ENVIRONMENTAL MANAGEMENT SCIENCE PROGRAM

RESEARCH PROJECT FINAL REPORT

U.S. Department of Energy

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

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Executive Summary

Motivation. On an annual basis the U.S. Department of Energy (DOE) spends approximately $6 billion to address problems involving contamination of soils and groundwater. The ability to predict the transport of radionuclides, chlorinated hydrocarbons, and other pollutants in the subsurface has become one of the most important challenges facing the DOE. Numerous contaminated DOE sites have active remediation programs underway, 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 threatens to or has contaminated the underlying aquifer. The primary driver for selecting a corrective action plan for site clean-up is the predicted future concentration and travel time to receptors of contaminants moving through the vadose zone. It is a daunting task to accurately predict future concentrations and distributions of contaminants in vadose zones because of subsurface heterogeneity and spatial and temporal variability of fluid flow. Complex temporal and spatial patterns of flow and transport in the subsurface can be difficult to find and predict. Many experts believe that the major shortcoming of the science of vadose zone hydrology is our inability to accurately predict contaminant transport (Looney and Falta, 2000). A major shortcoming, is the general lack of constitutive relations to describe the coupling and inter-relations between fluid flow, chemical transport, and heat transfer processes. The insufficiency of both existing data and descriptive models for constitutive relations is now posing a serious problem for further development and successful application of simulation technologies. Many existing numerical models have failed because there is no a readily available methodology for accounting for the effects of chaotic dynamic processes in vadose zone flow and transport. Furthermore, the general failure of the industry to recognize the inaccuracy of the assumptions of idealized, homogenous infiltration, threatens to doom current plans for performance monitoring to satisfy stewardship objectives.

This research project was triggered by the investigation of a complex behavior of flow and transport in unsaturated fractured rocks at the INEEL contaminated sites. Preliminary investigations conducted at the Large Scale Infiltration Test in 1994 and the Box Canyon site in Idaho in 1995-1996, prior to the origination of this project, as well as analysis of scientific literature, indicated that dynamical chaotic models could describe flow and transport in heterogeneous fractured rocks.

The primary objectives of this project are:

(1) 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, and

(2) To introduce a new approach to the multi-scale characterization of flow and transport in the fractured basalt of the vadose zone and to develop physically based conceptual models on a hierarchy of scales.

The objectives of this project are being achieved through the following accomplishments:

- Series of ponded infiltration tests, including (1) Small-scale infiltration tests (ponded area 0.5 m^2) conducted at the Hell's Half Acre site near Shelly, Idaho (Podgorney et al., 1997, 1998, 1999, 2000), and (2) intermediate scale infiltration tests (ponded area 56 m^2) conducted at the Box Canyon site near Arco, Idaho (Faybishenko et al., 1999; 2000),

- Laboratory investigations and modeling of flow in a fractured basalt core (Finsterle and Faybishenko, 1999; Faybishenko and Finsterle, 1999),

- Series of small-scale water dripping experiments in fracture models conducted to evaluate chaotic behavior of flow in single fractures (Geller et al., 2000);

- Development of a conceptual model 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 description of the temporal dynamics of flow and transport, which may be chaotic; and

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

The main hypothesis tested in this project is:

Subsurface spatial and temporal heterogeneity, non-linear feedback between unsaturated hydraulic processes and parameters, such as unsaturated hydraulic conductivity, moisture content, entrapped air, non-uniform matrix surface geochemistry and numerous other factors affect vadose zone flow and transport such that chaos theory can be used to describe the vadose zone process .

This past years efforts culminated a three-year project that included ponded infiltration tests conducted in Idaho at two fractured rock field sites: the Hell's Half Acre (the scale of 1 by 0.5 m) and the Box Canyon (the scale of 7 by 8 m) sites. Monitoring of water dripping, geophysical imaging, in-situ measurements of the moisture content, water flow, water pressure in the rock matrix and fractures, tracer distribution, and other critical parameters were used to characterize the temporal and spatial evolution of chaotic behavior at the meter scale in unsaturated fractured rock for the first time. Several new technologies have been developed for this project including piezoelectric probes, a leak detection system, a laser surveying system, and a 3D Electrical

Resistivity Tomography system. During the last year, we also refined the modeling approaches and wrote six technical reports and scientific papers, submitted for publication.

Laboratory experiments were conducted to evaluate the presence of chaotic behavior in water seepage through fracture models. The pervasiveness of highly localized and extremely non-uniform flow paths in the plane of the fracture was shown. Using the time-trend of a pressure signal for unsaturated flow in fracture models, the magnitudes of deterministic-chaotic and stochastic components in the data were analyzed. For this purpose, several parameters were determined such as the correlation time, Hurst exponent, Lyapunov exponent, capacity dimension, correlation dimension, and information entropy. The time-series data were used to construct three-dimensional attractors in a phase-space.

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) 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 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 an inclined fracture surface, 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 down a fracture much faster than expected by classical flat film theory.

Relevance, application, impact and technology transfer issues. The results of this project can be used by DOE to demonstrate the complex behavior of vadose zone transport and for development of characterization and monitoring methods, predictions, and the design of remediation approaches at contaminated sites, such as, Hanford, INEEL, LLNL, Oak Ridge, and LBNL.

The information and techniques developed from this project address numerous gaps identified in the book prepared by the Subsurface Contaminants Focus Area, and can directly be applied to formulating cleanup strategies for contaminants in the vadose zone. Three sites that can benefit from the findings of this work include the Underground Test Area at the Nevada Test Site, the vadose zone below the Hanford tanks, and the Radioactive Waste Management Complex of the INEEL. This project enables a better understanding of plume delineation and spreading rate so that applied cleanup technologies can be optimized.

Value/Benefits. The scientific and practical values of this approach is that we hope to determine the range within which the parameters of flow and transport will occur based upon the collection of a limited data set. Albeit, we cannot predict the behavior at any point or time. This is similar to saying we can determine the climate for a certain geographic province, but are unable to predict the temperature on any given day. The current reductionist approach to numerical modeling of vadose zone transport assumes that by knowing with enough certainty all of the subsurface factors affecting flow, we can predict with accuracy the temperature on any given day (or the temperature range). The uncertainty of this reductionsist approach has lead to several surprising detections of contaminants afield of DOE Facilities (Board on Radioactive Waste Management, 1999).

The scientific issues of the research rests in (a) the unique non-linear 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 non-linearity 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, and what the bounds on the time of contaminant transport are, and how long DOE will need to provide stewardship of theses sites. The significance of the research for the DOE will be in the form of new technologies developed for vadose zone monitoring and in improved vadose zone site characterization and predictability.

Improved information on contaminant transport and concentrations enables the development of better, more cost effective and protective cleanup strategies. Optimization of cleanup strategies based upon reliable predictions of contaminant fate and transport will save costs, shorten schedules and increase DOE credibility with stakeholders. Through improved understanding of contaminant spread drinking water sources, health and safety risks to surrounding populations will be minimized.

Collaborative work. Long-term collaboration between the LBNL and INEEL allowed us to better understand the practical problems facing DOE sites and use the potentials of both DOE Laboratories. Investigations were conducted in collaboration with University of Nevada, Reno, Geological Survey of Canada, Alberta Research Council of Canada, Lawrence Livermore National Laboratory, University of California at San Diego, and University of Alabama, Tuscaloosa, Alabama. Three graduate studies were also funded under this EMSP project.

Introduction

The Department of Energy faces the necessity of remediating numerous contaminated sites, including 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 lead to the contamination of or threatened contamination of underlying groundwater. An important issue in choosing a corrective action plan to clean up contaminated sites is to determine 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 pathways can be difficult to find and predict. Chaotic dynamic processes are likely a major reason for the weakness of present models.

The purpose of this Final Report of the Environmental Management Science Program (EMSP) Research Project is to document the findings from the project obtained from 1996 through 1999. The report includes the summary of work performed under the project, including the types of work completed, results achieved, the significant findings, and future research and practical applications. The report also discusses the relevance of scientific accomplishments to environmental management, improved understanding obtained on flow and transport processes, monitoring technology development, and cleanup techniques. The results of this project can be used to inform potential technology users and commercialization partners of emerging opportunities arising from the results of this project, as well as to identify potential sponsors for continuing research, field demonstration, and commercial testing.

Research Objectives

The primary objectives of the research conducted under this project are:

(1) 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.

(2) To introduce a new approach to the multiscale characterization of flow and transport in fractured basalt vadose zones and to develop physically based conceptual models on a hierarchy of scales.

The following activities are indicative of the success in meeting the project s objectives:

- A series of ponded infiltration tests, including (1) small-scale infiltration tests (ponded area 0.5 m^2) conducted at the Hell s Half Acre site near Shelley, Idaho, and (2) intermediate-scale infiltration tests (ponded area 56 m^2) conducted at the Box Canyon site near Arco, Idaho.

- Laboratory investigations and modeling of flow in a fractured basalt core.

- A series of small-scale dripping experiments in fracture models.

- Evaluation of chaotic behavior of flow in laboratory and field experiments using methods from nonlinear dynamics;

- Evaluation of the impact these dynamics may have on contaminant transport through heterogeneous fractured rocks and soils, and how it can be used to guide remediation efforts;

- Development of a conceptual model and mathematical and numerical algorithms for flow and transport that incorporate (1) the spatial variability of heterogeneous porous and fractured media, and (2) the description of the temporal dynamics of flow and transport, both of which may be chaotic.

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

This approach is based on the assumption that spatial heterogeneity and flow phenomena are affected by nonlinear dynamics, and in particular, by 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 in order to design and manage the remediation, even when we can not predict the behavior at any point or time.

Methods and Results

(1) Mathematical Models of Chaotic Flow and Methods of Analyses

Theoretical studies have shown that as a fluid film flows vertically on a fracture surface, it is inherently unstable and may exhibit chaotic behavior, even for low Reynold s numbers (Babchin et al., 1999). A one-dimensional equation of a slow motion (small Reynolds numbers R << 1) of a thin liquid film along an inclined (nonhorizontal) impermeable surface, which takes into account gravitational, capillary and molecular forces, has been derived. It is shown that the addition of the molecular force term leads to the equation of the spatial and temporal evolution of film thickness given in a canonical form by the Kuramoto-Sivashinsky equation

$$\frac{\partial \phi}{\partial \tau} + \phi \frac{\partial \phi}{\partial x} + \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^4 \phi}{\partial x^4} = 0$$

where ϕ is the dimensionless film thickness, x is the dimensionless coordinate, and τ is the dimensionless time. The solution of this equation shows that the open-flow film surface along the impermeable plane exhibits a chaotic hydrodynamic instability. These results are illustrated using the attractors and diagnostic deterministic-chaotic parameters for the dimensionless film thickness along the coordinate and time.

The analysis of literature and the assessment of chaotic flow along inclined planes shows that the liquid film waviness may enhance transfer of contaminants from rock to fluid by as much as five times and carry contaminated fluid down a fracture much faster than expected by classical flat film theory (*Dragila*, 1999).

The chaotic analysis of the time-series data sets was performed using two numerical programs: the Chaos Data Analyzer (CDA), the Professional Version (Physics Academic Software, Raleigh, North Carolina); and the Contemporary Signal Processing for Windows (CSPW), version 1.2 (Applied Nonlinear Sciences, San Diego, CA). Using these programs, we developed a special procedure for data analysis of the signal by separating broadband noise from a deterministic signal. Contrary to the Fourier analysis, which is used to analyze the time series data directly, the chaotic analysis of nonlinear systems is conducted with the N-dimensional phase space using N time-lagged variables. An analysis of a nonlinear dynamical system using one-dimensional observations of a scalar signal includes the determination of the following diagnostic quantitative parameters for chaos: correlation time, global embedding dimension, local embedding dimension, Lyapunov dimension, Lyapunov exponents, and correlation dimension.

(2) Hierarchy of Models

Because a variety of natural conditions affect the hydraulic processes in unsaturated, fractured basalt, field and laboratory investigations in the vadose zone should be conducted on different scales: elemental, small-scale, intermediate-scale, and large-scale (Figure 1). An elemental component is a single fracture or a block of homogeneous porous medium. Small-scale components include one or a few fractures and the surrounding matrix. Intermediate-scale components include a fracture network and other parts (fracture zones, vesicular lenses, soil, massive basalt, rubble zone) of a single basalt flow finger. Large-scale components include multiple basalt flows and their surrounding network of rubble zones and sedimentary interbeds. We find that, at each scale of investigation, different conceptual models for flow and transport phenomena must be used to explain the observed behavior. Because different methods of measurement are needed, we obtain data that can be used to create models describing different flow processes with no apparent scaling principles evident; instead, a hierarchy of models is needed to discriminate between the observed flow phenomena at each of the different scales. We find that, at each scale of investigation, different models for flow phenomena must be used to explain the observed behavior.

(3) Field Investigations

Field investigations were conducted in the fractured basalt near the INEEL at two sites: (1) small-scale infiltration tests (ponded area 0.5 m^2) conducted at the Hell s Half Acre site near Shelley, Idaho (Podgorney et al., 1997; 1998; 1999; 2000); and (2) intermediate-scale infiltration tests (ponded area 56 m^2) conducted at the Box Canyon site near Arco, Idaho (Faybishenko et al., 1999). We also analyzed the results of the Large Scale Infiltration Test conducted near the INEEL Radioactive Waste Management Complex (ponded area ~26,000 m^2) (Wood and Norrell, 1996; Wood and Faybishenko, 2000).

Eight small-scale ponded infiltration tests on a one-meter scale were conducted over a fractured basalt column (Figure 2) during the summers of 1997, 1998, and 1999 (Podgorney et al., 1998; 1999; 2000). Ponding was established using constant head, step-wise variable head, and constant-falling head conditions. The infiltration rates observed during the tests were highly variable with time and were apparently unrelated to the head in the infiltration gallery (Figure 3). Despite the minimum values of the infiltration rate being practically the same 2 to 4 days after the beginning of the tests, the infiltration rates varied greatly afterward for the rest of each test. From the field data, we hypothesized that the flow paths through both vertical and horizontal fractures were episodically opened.

Infiltration tests showed channeling to be a typical feature of flow in fractured basalt. Channeling occurs at all scales of investigation, including individual fractures, the intra-basalt fracture network, and the inter-basalt rubble-zone network. However, the instrumentation used in laboratory and small-scale field conditions (in particular, to record dripping phenomena) is not practical for use at larger field scales. Field measurements of flow characteristics in fractured rocks using single probes (such as tensiometers) are uncertain because the locations of the probes in relation to the flow paths are not precisely known and these probes average fracture and matrix hydraulic characteristics. The almost immediate appearance of infiltrating water at the bottom of the basalt column in both the fracture and matrix is evidence of fast, preferential flow. This phenomenon is in line with the results of numerical studies by Pruess (1998; 1999), showing that volume averaging of flow parameters may lead to the overestimation of the water travel time through the vadose zone to the water table.

The volumetric outflow rates combined from several dripping locations exhibit spatial and temporal instability with primary low-frequency fluctuations, as well as secondary high-frequency fluctuations caused by local instabilities. Figure 4 illustrates a time series of dripping water intervals from one of the dripping points collected during the constant head test, and the three-dimensional chaotic attractor for this data. Table 1 summarizes the diagnostic parameters of chaos.

Table 1. Diagnostic parameters of a chaotic behavior of water dripping shown in Figure 4, Drip Point 10, constant head test.

Type of Parameter	Value of Parameter
Time delay, τ	3
Capacity (fractal) dimension	2.11
Global embedding dimension	4
Local embedding dimension	4
Lyapunov dimension	3.278
Largest Lyapunov exponent	0.22

(4) Laboratory Investigations

Laboratory investigations included measurements on fractured basalt cores (Finsterle and Faybishenko, 1999; Faybishenko and Finsterle, 2000) and small-scale dripping experiments (Figure 5) in fracture models (Geller et al., 2000). Laboratory tests showed that water seepage within a fracture can proceed through channels that undergo cycles of snapping and reformation under low-flow conditions, even in the presence of constant boundary conditions (Su et al., 1999; Geller et al., 2000). Water dripping within a flow channel along a dense basalt fracture surface mated to a transparent replica of the other fracture half exhibited nonperiodic cycling (Geller et al., 1998). In order to investigate the physics of this time-varying intermittent flow under laboratory conditions, we designed a series of water dripping tests within smooth-walled and rough-walled transparent fracture models having submillimeter apertures. Water was supplied at a constant rate through a capillary tube inserted into the fracture models. The time variation of the water pressure at the tube entrance was measured over a range of flow rates (Figure 6). These data were then used to calculate the chaotic parameters and plot attractors (Figure 7). Video images of flow confirmed that the pressure fluctuations occurred in response to flow behavior, as drops formed and detached within the flow channel. Analysis of the flow behavior from the videotapes indicated correspondence between the intra-fracture dripping and the pressure fluctuations (Figure 8). The observations led to the hypothesis that dripping behavior was more strongly controlled by factors other than the inlet condition, such as initial surface properties of the plates.

We also analyzed the results of laboratory investigations conducted by Persoff and Pruess (1995), who investigated two-phase flow by injecting water and nitrogen gas simultaneously into a replica of the natural rough-walled rock fracture of a granite core (from the Stripa mine in Sweden). Persoff and Pruess explained that observed instabilities in the capillary pressure, liquid, and air pressures under steady-state injection rates resulted from the interplay between capillary effects and viscosity created by opening and closing pore throats in a fracture. The evaluation of a series of chaotic parameters characterizing capillary pressure at different liquid and gas flow rates confirmed the deterministic chaotic nature of flow processes in a single fracture.

(5) Other Practical Examples of the Use Of Chaos Theory

Open Water Dripping Experiments

In order to investigate the dynamics of drip function, we conducted a series of laboratory water dripping experiments using vertical, horizontal, and inclined capillary tubes, which were open to the atmosphere. The data analysis of our experiments can be viewed as an extension of the classic dripping faucet theory to include dripping in the presence of capillary forces. In our experiments, a constant water flow rate was maintained at the entrance to capillary tubes, and the water pressure was measured at the entrance to the tube. One-dimensional time-series sets of pressure fluctuations were analyzed to determine the effects of the flow rate and tube inclinations on the diagnostic parameters of chaos. We also provided an analysis of dimensionless groups (Reynolds, Weber, Stokes, Bond Capillary numbers, etc.) to evaluate the kinetics of water dripping.

Underground Mine Drainage Flux

We analyzed the discharge rates from the 4-level of Price Mine at the Myra Falls copper/zinc mine in British Columbia, Canada (the data were presented by A. Desbarats, Department of Natural Resources Canada). The outflow formed in response to multiple infiltration events exhibited long-term (years), seasonal, and daily fluctuations. A chaotic analysis of these data showed that daily discharge fluctuations could be described using a low-dimensional deterministic-chaotic model with a small (12.5%) stochastic component.

River Flow Calculations

One of the important applications of the dynamical chaotic analysis is to the prediction of river flow rates. Several long-term data sets of daily flow-rate fluctuations for several rivers (Big Lost River and Snake River in Idaho, and the Yakima River in Washington near Hanford) were analyzed. These data showed that different types of chaotic models could be used to describe the daily flow-rate fluctuations.

CO_2 Concentration in Soils

The approach developed in this project was used to analyze the time trend of the CO_2 concentration in soils based on the data obtained from numerical modeling by J. Simunek of the U.S. Salinity Laboratory, Riverside, CA. The results confirmed that a complex, random-looking temporal pattern of the CO_2 concentration in a top-soil layer could be described using a deterministic chaotic model.

Washboard Calculations

Our review of published literature showed that the washboard phenomenon on unpaved highways is the result of the dynamic interaction between vehicle wheels and road surface, affected by a number of nonlinear variables in the physical system. Rather than attempt to solve the system analytically, we defined a set of simple, locally defined rules to (1) describe the wheel jump upon striking an irregularity on the roadway surface, and (2) to describe the resulting digging. We developed a new model and a computer code to iterate a mapping algorithm to simulate the effect of multiple vehicles (Mays and Faybishenko, 2000). We analyzed the resulting simulated road surfaces for evidence of complexity using information entropy and spatial pattern analysis. This approach can answer several outstanding questions in the literature, including those on the irregularity of washboard geometry, the direction of washboard migration, and the determination of washboard pitch, or wavelength. The study also resulted in several observations, which are commonly associated with complex dynamic systems, including pattern emergence, sensitive dependence on initial conditions, and for some simulations, evidence of spatial chaos. Our conclusion is that washboards in unpaved highways may be modeled as the manifestation of a complex dynamical system. We intend to use the developed approach for simulating soil erosion.

(6) Research Conclusions

The research conducted proved the evidence of deterministic-chaotic processes for flow in fractured rocks and heterogeneous soils. An important feature of flow in the basalt vadose zone is that the hydraulic system includes both unsaturated and saturated rocks. During flooding at the surface, the saturated zones have a limited and local extent within flow channels in the fractures and vesicular zones. Single probes, which cross the saturated fractures, also intersect the matrix, and, hence, the probes measure an averaged water pressure in the fracture-matrix system. However, it is difficult to separate the contribution of the fracture from that of the matrix (Finsterle and Faybishenko, 1999; Faybishenko and Finsterle, 2000). Using available monitoring techniques under field conditions, we cannot perfect our knowledge of initial conditions; we can only measure approximate values or determine the ranges of different parameters (such as pressure, moisture content, temperature, and concentration).

Fluid flow in fractured basalt of the vadose zone can be considered a nonlinear dynamic process in which the behavior, both temporally and spatially, may be chaotic (Faybishenko, 1999; Sposito and Weeks, 1997; Weeks and Sposito, 1998). The chaotic nature of flow results from nonlinear processes and the strong spatial and temporal variations in moisture content, hydraulic conductivity, and fracture connectedness. As a result, in fractured basalt (which is a nonlinear system) small variations in flow parameters may lead to significant variations in predicted results. The dissipative nature of the system implies that its phase-space volume decreases with time, leading to the formation of strange attractors characterizing the range in which the flow parameters are expected to change. The dynamics of such systems are sensitive to the initial conditions. The response of such systems may include a stochastic component that it is not necessarily a dominant factor on the system behavior. If the stochastic component is not dominant, then a stochastic analysis will not provide useful information.

We also find that under field conditions with a limited number of single-probe measurements, we can detect neither the spatial nor temporal chaotic variations of the flow parameters, and therefore, we must use conventional (i.e., nonchaotic) stochastic or deterministic methods to describe flow and transport processes. If the stochastic component is not a dominant factor, then a stochastic analysis will provide incorrect answers and should be replaced by a chaotic analysis. If the stochastic component is significant (or if the phase-space dimension is so large that the dynamics look stochastic), then a stochastic analysis is the most appropriate tool to use. Because the system exhibits sensitivity to initial conditions, we can predict only the range in which the flow rate is expected to change, but not the exact flow rates. Where elemental and small-scale components are involved, the flow data can be analyzed using methods of nonlinear dynamics. Where intermediate and large-scale components are involved, a combination of deterministic and stochastic methods of flow analysis can be used.

Further work is warranted to refine the methods and models of channelized flow in fractured rocks at a number of different sites and to gain insight into the relationships between different factors and processes affecting flow and transport in the subsurface. The understanding of the mechanisms governing flow instabilities will be used in developing conceptual and mathematical models of flow and transport behavior in unsaturated fractured basalt and further development of robust characterization and monitoring tools related to long-term waste management, storage, and remediation.

Relevance, Impact and Technology Transfer.

The goal of this section is to present information to assist DOE to communicate project information to potential technology users and commercialization partners, and to identify potential sponsors for continuing research in this technology area.

The research advanced our understanding in the area of flow and transport processes, and several new applications were found. The new scientific knowledge obtained in this project is relevant to critical DOE environmental management problems and will be beneficial for the improvement of characterization and monitoring activities, predictions, and remediation efforts. The specific problems developed in this project for fractured rocks at the INEEL sites can be used for improving characterization, monitoring, and prediction methods needed in designing and managing remediation activities, as well as in assessing and making decisions for many DOE contaminated sites.

The new scientific knowledge obtained through this project about the nonlinear dynamics of processes taking place in the subsurface can bridge the gap between broad fundamental research of flow and transport in fractured media, which has wide-ranging applications, and needs-driven applied technology development. This knowledge will improve technologies and cleanup approaches by reducing costs, schedules, and risks and will meet DOE compliance requirements. The project's impact on individuals, laboratories, departments, and institutions will present a new direction of studies of instabilities as affected by chaotic dynamics. Results will be used by DOE laboratories, U.S. Environmental Protection Agency (EPA) and Department of Defense (DoD) sites, universities, and private companies.

Based on the results obtained, special studies, including larger scale trials of the methods developed and large-block laboratory investigations, are warranted. Field demonstrations can be planned to prove the feasibility of characterization and monitoring methods as well as remediation activities.

The main hurdle that must be overcome before the results of this project can be widely applied to DOE Environmental Management problems is that the methods and technologies based on the results of this project should receive regulatory and end-user acceptance to be field-tested and commercialized more rapidly. To accelerate the finding of solutions to these problems, we will present proposals to the Subsurface Contamination Focus Area of DOE and the DoD Environmental Security Technology Certification Program. We will develop more contacts with site representatives and bring the results to their attention. To expedite this process, the researchers involved in this project wish help in deploying the research results at other sites.

Some parts of the project are ready for deployment and a full-scale demonstration, such as:

- Methodologies for time series analysis of long-term monitoring data for groundwater levels and concentrations of contaminants to determine stochastic and chaotic components.

- Field monitoring tools such as tensiometers, electrical resistivity probes, and suction lysimeters for shallow and deep vadose zone monitoring.

Additional research is required for the development of:

- Predictive modeling techniques for large-scale simulations of flow and transport.

- A strategy for scaling up model data to a larger model.

This project was conducted with permanent contact maintained between INEEL, LBNL, and the University of Nevada, Reno. Researchers were in contact with LLNL and the Yucca Mountain Project. Other sources of funding for continued research are Environmental Management Science Program (EMSP) Follow On, Characterization, Monitoring, and Sensor Technology Cross-Cutting Program (CMST-CP), and Subsurface Contamination Focus Area. The researchers wish help in locating follow-on funding for additional research, including Site Technology Coordinating Groups, Mixed Waste Focus Area, Subsurface Contaminants Focus Area, Tanks Focus Areas, Plutonium Focus Area, Decontamination and Decommissioning Focus Area.

The output of the research includes papers, calculations, reports, and models. The project accomplished all of the proposed goals and was conducted on schedule. The work plan has not been revised. INEEL extended the deadline of the project with no additional funding until the end of fiscal year 2000.

The following professional personnel were associated with this project and supported its research efforts:

Faculty: 1
Post-Doc: 1
Graduate Students: 4
Undergraduate students: 2 - LBNL, and 5 - INEEL
Staff Scientists: 6 - LBNL; 3 — INEEL.

Two Masters degree; one Ph.D. completed, and one Ph.D. is in progress.

Interactions and Transitions

During the course of this project, we provided consultative and advisory functions to other laboratories and agencies, which allowed us to establish how project results were transitioned to other organizations. The results of this project were implemented in the reports describing numerical models of flow and transport for the Yucca Mountain high nuclear waste disposal project (CRWMS, 1999; Pruess et al., 1997; 1999; Contact persons A. Simmons and G. Bodvarsson), and were used in Chapter 3, Vadose Zone Characterization and Monitoring of *Vadose Zone Solution and Technology*, of a book Vadose Zone Science and Technology Solutions prepared by DOE (Looney and Falta, 2000). The most important planned transitions include the development of (1) a new optimization method for characterization and monitoring of the vadose zone, which we plan to test at INEEL (T. Stoops), LLNL (D. Bishop and C. Carrigan), LBNL (I. Javandel), and Hanford; and (2) a new soil-remediation technology using chaotic mixing of pollutants in the vadose zone and groundwater induced by a pulsed air-water injection with additives such as oxygen, methane, and nitrogen gases to enhance vapor stripping and bioremediation of soils (the partners will be determined jointly with T. Hazen). Based on the expertise obtained at Box Canyon site, we consulted with the University of Arizona, Tucson, AZ (S. Neuman, P. Wierenga), on the design of the infiltration test at the Apache Leap Site (funded by the Nuclear Regulatory Commission, T. Nicholson).

Directions of Future Work

1. *Theoretical investigations:*

- Extend the results of statistical and deterministic-chaotic analysis of laboratory and small-scale field investigations to larger field scales.

- Assess the utility of existing models and develop new models to describe unsaturated flow in fractured rock using time-series, one-dimensional chaotic models, and two- and three-dimensional models of film flow for low and large Reynolds numbers,

- Assess the application of chaotic-mixing models to describe flow in heterogeneous soils

- Develop a chaotic-mixing theory to be used in the design of controlled, accelerated remediation

2. Perform field investigations at the HHA and Box Canyon sites, including tracer tests (reactive chemical and colloidal transport), taking into account the fracture-matrix interaction in fractured rocks.

3. Conduct laboratory investigations using large basalt cores/blocks taken from the field for detailed investigations of the fracture-matrix interaction; and small-block investigations to assess the effects of fracture-matrix interaction, determine the effects of gravity and capillary forces, and provide a proof-of-concept of mixing phenomena to be used for remediation.

4. Provide small-scale demonstration experiments for monitoring and remediation.

Articles and Reports Stemming from the Research

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1. 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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1. Faybishenko, B. Vadose Zone Characterization and Monitoring: Current Technologies, Applications, and Future Developments, Chapter 3 of Book Vadose Zone Science and Technology Solutions, Battelle Press, OH., Editors B. Looney and R. Falta, In press, May 2000.

2. Faybishenko, B. Tensiometer for Shallow or Deep Measurements Including Vadose Zone and Aquifers, paper accepted for publication in Soil Sciences Journal, 2000.

3. Faybishenko, B., C. Doughty, M. Steiger, J.C.S. Long, T. Wood, J. Jacobsen, J. Lore, and P. Zawislanski. Conceptual Model of the Geometry and Physics of Water Flow in a Fractured Basalt Vadose Zone: Box Canyon Site, Idaho, Paper was reviewed by *Water Resour. Res*., and now is being revised. According the Associated Editor letter, the paper will be excepted for publication.

4. Podgorney, R.K., B.A. Faybishenko, T.R. Wood, and T.M. Stoops, Spatial and Temporal Instabilities in Water Flow through Variably Saturated Fractured Basalt on a 1-Meter Field Scale, In Monograph "Dynamics of Fluids in Fractured Rocks: Concepts and Recent Advances, American Geophyscial Monograph Series.

5. Faybishenko, B., and S. Finsterle, On Tensiometry in Fractured Rocks, To be published in a Special GSA book "Theory, Modeling, and Field Investigation in Hydrogeology: A Special Volume in Honor of Shlomo P. Neuman's 60th Birthday," 2000.

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8. Wood, T. R., R.K. Podgorney and B. Faybishenko, Small Scale Field Tests of Water Flow in a Fractured Rock Vadose Zone, In: Vadose Zone Solutions and Technology, Editors B. Looney and R. Falta, Battelle Press, 2000.

Papers published in non-peer-reviewed journals and books

1. Finsterle, S., and B.A. Faybishenko, What does a tensiometer measure in fractured rocks? Proceedings of the International Symposium *Characterization and Measurement of the Hydraulics Properties of Unsaturated Media*, October 22-24, 1997, Riverside, CA, 1999, p. 867-875.

2. Faybishenko, B., Comparison of laboratory and field methods for determination of unsaturated hydraulic conductivity of soils, In Proceedings of the International Workshop *Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media*, 279-292, 1999.

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1. Faybishenko, B., T.R. Wood, T.M. Stoops, C. Doughty, and J. Jacobsen, A conceptual model of tracer transport in fractured basalt: Large Scale Infiltration Test revisited. Proceedings of 1997 GSA Annual Conference, Salt Lake City, UT.

2. Faybishenko, B., C. Doughty, J.C.S. Long, T. Wood, J. Lore, and J. Jacobsen, Conceptual model of geometry and physics of liquid flow in unsaturated fractured basalt at Box Canyon Site, Proceedings of the 1997 Fall Meeting of AGU, San Francisco, CA, 1997.

3. Faybishenko, B., P.A. Witherspoon, C. Doughty, J. Geller, T. Wood, and R. Podgorney, Multi-scale investigations of flow in fractured rocks, Proceedings of the 1998 Fall Meeting of AGU, p. F377-378, San Francisco, CA, 1998.

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5 Faybishenko, B. and J. Geller, Analysis of Observed Chaotic Data for Flow Through Capillary Tubes, Experimental Chaos Conference, 1999.

5. Geller, J.T., S.E. Borglin, and B. Faybishenko, Experimental study and evaluation of dripping water in fracture models, Abstracts of the Chapman Conference on Fractal Scaling, Non-Linear Dynamics, and Chaos in Hydrologic Systems, May 1998, Clemson University, SC.

6. Geller, J.T., S.E. Borglin, and B. Faybishenko, Experimental study and evaluation of dripping water in fracture models, Proceedings of the 1998 Fall Meeting of AGU, p. F383, San Francisco, CA, 1998.

7. Faybishenko, B., and S. Finsterle, On the Physics of Tensiometry in Heterogeneous Soils and Rocks, Spring AGU 99, Boston

8. 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, Spring AGU 99, Boston.

9. Faybishenko, B., On Nonlinear, Chaotic Dynamics of Flow in Unsaturated Fractured Rocks, Fall AGU 1999 Meeting, San Francisco

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1. Faybishenko, B., C. Doughty, J. Geller, S. Borglin, B. Cox, J. Peterson Jr., M. Steiger, K. Williams, T. Wood, R. Podgorney, T. Stoops, S. Wheatcraft, M. Dragila, and J. Long, A chaotic-dynamical conceptual model to describe fluid flow and contaminant transport in a fractured vadose zone, *Lawrence Berkeley National Laboratory Report LBNL-41223*, 1998a.

2. Faybishenko, B., P. A. Witherspoon, C. Doughty, T. Wood, R. Podgorney, and J. Geller, Multi-Scale Investigations of Liquid Flow in a Fractured Basalt Vadose Zone, LBNL Report 42910.

3. Faybishenko, B., C. Doughty, S. Steiger, J. Long, T. Wood, J. Jacobsen, J. Lore, and P. Zawislanski, Conceptual model of the geometry and physics of water flow in a fractured basalt vadose zone: Box Canyon site, Idaho, LBNL report 42925 (Paper submitted to Water Resources Research, March 1999.) 1999b.

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5. Podgorney, R.K., D.L. Whitmire, T.R. Wood, and T.M. Stoops, 1999, Basalt Outcrop Infiltration Tests to Evaluate Chaotic Behavior of Unsaturated Flow in Fractured Rock, Data Summary Report, 1999 Field Season (Draft), INEEL/EXT-99-01204.

6. Podgorney, R.K., T.R. Wood, T.M. Stoops, R.G. Taylor, and J.M. Hubell, 1999, Basalt Outcrop Infiltration Tests to Evaluate Chaotic Behavior of Unsaturated Flow in Fractured Rock, Data Summary Report, 1997 Field Season, INEEL/EXT-99-01211.

7. Finsterle, S., and B.Faybishenko, What does a tensiometer measure in fractured rocks? LBNL Report-41454. 1998

8. Faybishenko, B., Short-term and long-term vadose zone monitoring: current technologies, development and applications, Presented at *Subsurface Remediation: Improving Long-Term Monitoring & Remedial Systems Performance,* June 6-11, 1999, LBNL-43408, Lawrence Berkeley National Laboratory, Berkeley, Calif., 1999.

9. Pruess, K., B. Faybishenko, and G.S. Bodvarsson, Alternative Concepts and Approaches for Modeling Unsaturated Flow and Transport in Fractured Rocks, Chapter 24 of The Site-Scale Unsaturated Zone Model of Yucca Mountain, Nevada, for the Viability Assessment. 1997.

10. CRWMS M&O 2000, Natural Analogs for the Unsaturated Zone. MDL-NBS-HS-000007. Las Vegas, Nevada, Acc: MOL. 1999.

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1. B. Faybishenko, T.R. Wood, T.M. Stoops, C. Doughty, and J. Jacobsen, A conceptual model of tracer transport in fractured basalt: Large Scale Infiltration Test revisited. *Proceedings of 1997 GSA Annual Conference, Salt Lake City, UT.*

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3. Faybishenko, B., P.A. Witherspoon, C. Doughty, J. Geller, T. Wood, and R. Podgorney, Multi-scale investigations of flow in fractured rocks, *Proceedings of the 1998 Fall Meeting of AGU, San Francisco, CA, 1998.*

4. Faybishenko, B., A fuzzy-chaotic analysis of water flow and chemical transport in unsaturated-saturated soils, 16th World Congress of Soil Science, Montpellier, France, October 1998

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6. 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, Spring AGU 99, Boston.

7. Faybishenko, B., On Nonlinear, Chaotic Dynamics of Flow in Unsaturated Fractured Rocks, Fall AGU 1999 Meeting, San Francisco

8. Podgorney, R. K., B. Faybishenko, and T. Wood, Field Evidence of Unstable Infiltration into Variably Saturated Fractured Basalt on a 1-Meter Scale, Fall AGU 1999 Meeting, San Francisco.

Invited presentations given by B. Faybishenko on project-related problems

1. Lawrence Livermore National Laboratory, Environmental Restoration Division, Livermore, California (August 1998)
2. Stanford University, Earth Sciences Department (May 1995)
3. U.S. Nuclear Regulatory Commission, Washington, D.C. (November 1997)
4. Chapman Conference on Fractals in Hydrology, Clemson University, South Carolina (May 1998)
5. Gordon Research Conference, Proctor Academy, Andover, New Hampshire (August 1998)
6. University California at San Diego, Institute of Nonlinear Sciences, (January 1999)
7. Florida State University (February 1999)
8. DOE Characterization, Monitoring, and Sensor Technology—Crosscutting Program Annual Review Meeting, Gaithersburg, Maryland (March 1999)
9. University of California at Santa Barbara, Department of Geography, Santa Barbara, California (April, 1999)
10. Stanford University, Stanford, California (May 1999)
11. Spring 1999 American Geophysical Union Meeting, Special Session H12, Role of the Vadose Zone for Groundwater Contamination: Barrier or Pathway? (Boston, MA, June 1999)

Invention Disclosures (partially funded by the project)

K.H. Lee, A. Becker, B. Faybishenko, and R. Solbau, Electrical Resistivity Monitoring Borehole Array, Disclosure and Record of Invention submitted to the LBNL Patent Department on 7/8/98 (IB-1425).

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WEB site:

http://www-esd.lbl.gov/ERT/emsp.html

Figure Captions

Figure 1. Hierarchy of scales of hydrogeological components in fractured basalt

Figure 2.Cross-sectional schematic of the Hell s Half Acre research site showing the fracture traces in the basalt block, the infiltration gallery, drip sensors, outflow collection pans, and tensiometers.

Figure 3. Time variations of (a) Infiltration flux and total outflux, (b) outflux from pans located below the infiltration gallery, and (c) outflux from pans located outside of the footprint of the infiltration gallery.

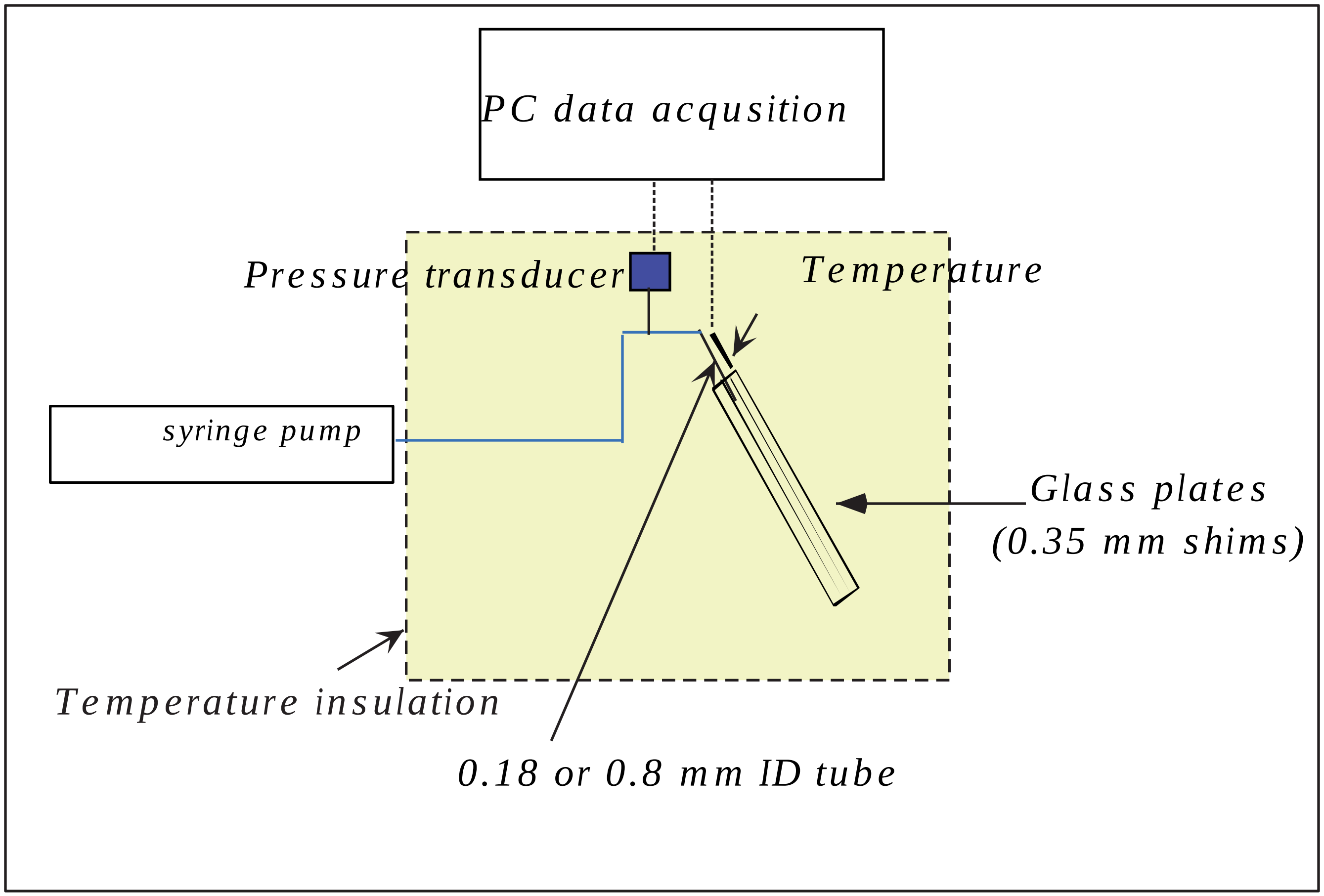
Figure 4. Time series (a) of dripping water intervals from Drip point D10 collected during the constant head test (first 200 points are shown), and (b) the three-dimensional chaotic attractor for this data plotted using the time delay $\tau = 3$ for the whole data set of 2858 points.

Figure 5. A schematic of the experimental apparatus to investigate water flow in a transparent fracture replica.

Figure 6. Examples of water pressure fluctuations for dripping in smooth and rough plates and schematics of drip formation.

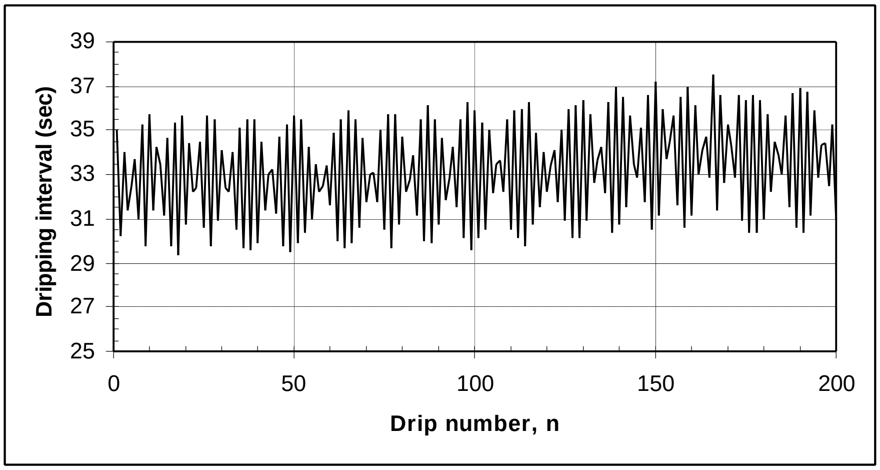
Figure 7. Chaotic attractors for pressure measured during water dripping experiments in smooth plates for different flow rates.

Figure 8. An example of a correspondence between the measured pressure and to drip formations in a variable aperture fracture replica for a flow rate of 5 mL/hr through a 0.8 mm ID needle.

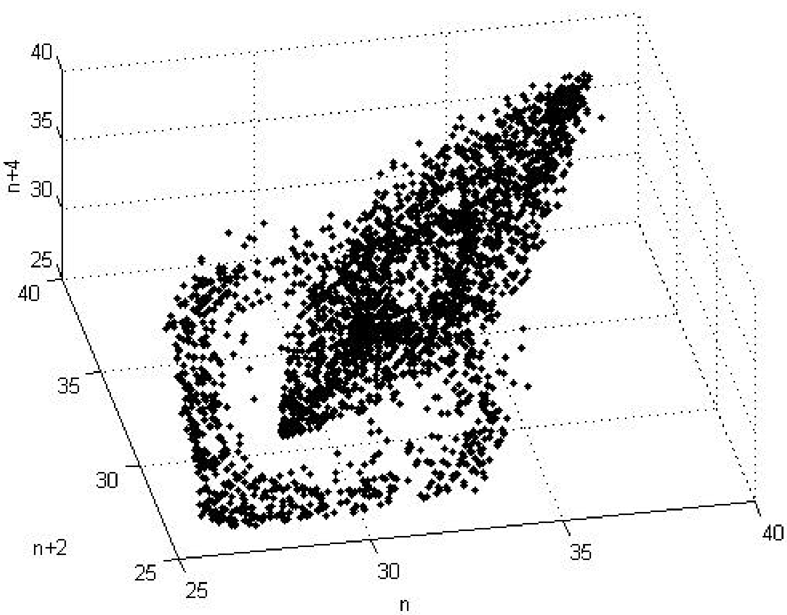


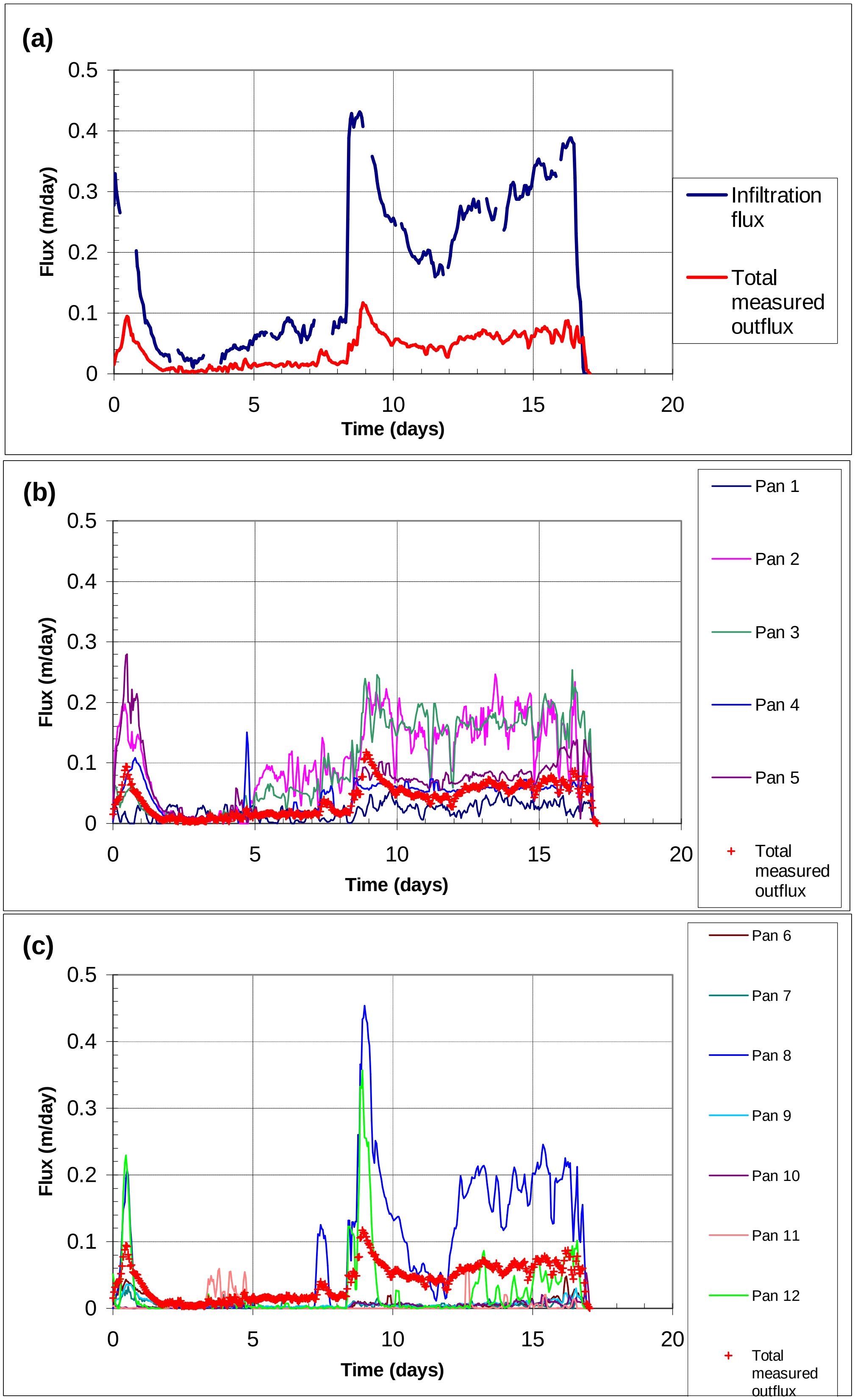
PC data acqusition
Pressure transducer
Temperature
syringe pump
Glass plates
(0.35 mm shims)
Temperature insulation
0.18 or 0.8 mm ID tube

(a)

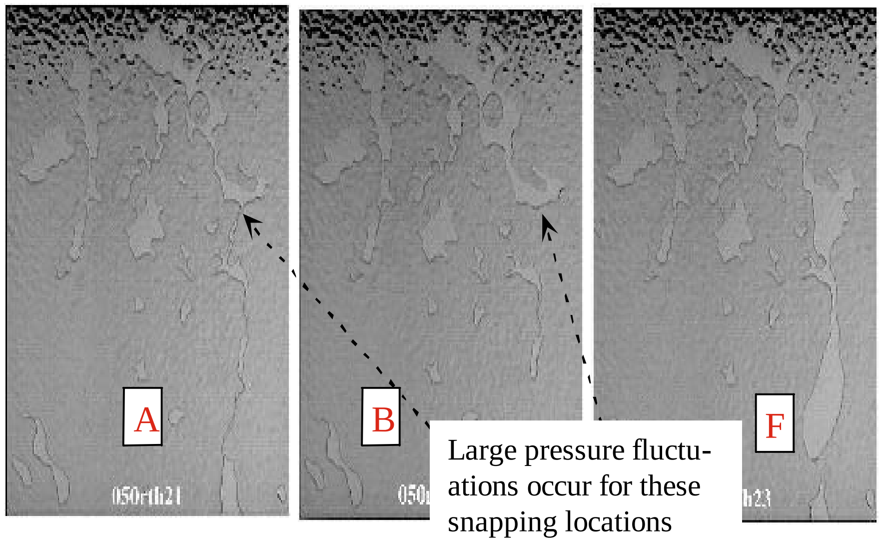

Dripping interval (sec)
39
37
35
33
31
29
27
25
0
50
100
150
200
Drip number, n

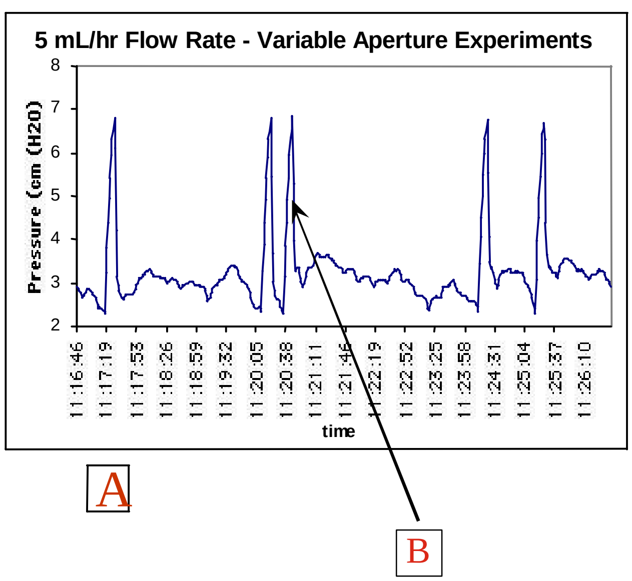
(b)


n+4
40
35
30
25
n+2
40
35
30
25
n
25
30
35
40



(a)
Flux (m/day)
0.5
0.4
0.3
0.2
0.1
0
0
5
10
15
20
Time (days)
Infiltration flux
Total measured outflux
(b)
Flux (m/day)
0.5
0.4
0.3
0.2
0.1
0
0
5
10
15
20
Time (days)
Pan 1
Pan 2
Pan 3
Pan 4
Pan 5
Total measured outflux
(c)
Flux (m/day)
0.5
0.4
0.3
0.2
0.1
0
0
5
10
15
20
Time (days)
Pan 6
Pan 7
Pan 8
Pan 9
Pan 10
Pan 11
Pan 12
Total measured outflux


A
B
F
050rth21
h23
Large pressure fluctuations occur for these snapping locations


5 mL/hr Flow Rate - Variable Aperture Experiments
Pressure (cm (H20)
8
7
6
5
4
3
2
11:16:46
11:17:19
11:17:53
11:18:26
11:18:59
11:19:32
11:20:05
11:20:38
11:21:11
11:21:46
11:22:19
11:22:52
11:23:25
11:23:58
11:24:31
11:25:04
11:25:37
11:26:10
time
A
B