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

Principle Investigator
Boris Faybishenko, Tel: 510/495-4852, Fax: 510/486-5686, email: bafaybishenko@lbl.gov

Lawrence Berkeley National Laboratory
Mail Stop 90-1116

Co-Investigators:
C. Doughty, J.T. Geller, S. Borglin, B.L. Cox, J.E. Peterson, Jr., M. Steiger, and K.H. Williams (LBNL)
T. Wood and R. Podgorney, (Parson's Engineering Inc.)
T. Stoops, (INEEL)
S. Wheatcraft, M. Dragila and J.C.S. Long, (UNR)

ABSTRACT

Understanding subsurface flow and transport processes is critical for effective assessment, decision-making, and remediation activities for contaminated sites. However, for fluid flow and contaminant transport through fractured vadose zones, traditional hydrogeological approaches are often found to be inadequate. In this project, we examine flow and transport through a fractured vadose zone as a deterministic chaotic dynamical process, and develop a model of it in these terms. Initially, we examine separately the geometric model of fractured rock and the flow dynamics model needed to describe chaotic behavior. Ultimately we will put the geometry and flow dynamics together to develop a chaotic-dynamical model of flow and transport in a fractured vadose zone.

We investigate water flow and contaminant transport on several scales, ranging from small-scale laboratory experiments in fracture replicas and fractured cores, to' field experiments conducted in a single exposed fracture at a basalt outcrop, and finally to a ponded infiltration test using a pond of 7 by 8 m. In the field experiments, we measure the time-variation of water flux, moisture content, and hydraulic head at various locations, as well as the total inflow rate to the subsurface. Such variations reflect the changes in the geometry and physics of water flow that display chaotic behavior, which we try to reconstruct using the data obtained.

In the analysis of experimental data, a chaotic model can be used to predict the long-term bounds on fluid flow and transport behavior, known as the attractor of the system, and to examine the limits of short-term predictability within these bounds. This approach is especially well suited to the need for short-term predictions to support remediation decisions and long-term bounding studies.

1.0 Objectives and Structure of the Project

Our primary objective is to determine when and if deterministic chaos theory is applicable to infiltration of fluid and contaminants through the vadose zone in fractured rock. To the extent that this theory is applicable we will develop algorithms for predicting flow and transport based on this theory.

In classical analysis, the system components are commonly taken to be cubes of equivalent porous media that tessellate the volume of interest. The rules used to describe multi-phase fluid flow are commonly given by Richard's Equation, a version of Darcy's Law, which describes how much fluid will be transferred as a function of the hydraulic head gradient and relative permeability.

For the case of infiltration in fractured rock, we will describe the geometry of the fracture network and determine the rules describing how fluid is transmitted as dynamical processes. The result of evaluating these processes will be an entirely new approach to the description of flow and transport behavior. The objectives of this project will be achieved through the development of:

- A hierarchical description of fracture geometry that controls fluid flow and transport
- A dynamical description of infiltration and transport of contaminants in single fractures
- An algorithm for flow and transport which combines the hierarchical geometry and the description of dynamical flow and transport
- Appropriate techniques needed to detect chaotic behavior of flow in the field
- Evaluation of deterministic chaos in laboratory and field experiments

2.0 Background Information on Chaotic Dynamics and Fractal Structures

One of the central problems in the prediction of water, heat, and mass transfer in soils and fractured rocks is how to use past observations in order to predict the future. Field measurements can only employ a limited number of probes that cannot collect all needed information. Consequently, the quality of prediction using classical deterministic and stochastic differential equations with a set of initial and boundary conditions and volume-averaged parameters may become poor. One of the alternative approaches views a time series of data as a result of chaotic dynamics, which can appear even in a simple deterministic system. Random-looking data may in fact represent chaotic rather than stochastic processes. For predictive purposes, it is critical to recognize which is which, because for chaotic systems often only short-term predictions can be made. For example, it was shown that the weather predictability will approach zero for predictions of more than two weeks (Lorenz, 1982).

The differences between regular (non-chaotic deterministic), random, and chaotic systems, are illustrated in Figure 2.1, which shows trajectories typical for each type of motion. Note that the flow trajectories for chaotic systems are different from both regular and stochastic systems. In general, the term chaotic process is used to describe a dynamical process with the following features: random processes are not a dominant part of the system, the trajectories describing the future states of the system are strongly dependent on initial conditions, adjacent trajectories diverge exponentially with time, the information on initial conditions cannot be recovered from later states of the system, and behavior is often characterized by an attractor that has a fractal geometry.

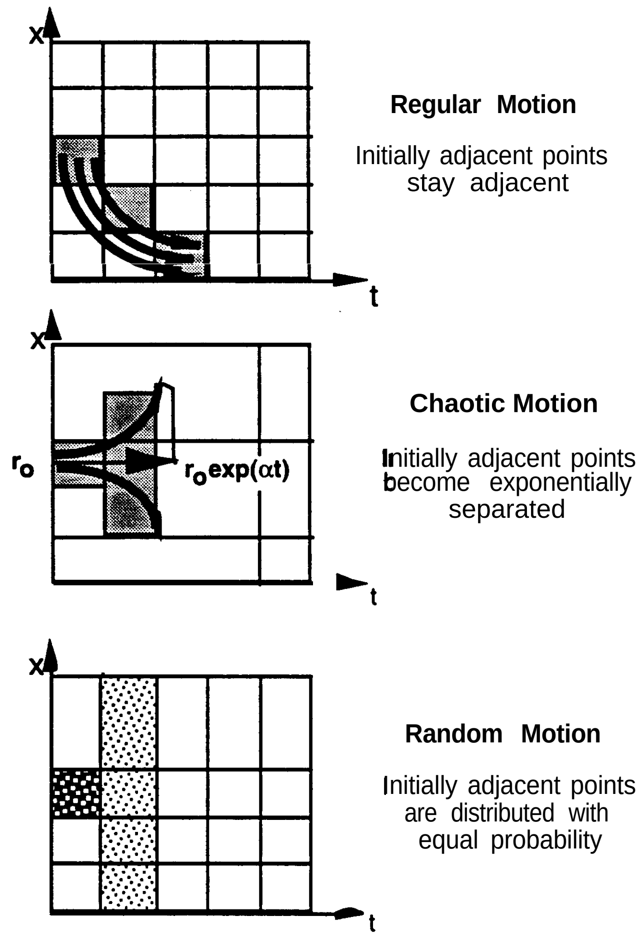

Figure 2.1 Comparison of regular (i.e., non-chaotic deterministic), chaotic, and random behavior (modified from Schuster, 1993).

Chaotic flow behavior in heterogeneous fractured media may result from hydrodynamic instabilities and a sensitive dependence of flow on (1) boundary conditions (precipitation, ambient temperature and pressure, groundwater fluctuations, etc.), (2) initial conditions (distribution of water content, pressure, and temperature), and (3) the current state of the system (water content, pressure, and temperature). Flow depends upon coupled effects of several non-linear factors such as the geometrical connectivity of the fracture system, air entrapment and its removal, clogging of the conductive fractures, biofilms, kinetics of the matrix-fracture water exchange, variability of effective hydraulic porosity and hydraulic permeability, and others.

The coupled effect of several non-linear processes in an unsaturated heterogeneous and fractured material causes non-linear behavior, governed by non-linear ordinary and partial differential equations, which may have bounded, nonperiodic solutions. These equations may be either: (1) purely deterministic where no random quantities appear in the equations (Moon, 1987; Tsonic, 1992), (2) chaotic-stochastic, or (3) have a noisy component (Kapitaniak, 1988). Therefore, one of the main problems in data analysis is to properly identify the type of the equation describing the flow system.

There are numerous examples of dynamical systems that display non-linear chaotic behavior for some system parameters. Some examples relevant to our study are: avalanche fluctuations resulting from the perturbation of sandpiles of various sizes (Rosendahl et al., 1993), falling off of water droplets (Cheng et al., 1989), atmospheric temperature, river discharge, and precipitation (Pastemack, 1996; Pelletier, 1996), and oxygen isotope concentrations (Nicolis and Prigogine, 1989). One of the simplest examples is a dripping faucet (Shaw, 1984). Figure 2.2 shows a conceptual model of flow in fractured rocks based on a model of irregularly dripping water through a fracture, which produces non-periodic and non-repetitive behavior in both time and space.

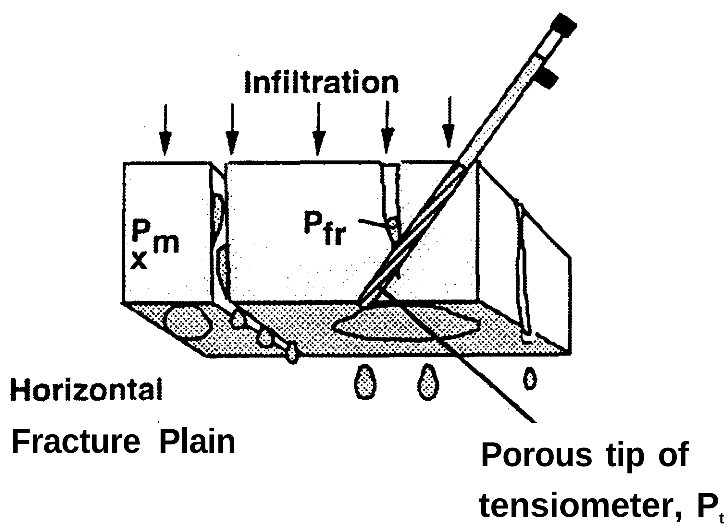

Figure 2.2 Conceptual model of flow and measurement in partially saturated fractured rocks

It has been recognized that fractal structure is a possible indication of chaotic behavior of a system (Mandelbrot, 1977). Fractal analysis has been applied to many earth sciences problems, such as topography, fault traces, fracture networks, fracture surfaces, porous aggregate geometry, permeability distribution, flow and transport through heterogeneous media, erosion and chemical dissolution, etc. La Pointe (1988) used fractal geometry to characterize fracture density and connectivity. There are several papers in which the fractal properties of fractured tuff at Yucca Mountain were investigated (Carr, 1989). Fractal analysis was also used to predict bypass flow in rocks (Nolte et al., 1989; Cox and Wang, 1993) and clay soils with vertically continuous macropores (Hatano and Booltink, 1992).

3.0 LABORATORY TESTS (LBNL)

3.1 Introduction and Motivation.

Observations of water seepage in fractures in the laboratory have shown the pervasiveness of highly localized and extremely non-uniform flow paths in the plane of the fracture ***(Geller et al.,** 1996)*. These channels exhibit intermittent flow behavior as portions undergo cycles of draining and filling, and small connecting threads snap and reform. This unsteady behavior occurs even in the presence of constant pressure boundary conditions. These observations motivated us to study dripping water between parallel plates as an idealized model of some of the flow behavior characteristic of water seepage through fractured rock. This study extends the classic chaos experiment of the "dripping faucet" to drips in the presence of capillary forces as they are affected by the surface properties and the small aperture of the parallel plates.

The objective of these experiments is to collect data records that can be analyzed to determine whether or not, and under what conditions, the dripping of water in parallel plates is chaotic, random, or periodic. This work was further motivated by preliminary experiments that showed the sensitivity of pressure measurements to the formation and release of water drops through a needle in open air and inserted between parallel plates. Much of this year's work was invested in developing the experimental system to reliably obtain usable data records.

Experiments were performed at a variety of flow rates to evaluate the system for chaotic behavior. Four basic types of experiments were conducted. Type A are pressure fluctuations caused by the 28 gauge needle dripping water into open air. Type B measure the baseline pressure fluctuations of the 28 gauge needle delivering water with a constant pressure condition at the outlet. Type C use the 28 gauge needle to deliver water between smooth glass plates with a 0.35 mm gap at an angle of 60 degrees from the horizontal. Type D are identical to type C except for the use of rough glass plates. In each experiment, a constant flow rate of water was delivered as the magnitude of the pressure at the syringe needle was measured.

The smooth glass plates (type C) experiments were run at flow rates of 0.25, 0.5, 1.0, 1.5, 2.0, and 3.0 ml/hr. Typical pressure data for these flow rates are shown in Figure 3.1. In Figure 3.2 the frequency of drips and height of the average pressure fluctuation are plotted against the flow rates of the experiments in Figure 3.1. The experiments plotted in Figure 3.2 show a trend toward more frequent drip events and decreased height of pressure fluctuation as the flow rate increased. Visual observation of the drip events confirmed an increase in thread length as flow rate increased. However, duplicate experiments at each flow rate demonstrated that both the height of pressure fluctuations and the frequency of the drips vary between type C experiments with the same flow rate. The formation of the threads appear to depend qualitatively upon the initial condition of the plates. Some of the factors suspected to influence the drip frequency and length of thread formation are the amount of moisture on the plates, whether the drip was following a preexisting flow path determined by a previous flow rate, and the cleanliness of the plates.

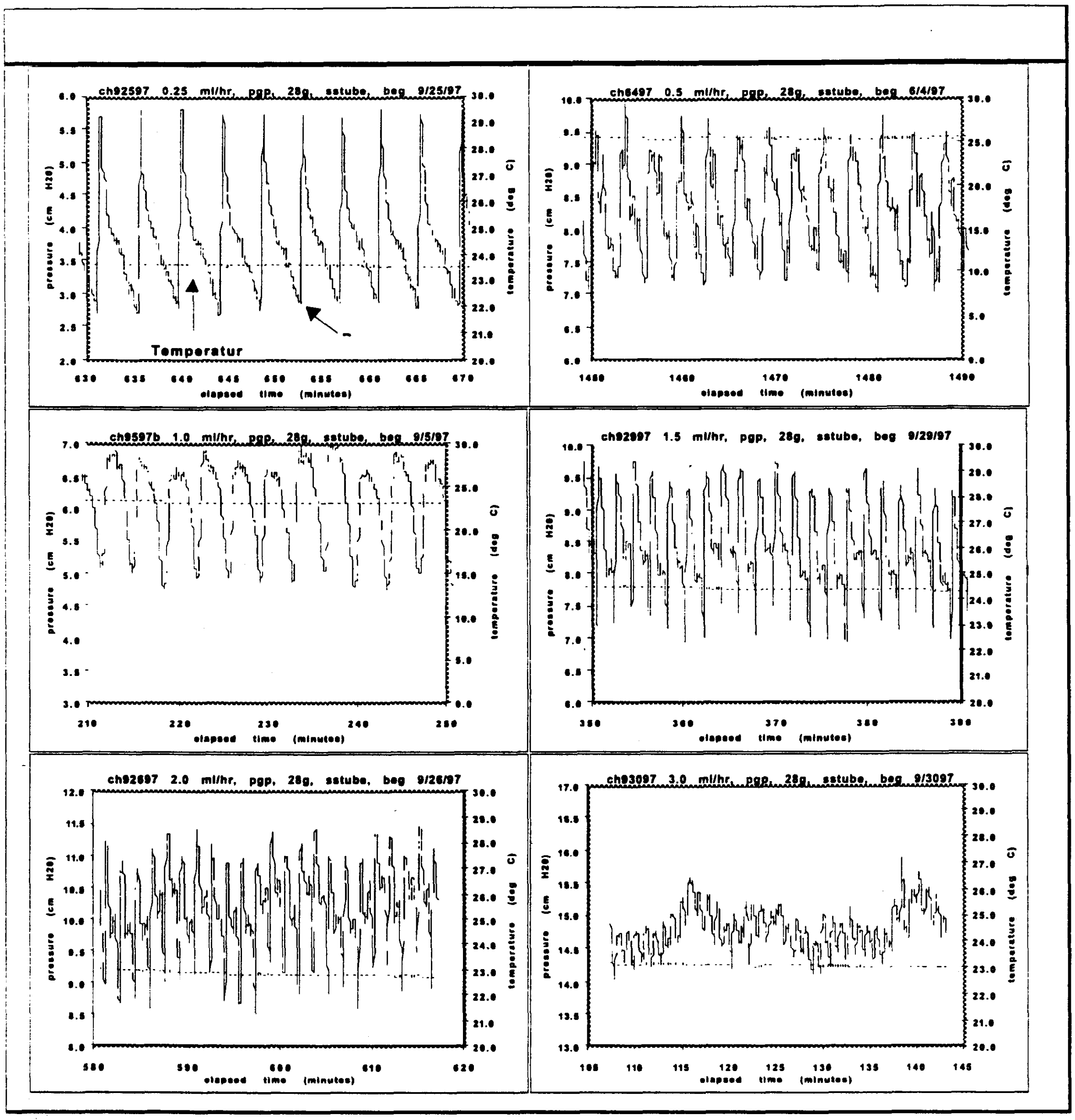

Figure 3.1: Smooth parallel glass plates. Pressure fluctuations caused by dripping water between smooth parallel gass plates at flow rates of 0.25, 0.5, 1.0, 1.5, 2.0, 3.0 ml/hr.

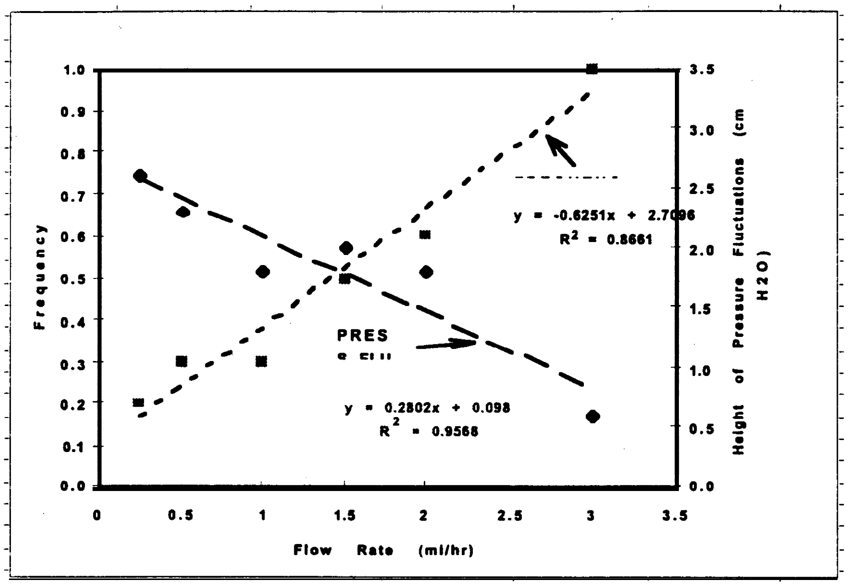

Figure 3.2: Observed trends in frequency and magnitude.

Experiments in roughened glass plates were conducted to test the effect of surface variability on drip behavior. Two types of plates were utilized: sand-blasted and shower-door glass (type D) plates. Both plates were separated by 0.35 mm shims. The sandblasted plates had an overall consistency of fine sandpaper with an even coating of fine (approximately 0.1 mm) irregularities on the surface. When the water was introduced into the sandblasted plates, a halo developed on the plate as the water advanced as film flow and drops did not form. The pressure signature observed from the sandblasted plates was similar to that observed for the baseline monitoring (see below).

The shower-door glass plates had larger, smooth irregularities or nubs on the surface (average scale of 2-3 mm). When the drips were introduced into the shower glass plates, the larger spaces between the nubs allowed drips to form at the end of the needle. The drops grew to different sizes before they snapped off and moved down the plate. Occasionally, short threads formed before the drop snapped off completely. After snapping off, the drop either moved quickly down the plate and was removed from the system or it remained close to the end of the needle, held back by a narrow ëthroatsí formed by adjacent nubs. When the next drop formed, it tended to combine with the previous drop and the new larger drop would travel down between the plates.

The pressure fluctuation from the drips of water from the 28 gauge needle into open air (type A experiments) were recorded as a basis for comparison to the glass plate experiments. It was determined that the presence of capillary forces induced by the glass plates causes a decrease in drip frequency and a decrease in the height of the pressure fluctuation.

The experiments demonstrate the variation of observed pressure fluctuations and the importance of both identifying and controlling initial conditions to achieve consistent results. Although quantitative analysis of the results is not yet complete, these features suggest that chaotic dynamics play an important role.

4.0 Fractured Rock Outcrop Experiments (INEEL)

The outcrop scale experiments were designed and conceptualized to fill a gap of knowledge between the laboratory and field (Box Canyon) scales of investigation. A research site was selected at Hell's Half Acre Lava Field where a single fracture could be studied. The site consisted of a basalt outcrop approximately 1 meter thick that extended approximately 1.5 meters outward from the rock wall. An infiltration gallery (0.5 X 1 m) was constructed above the fracture to perform constant head infiltration tests. On the underside of the overhang, drip sensors were installed to count and timestamp drops of water falling from the fracture. More traditional monitoring parameters, such as tension, temperature, and barometric pressure were also collected. Figure 4.1 shows the general site and instrument layout.

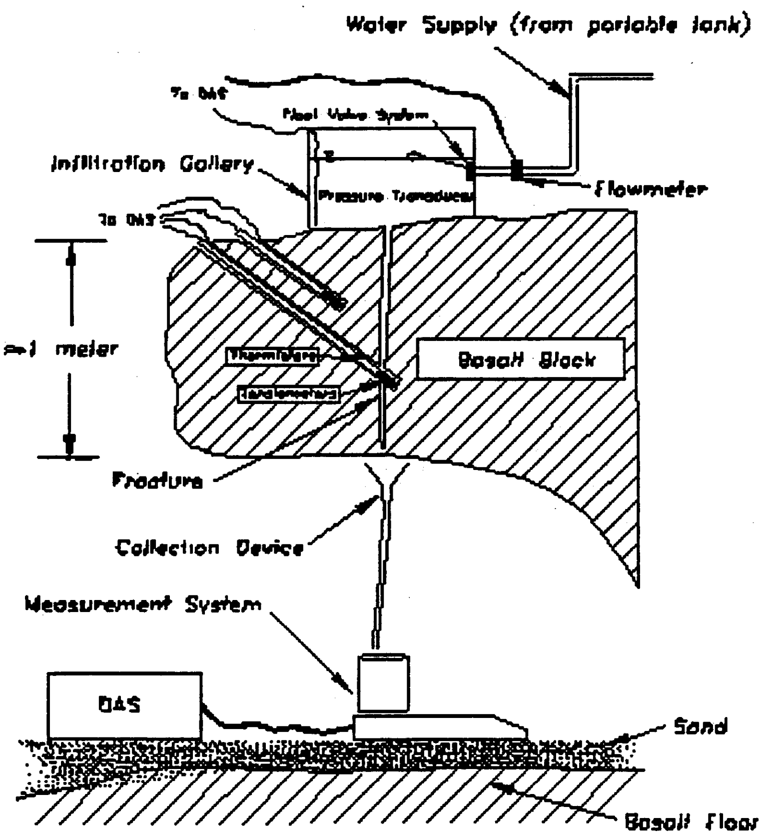

Figure 4.1. Field site characteristics and instrument layout. Note figure not to scale.

The field site was instrumented to collect data that would be amenable to a chaotic-dynamical analysis, which typically requires long time-series of data. Data collected included time stamping individual drip events for 20 distinct drip locations (to perform an analysis similar to that in Shaw, 1984); measurements of the inflow and outflow rates into the system (to compare temporal and spatial variability as well as do mass balance calculations); and moisture tension, temperature, and barometric pressure (to examine and compare with flow and drip data).

4.1 Field Test Setup and Instrumentation

Field work at the site began in June 1997 and continued until October 1997. Seven ponded infiltration tests were conducted, each with 4 to 48 hour duration and a varying amount of dry-out time (hours to weeks) between tests. Individual drips were monitored as they landed, using an array of specially designed piezo-electric sensors that sent a signal to the data acquisition system in response to the pressure increase accompanying a landing drip.

4.2 Field Observations and Preliminary Data Analysis

Preliminary reductions indicate that between 0 and 20,000 drips were collected for each location during each test. During the later tests (4-7) over 5,000 drip events were. recorded at approximately 50% of the drip locations. The parameters of moisture tension, temperature, barometric pressure, and flow rates/water levels were collected at 1 minute intervals for the duration of the tests.

As the data analysis has yet to be conducted, a detailed discussion of the results cannot be presented at this time, however the following were observed during the testing:

- Flow rates were observed to vary between and during tests, ranging from near negligible inflow rates to as high as 0.8 L/mm.
- The ambient moisture conditions in the basalt may exhibit some control on the flow through the fracture
- Temporal and spatial variability was observed in the location of the first appearance of drips

5.0 BOX CANYON PULSED PONDED INFILTRATION EXPERIMENT (LBNL)

The Box Canyon experiment consists of a series of pulses of ponded infiltration, in which a fixed volume of water containing a known concentration of tracer (potassium bromide) is added to the pond all at once, allowed to infiltrate for two days, then pumped out of the pond, allowing air to enter the subsurface. This sequence of water and air boundary conditions is believed to be conducive to the development of chaotic flow and chemical transport behavior in the fractured basalt. In addition to monitoring water infiltration and evaporation rates from the pond, two types of measurements were conducted in the subsurface below the infiltration pond in order to study the flow and transport behavior in fractured basalt. First, time series of measurements at point locations were collected, to study the local dynamics of flow and transport and examine it for chaotic behavior. Second, snapshots of the spatial distribution of moisture and tracer movement were collected with geophysical techniques, to study the geometrical pattern of flow and transport and examine it for evidence of fractal geometry.

5.1 Infiltration Tests and Pond Data Collected

Three pulse infiltration tests were conducted in September-October 1997 of approximately 48 hours each. Table 5.1 shows specifics for each test.

Table 5.1. Pulsed ponded infiltration tests conducted at Box Canyon in 1997.

Beginning of ponding		Test number	Volume added (m^3)	Duration of ponding (days)	Volume infiltrated and evaporated (m^3)
9/11/97	12:15	1	11.23	2.02	5.55
9/18/97	14:56	2	11.03	2.08	5.37
10/2/97	15:40	3	11.00	2.01	4.63

Potassium Bromide slurry was added to the tanks before each test to a concentration of approximately 3 mg/L. Water samples were taken from the tanks and the pond once infiltration began to check for uniformity of concentration. Analysis of these water samples is ongoing.

Water levels in the pond were taken and cumulative infiltration rates accounting for evaporation were calculated for each test. Evaporation was monitored using a pool within the berm walls. As can be seen from the final column of Table 5.1, the cumulative flow rate into the pond decreased from pulse to pulse.

5.2 *Point Measurements*

Time domain reflectory (TDR) measurements were taken during the three infiltration tests and during dormant periods. During infiltration, measurements were taken every 15 minutes, and during dormant periods, every 1 or 2 hours, depending on the length of time between the tests.

Electrical resistivity (ER) measurements using miniature ER probe were taken at an interval of 15 minutes during and between tests. 45 existing probes installed at multiple depths in 5 wells were used as well as newly installed single probes placed in the bottom of 3 wells. 13 probes were placed within the pond, and 1 probe was placed in the water tank.

Tensiometry measurements of water pressure were done using 26 tensiometers installed within and outside the pond.

Water sampling was conducted using suction lysimeters installed in boreholes. Sampling was carried out a total of 17 times. The purpose of the sampling was to detect the movement of the bromide tracer, and construct breakthrough curves as the water infiltrated downward through the fractured basalt. Analysis of the water samples is ongoing.

5.3 *Geophysical Measurements*

Neutron well logging provides a one-dimensional picture of moisture distribution. It was carried out in 7 wells at 10-12 times before, during, and after each ponding period. Preliminary results indicate increases in water content during infiltration in wells located within and close to the pond.

Cross-borehole ground penetrating radar (GPR) provides a two-dimensional tomogram of moisture distribution by using variations in the velocity of electromagnetic waves with dielectric constant. GPR surveys were conducted between six different well pairs. Preliminary analysis confirms that ambient conditions are wetter this year than last year, but radar tomograms still identify the central fracture zone and the rubble zone as low velocity zones.

Electrical resistivity tomography (ERT) provides a three-dimensional picture of the subsurface electrical conductivity distribution, which may be related to moisture distribution. ERT measurements were provided by Steam Tech, Inc. These measurements involved the development of special ER probes installed in three deep (20 m) boreholes outside the pond, three shallow (2 m) boreholes within the pond, and 15 surface ER probes. The data analysis is ongoing.

6.0 NON-LINEAR DYNAMICAL PROCESSES IN UNSATURATED FRACTURE FLOW (UNR)

Systems exhibiting chaotic behavior are characterized by the ability to make short-term predictions. Long-term predictions are impossible because of an exponential loss rate of information on the system state. We identify and develop the conditions under which chaotic behavior in unsaturated flow can be expected so that realistic limits can be placed on predictions about the future state of the system. We cast the problem in terms of thin film flow in fractures with aperiodic saturation events using Navier-Stokes governing equations. Initial conditions consist of constant inflow rates at the top of the fracture. If the rates are small enough and surface tension dominates, the thin film will reach a steady flow rate. Above a certain threshold flow rate, as gravity begins to dominate, periodic solitons develop. Above still another threshold, aperiodic solitons take over, and the flow characteristics are chaotic. Laboratory experiments are examined and interpreted in light of the models that we have developed.

7.0 ESTIMATING TOTAL MASS OF CONTAMINANT PLUMES FROM SPARSE WELL DATA (LBNL)

A major problem we encounter in trying to develop models (chaotic or otherwise) for **flow** and transport in fractured basalts is that it is extremely difficult to develop a picture of the overall spatial structure of these processes from isolated point measurements, due to the extreme heterogeneity of the system.

We consider the estimation of the total mass of a contaminant plume as a model problem to investigate means of using sparse data effectively. Generally, the estimation of the volume or mass and shape of the plume is based on sampling and analyzing water and soil. We have generated several complex hypothetical contaminant plumes. We then test the ability of different prediction methods and different sample spacing to estimate the mass of the contaminant plume. Comparisons among the methods should tell us something about the performance of different estimation methods for different types of complex distributions. They should also indicate what resolution of sampling is required to make an acceptable mass estimation.

7.1 Methods

We approach the problem of sample minimization by using several simulated heterogeneous distributions obtained from fractal generating algorithms, and a real distribution obtained from a fracture infiltration experiment. We initially select 15 well locations, based on a quasi-random scheme, along a two dimensional cross-section. The extension of this approach to three dimensions would involve taking several two-dimensional cross-sections. The wells are sampled at equally spaced vertical intervals. Sequential predictions of the total mass of contaminant are computed as each successive well is sampled. Figure 7.1 shows the fractal plume and the wells used to sample the field. The numbers indicate the sequence in which the wells are sampled.

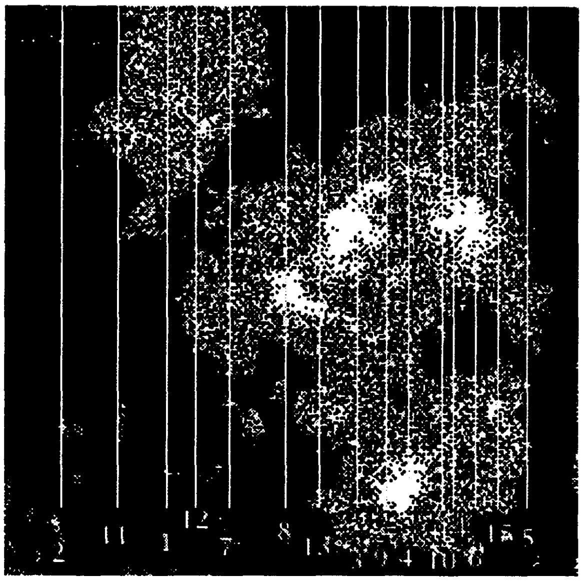

Figure 7.1. Synthetic contaminant plume with fractal geometry and locations of sampling wells.

We use several estimation techniques such as simple averaging, spatial integration, fractal and neural network models, to predict the total mass of the plume from the sample data. Parameters of the concentration distribution for the plume determined from the sparse well data were compared to those for the computer-generated plume. The convergence of the estimated plume mass to the actual known mass, as well as the number of wells required for convergence, were used as criteria to compare the different methods.

7.2 Preliminary Results

Analyzing the concentration distribution, we found little or no spatial correlation between samples collected from adjacent wells, indicating that the wells are far enough apart to provide independent information. In general, for the examples we studied simple averaging, spatial integration, and neural network predictions performed comparably well and estimates of total mass did not significantly improve after five wells had been sampled. In contrast, the fractal-based methods proved less successful, in part because they depend strongly on the value of the fractal dimension of the plume, which is very difficult to determine from sparse well data. A comparison of some of the estimation methods is plotted in Figure 7.2 for a synthetic fractal plume with a fractal dimension prescribed to be 1.5. This plot shows how the estimation changes as each additional well is sampled. The bar indicates a perfect estimation. Interestingly, the least successful method is a fractal-based method that assumes a fractal dimension of 1.5, supposedly the actual fractal dimension of the plume. The much better performance of a fractal method that uses a fractal dimension of 1.3 suggests that perhaps the algorithm used to create the plume does not actually produce the desired fractal dimension. This topic is currently under investigation.

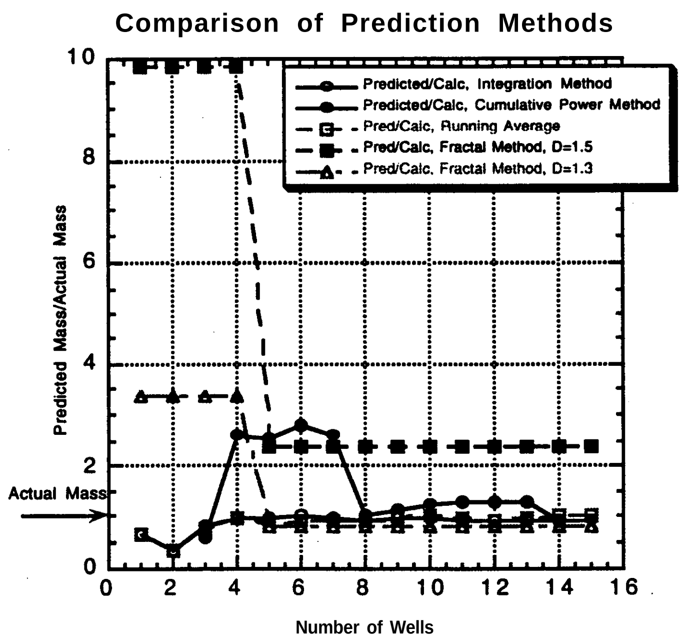

Figure 7.2. Summary of predictions for a fractal plume with a fractal dimension prescribed to be 1.5. The curves labeled cumulative power method, fractal 1.5, and fractal 1.3 all use various forms of fractal-based approaches.

8.0 TOPICS OF ON-GOING RESEARCH

8.1 Theoretical

- Study the physics of water flow and chemical transport in fractured rocks using dynamical models of chaos theory, fuzzy logic, and a combined fuzzy-chaotic approach (a tool for managing and optimizing remediation activities under conditions for which chaotic processes are important).

- Use fractal and neural network approaches to determine three-dimensional spatial distributions of properties or processes in soils and fractured rocks from point-type measurements in boreholes.

- Apply the theory of linguistic variables to lithological analysis of data from boreholes.

- Re-examine water flow and tracer transport in fractured basalt from the Large Scale Infiltration Test in light of chaotic dynamic models.

- Compare laboratory and field methods for the determination of quasi-saturated hydraulic conductivity of soils, and use a deterministic-chaotic model to describe a variable hydraulic conductivity within the zone of fluctuation of water table.

- Examine the relationship between the spatial structure of geologic heterogeneity (using methods of fractal geometry) and chaotic dynamics, as related to infiltration through a fractured basalt vadose zone.

- Construct and investigate fractal structures created with iterated function systems (IFS), which can simulate realistic characteristics of natural fracture patterns in basalt.

Experimental

- Evaluate the performance of tensiometers in fractured rocks, using laboratory cores and modeling, taking into account the interaction between the matrix and fractures.

- Use ground penetrating radar to investigate flow in soils and fractured rocks.

- Use 2-D and 3-D Electrical Resistivity Tomography to evaluate zones of preferential flow in fractured rocks.

- Conduct a series of pulsed infiltration tests at Box Canyon and Half Hells Acre field sites in Idaho.

ACKNOWLEDGEMENT

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Figure Captions

Figure 2.1. Comparison of regular (i.e., non-chaotic deterministic), chaotic, and random behavior (modified from Schuster, 1993).

Figure 2.2. Conceptual model of flow and measurement in partially saturated fractured rocks.

Figure 3.1. Pressure fluctuations caused by dripping water between smooth parallel glass plates.

Figure 3.2. Observed trends in frequency and magnitude of pressure fluctuations.

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