including piezoelectric probes, a leak-detection system, a laser-surveying system, and a 3D electrical resistivity tomography system. The temporal and spatial nonlinear evolution and instability of unsaturated flow were characterized for the first time in fractured basalt.

Laboratory experiments were conducted to evaluate the presence of chaotic behavior in water seepage through fracture models, which have shown the pervasiveness of highly localized and extremely nonuniform flow paths in the plane of the fracture. Using the time-trend of a pressure signal for unsaturated flow in fracture models, the magnitude of deterministic-chaotic and stochastic components in the data were analyzed. For this purpose, several diagnostic parameters were determined, such as the Hurst exponent, Lyapunov exponent, correlation dimension, information dimension, correlation time, and constructed three-dimensional attractors in phase-space.

We performed numerical modeling of the Box Canyon ponded infiltration tests using the TOUGH2 code with an explicit, yet simplified representation of the key geologic and hydrogeological features (a hierarchical pattern of column-bounding and column-normal fractures in fractured basalt). This modeling confirmed (a) the presence of complex, irregular flow paths for liquid-phase tracer, as well as air trapping and escaping in the vadose zone, and (b) the hypothesis that temporal aspects of chaotic flow, identified in laboratory and field experiments, cannot be captured using conventional modeling approaches.

Theoretical studies have shown that as a fluid film flows on a nonhorizontal fracture surface, it is inherently unstable and may exhibit chaotic behavior, even for low Reynold's numbers. Film waviness may enhance transfer of contaminants from rock to fluid by as much as five times, carrying contaminated fluid much faster than expected by classical flat-film theory.

The scientific significance of the research rests in (a) the unique nonlinear dynamics analysis of data sets such as fracture and matrix flow rates, pressure, and tracer concentrations, and (b) the development of a new dynamical chaotic model for flow and transport in fractured media. The results of this project are expected to change the conventional approach of using traditional stochastic and/or deterministic methods to predict flow and transport in environmental systems. Because the nonlinearity of environmental systems limits their predictability into the future, we aim to determine how far into the future it is realistic to predict the state of the environmental system, what the bounds on the time of contaminant transport are, and how long we can expect clean-up to take. The significance of the research for the DOE will be new technology developed for vadose-zone monitoring and in improved vadose zone site characterization and predictability.

PLANNED ACTIVITIES:

Additional field experiments will be conducted in 1999 to examine the tracer transport and fracture-matrix interactions. Analysis of existing data from DOE sites (INEEL, LBNL, LLNL, and other) will be completed. Final reports and publications will be submitted and made available to the environmental community at large. The methodology developed will be recommended to DOE sites where monitoring and remediation of contaminants using vacuum extraction, air stripping, steam injection, barriers, etc., are problems.

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5. Podgorney, R. K., and T. R. Wood, Observations of water movement in variably saturated fractured basalt and its possible implications on predictive modeling, In Proceedings of the International Symposium *Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances*, pp. 300-304, Berkeley, CA, 1999.

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9. Carrigan, C. R, Hudson, G. B., Martins, S.A., Ramirez, A. L., Daily, W. D., Buettner, H. M., Nitao, J. J., Ralston, D. K., Ralston, D. K., Ekwurzel, B., Moran, J. E., Faybishenko, B. A., and McCarthy, J. F., Lessons on Transport and Monitoring From the LLNL Vadose Zone Observatory, *Proceedings of the 1999 Spring AGU Meeting*, Boston.

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1. Babchin, A.J., Faybishenko, B., G.I. Sivashinsky, A. Frenkel, and D. Halpern, A model of chaotic time evolution of a slow liquid film on an inclined plane: One-dimensional solution. LBNL Report 42884, 1999.

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The DOE press release "Water Travels Chaotically Through The Ground" of December 17, 1999 about the project "A Chaotic-Dynamical Conceptual Model to Describe Fluid Flow and Contaminant Transport in a Fractured Vadose Zone" (see Web site http://www.eurekalert.org/releases/ineel-wtcttg.html) was published by four reporters.

Several papers are in preparation.

Invention Disclosures

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