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Authors
Long, R.H.
Benson, S.
Alavi, M.

Publication Date
1988-04-01

Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

EARTH SCIENCES DIVISION

Presented at the Eighth Annual AGU Front Range
Branch Hydrology Days, Fort Collins, CO,
April 19–21, 1988

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R.H. Long, S. Benson, M. Alavi, and T.N. Narasimhan

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Transport of a Conservative Solute through a Shallow Pond Bottom

Robert H. Long,[1,2] Sally Benson,[2] Mohsen Alavi,[2] and T.N. Narasimhan[2]

[1]Department of Materials Science and Mineral Engineering
University of California
Berkeley, CA 94720

[2]Earth Sciences Division
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

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Robert H. Long[1,2], Sally Benson[2], Mohsen Alavi[2], T.N. Narasimhan[2]

ABSTRACT

A field experiment has been performed in an evaporation pond at Kesterson Reservoir, Merced County, California, aimed at determining average solute fluxes through pond sediments and at estimating the magnitude and degree of spatial variability of water and solute transport properties. Kesterson Reservoir, a series of shallow ponds located at the terminus of the San Luis Drain, became the object of intense public interest and scientific investigation after it was discovered in 1983 that the disposal of irrigation drain waters bearing hazardous levels of a naturally occurring element, selenium, was having serious environmental effects on plant and animal life. The primary focus of the experiment was to gain insight into the mechanism of selenium migration and immobilization. As a first step in analyzing the selenium migration data, permeability and apparent dispersion coefficient values were obtained through the history-matching of breakthrough curves of a conservative solute, chloride, at 40 sampling locations within 5 sites throughout a 40-ha (100-acre) cell following pond-flooding. Chloride occurring naturally throughout the soil profile was utilized in a modeling effort as a conservative tracer under conditions of transient flow, and a deterministic one-dimensional fluid flow and transport mathematical model employing the integrated finite difference method (IFDM) was employed in the effort. Reasonable matches were obtained between the observed and calculated concentrations with the advective-dispersive code. Extreme lateral variability of soil hydraulic properties was demonstrated between and within field plots, with values of permeability and apparent dispersion coefficient varying by one to two orders of magnitude. The flow and transport properties determined throughout the field were found to conform to a log-normal distribution. The apparent dispersion coefficient is shown to be velocity dependent and exhibits a linear relationship with average pore water velocity. Estimates of dispersivity at the 40 locations appear high in relation to values measured typically in the laboratory. A general trend is observed of greater dispersivity values with increasing travel distance.

INTRODUCTION

Interest has risen markedly in recent years in improving our ability to

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1 Graduate Student, Department of Materials Science and Mineral Engineering, University of California, Berkeley, Ca. 94720

2 Earth Sciences Division, Lawrence Berkeley Laboratory, Berkeley, Ca. 94720

make accurate estimates of solute and water fluxes through systems of porous media. The need to quantify movement of chemical constituents through soils arises in a variety of situations, including the use of fertilizers and pesticides in agricultural applications, the disposal of industrial and municipal wastes in landfills, and the leaching of salts during soil reclamation. Technologists wish to improve their understanding of the physical processes that govern transport so that they are better able to predict the fate of contaminants in the subsurface and their potential impact on water resources. Concern over adverse environmental impacts through agriculture and land disposal of wastes has been reflected in increased governmental regulation and in the current high level of research in the fields of waste isolation and contaminant fate prediction. Ultimately, the ability to assess impacts on groundwater quality depends on the use of reliable models and methods that are able to describe water and solute fluxes over large field systems. This includes the ability to estimate not only average fluxes, but also the distribution about the average.

The determination of *average* solute and water fluxes, however, is made difficult by the extreme spatial and temporal variability exhibited in soil flow and transport properties. Many investigators have examined issues of spatial variability of soil properties and have elucidated difficulties for the transport modeler. *Biggar and Nielsen* (1976), in a steady-state study of chloride movement during ponding among 20 sites within a 150-ha field, fitted observed data to a one-dimensional analytical solution to the advection-dispersion equation through the variation of two parameters - apparent dispersion coefficient (D) and average pore water velocity *(v)*. Statistical analysis of D and v showed them to be log-normally distributed. D and v were observed to vary by an order of magnitude within a plot. *Van De Pol et al.* (1977) in an experiment involving unsaturated transport, fitted apparent dispersion coefficients and average pore water velocities in a similar fashion and observed that some breakthrough curves indicated that solute reached deeper depths before shallower depths. D and v were again found to be log-normally distributed.

With the eventual analysis of the reactive chemical transport of selenium in mind, the primary objective of this work has been to characterize the physical properties governing flow and transport through a shallow pond bottom sediment. If such a characterization is to provide accurate information for the prediction of solute fluxes, it must include not only an estimate of average properties but an understanding of the spatial variability of the soil properties. Therefore, values of permeability and apparent dispersion coefficient have been determined at a number of locations throughout the pond and are analyzed for type of distribution and degree of heterogeneity. An integrated finite difference method numerical code is used for the solute transport simulations. Discussion is included of the equations used and the modeling methodology, including

choice of boundary and initial conditions. Several related issues, such as a possible functional relation between average pore water velocity and apparent dispersion coefficient, and an examination of the effect of sample number on parameter estimation are also presented.

A second purpose of this study was to determine the longitudinal dispersivity of the underlying pond sediments. Hydrodynamic dispersion is a key process that determines the rate at which solutes migrate. At present, only a few tens of field tracer tests are reported in the literature involving the determination of field-scale dispersivities, and only five were judged to be of high reliability in a recent literature review that was performed on the subject *(Gelhar et al.,* 1985). Clearly, there is a need for reliable field-scale dispersivity data to fill the present gap. By performing additional field-scale experiments, we will develop a better understanding of the processes and mechanisms of flow and transport, as well as more of a consensus as to what methods of measurement are most appropriate. Therefore, calculated dispersivities are presented and a few potential correlations are examined, such as with travel distance and pore water velocity.

THEORY

The primary mechanisms for the transport of solutes in soils are advection and hydrodynamic dispersion, the latter of which results from two distinct processes, mechanical dispersion and molecular diffusion. Mechanical dispersion, a mixing process similar in effect to diffusion, results from spatial variations in advective transport, and has been found to conform, on a laboratory scale, to an equation of the same form as that of diffusion. Even though the effects of the two processes appear to be similar, they are not related. Dispersion results from the heterogeneous nature of soil water flow including velocity variations within individual pores, variably distributed pore sizes, and the tortuous nature of flow paths. Because of the similar mathematical formulations of the two processes, they are typically lumped together additively into a single coefficient, the apparent dispersion coefficient, D_h, that incorporates both effective molecular diffusion (D_e) and mechanical mixing (D_m),

$$D_h = D_e + D_m \tag{1}$$

resulting in the following form of the advection-dispersion equation for transient, one-dimensional flow in fully-saturated, isotropic, and homogeneous porous media,

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left[D_h\frac{\partial C}{\partial z} - vC\right] \tag{2}$$

where z (L) is the unidirectional space coordinate, t (T) is time, C $(M \cdot L^{-3})$ is the solute concentration in the soil solution, and v $(L \cdot T^{-1})$ is the average pore water velocity.

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Many analytical solutions are available for problems involving simple geometries, well-defined initial/boundary conditions, and steady flow. The application of (2) to problems of practical interest has been investigated by various researchers, and the equation has been thoroughly tested in the laboratory under conditions of steady-state and transient water flow. The work of *Danckwerts* (1953), *Day* (1956), and *Nielsen and Biggar* (1961,62) demonstrated the utility of the physically-based model in columns of uniform glass beads, clean sands, and sieved loams. In aggregated soils, the use of (2) has also been justified in the work of *Passioura* (1971), *Rao et al.* (1980), and *Nkedi-Kizza et al.* (1983). Its application, though, has often required a scaling-up of the relatively small dispersion coefficients measured in the lab to larger values observed from field-scale experiments.

In highly-structured soils or unsaturated soils, the use of (2) has been less successful, and evidence from a number of researchers *(Biggar and Nielsen,* 1962; *Green et al.,* 1972; *Rao et al.,* 1974) suggests that the application of the physically-based model may be inappropriate for describing the average movement of water and solutes at large field sites exhibiting a high degree of spatial heterogeneity with regard to fluid flow and transport properties. Several new approaches have been developed in an effort to cope with extreme lateral and vertical variability and with the concern that the advection-dispersion equation is an inappropriate approximation to solute transport description in the field. Most of the alternate approaches, including the use of scaling factors *(Peck et al.,* 1977) and transfer functions *(Jury,* 1982) use stochastic methods to describe the inherent statistical distributions of the pertinent properties. Variations in velocity are explicitly included to account for solute spreading rather than through the use of large dispersion coefficients.

In this study, rather than attempting to verify or compare particular models, a deterministic approach is taken in an attempt to make local measurements of the flow and solute transport properties and to gain an understanding of the type of statistical variability that exists in the Kesterson soils. In many field situations, however, as in this experiment, initial and boundary conditions are such that analytical solutions to the advection-dispersion equation are not available. Therefore, (2) was evaluated numerically by the integrated finite difference method (IFDM) *(Narasimhan and Witherspoon,* 1977). For non-reactive fully-saturated solute transport, the code, CHAMP, *(Narasimhan et al.,* 1985) solves a set of coupled equations describing the net flux of solutes into a volume element in the form of:

$$-\int \vec{q} \cdot \vec{n} \, C \, d\Gamma + \int \phi D_h \nabla C \cdot \vec{n} \, d\Gamma = V_w \frac{\Delta C}{\Delta t} \qquad (3)$$

where Γ represents the closed surface around a volume element, $\vec{n}$ is the outer normal to the element surface, ϕ is porosity, and V_w is the volume

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of water in the element. This equation of mass balance, with boundary conditions and source terms, is written for each volume element, and the resulting set of equations is assembled in matrix form. A mixed explicit-implicit iterative scheme is used for matrix solution.

EXPERIMENT

Five 2.75 m^2 (9 ft x 9 ft) sites in a 40 hectare (100 acre) shallow pond were instrumented while the pond was dry. Instrumentation included soil water samplers, tensiometers, and shallow groundwater monitoring wells. 8 soil water samplers and tensiometers were installed in each plot to evenly spaced depths of from 0.175 m (0.6 ft) to 1.225 m (4 ft). Shallow groundwater monitoring wells were drilled and installed to depths of from 2.44 m (8 ft) to 12.19 m (40 ft). Loam and sandy-loam soils make up the pond bottom material to a depth of approximately 2.44 m (8 ft) overlying a shallow sandy aquifer. Dessication cracks in the soil surface were visible to depths of 0.15 m (6 in). The pond consists of one of twelve shallow cells at Kesterson Reservoir used for the collection of agricultural drain water from irrigated farmlands.

Flooding to a depth of 1 m (3.28 ft) took place over an approximately one week period with groundwater ($\approx$1000 ppm Cl) pumped from a nearby series of wells. Intensive collection of soil water samples, pond water, and shallow groundwater samples was initiated after flooding at rates of from once every 3 days at early times to once every 2 weeks after several months. The experiment continued for a period of approximately one year. Samples were analyzed for chloride with a silver nitrate titration. Data from four of the water samplers at one of the monitoring sites are shown in Figure 1.

MODELING METHODOLOGY

The conservative tracer was not added artificially to the system. Rather, chloride movement resulted from the dissolution of chloride in a salt crust upon flooding and from that which was already present in the soil solution. Immediately following the flooding event, flow and transport were highly transient. No attempt was made to model this early period of partially-saturated flow since the water application rate and the initial rate of chloride mobilization were essentially unquantifiable. The modeling effort begins several days after flooding, after fully water saturated conditions were established.

Chloride concentrations and fluid potentials were monitored at each of the plots from the pond surface to a depth of approximately 2.75 m (9 ft). A one-dimensional grid of 55 5 cm (1.97 in) thick elements was constructed to discretize the 2.75 m flow region. For the upper boundary, measured pond water depths served as a prescribed potential boundary while measured chloride concentrations provided a prescribed concentration boundary condition. For the bottom boundary, in a similar

manner, hydraulic head values measured in monitoring wells were input directly as the potential condition and observed chloride concentrations in groundwater served as the concentration boundary condition. Figure 2 shows chloride concentrations utilized as the upper and lower boundary conditions at one of the sites. At each site, an instant T_0 some few days after flooding was chosen to be the time from which history-matching of solute breakthrough would begin. T_0, depending on the site, ranged from 4 to 19 days following flooding. Figure 3 shows an example of a chloride profile measured at T_0 for one of the plots. The solute concentration profile measured at each site at T_0 was utilized as the initial concentration for the system grid. For the fluid potential initial condition, a linear interpolation between the potentials measured at the surface and in the shallow well at T_0 was used.
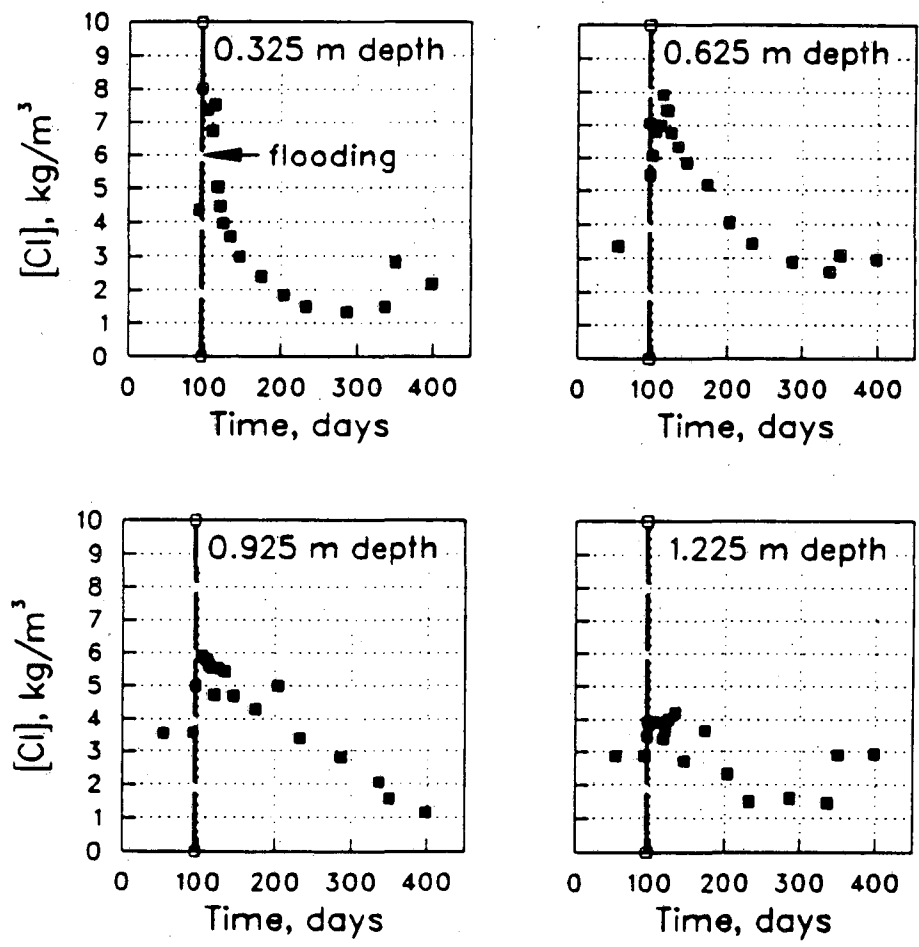

Figure 1. Chloride response curves resulting from pond flooding for 4 of 8 soil water samplers at site UZ-8.
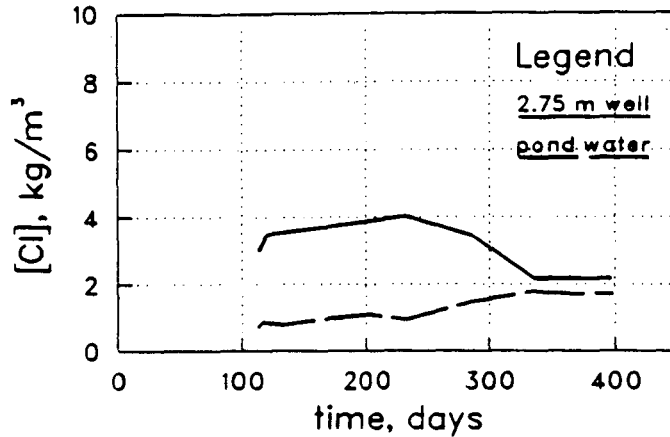
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Figure 2. Chloride levels measured throughout the experiment in pond water and shallow groundwater were utilized as concentration boundary conditions. The boundary conditions utilized for site UZ-8 are shown.
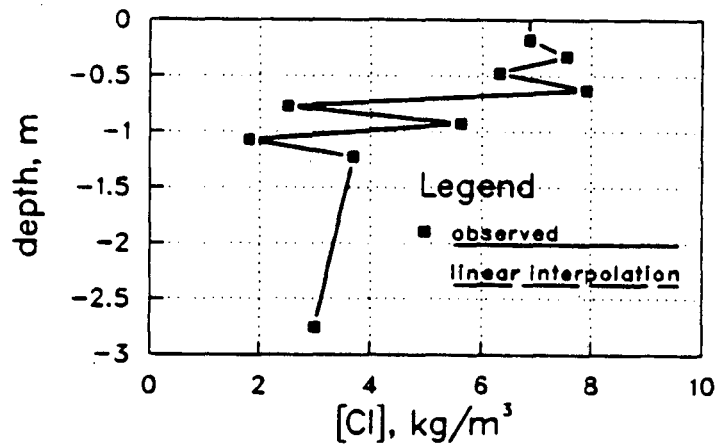

Figure 3. The chloride concentration profile measured at each plot at time T_0 was used as the initial solute concentration condition for modeling performed at the particular site. The profile observed at site UZ-8 is shown.

It is important to mention several key assumptions that were made in the analytical procedure and possible resulting limitations.

(1) The flow regime was modeled as a fully-saturated medium. Actual saturation at T_0 may have been slightly less than this due to the presence of entrapped air, however, tensiometer data collected during the experiment, and modeling of the infiltration process indicated that it was very likely that by this time the soils were at least 90-95% saturated.

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(2) It was assumed that the dissolution of chloride was complete at the commencement of modeling, i.e. that there was no chloride source within the flow region during the modeling time frame. Chloride has been used extensively in tracer studies reported throughout the literature due to its high water solubility and mobility, however, the possibility of a rate limitation to its dissolution in this system is not known and has been neglected.

(3) Chloride measurements were assumed to provide representative estimates of average conditions at the particular depth or location from which they were collected, i.e. pond water and well water samples were considered to adequately define the upper and lower boundary conditions, and that chloride levels measured in soil water samplers were indicative of processes and transport occurring in the interval adjacent to the soil water sampler.

(4) The chloride profile used as the initial condition was constructed from soil water samples collected laterally throughout each plot. Due to the extreme lateral variability that is often evidenced in soils, these conditions used may not have been representative of initial conditions throughout the test plot. The extent to which uncertainty in the initial conditions would effect interpretation of results is a function of the degree to which lateral heterogeneity is exhibited in the solute profiles. Sensitivity studies are presently being performed to address this issue.

(5) The modeling was performed assuming one-dimensional vertical flow. A two-dimensional effort would have lead to an unwarranted degree of complexity. With the addition of a large number of variables and parameters, a highly arbitrary history-matching procedure would have resulted. However, the large spatial variations in soil hydraulic parameters that have often been observed in soils, can lead to possible 2- and 3-dimensional flow effects which have been neglected in this study. An attempt is being made, the results of which are not yet available, to evaluate for some simple forms of soil heterogeneity, the extent to which water may flow laterally during infiltration.

In modeling performed at a particular site, one site-specific set of boundary and initial conditions was applied to the eight individual locations, however, history-matching of the chloride concentration was performed separately at each soil water sampler (at each depth) as if it possessed its own set of parameters representing a vertical, independent, non-interacting flow region. No attempt was made to match chloride concentration profiles during the experiment. The results therefore represent spot measurements of properties at discrete points where each parameter is an effective value over the entire 2.75 m (9 ft) soil column. History-matching involved making numerous iterative runs of CHAMP and systematically varying the parameters, permeability, k (L^2), and apparent dispersion coefficient, D_h, in an attempt to produce the best possible

match, determined visually, to the observed data. The parameters were applied uniformly over the grid, and a constant porosity of 0.45, based on an average value obtained from laboratory measurements, was assumed for all the sites. The final results of the history-matching at 4 locations within one site, produced with the best possible combination of parameters, are presented in Figure 4.

It was often possible, based purely on the closeness of the observed and calculated curves, for a range of parameter values to match the data almost equally well. *Good* matches, however, could often result in the choice of physically unrealistic combinations of parameters or the choice of values that were considered unlikely based on previous measurements made in the laboratory and at Kesterson. An element of discretion was therefore introduced into the history-matching procedure of systematically constraining D_h and k. Dispersion coefficients were adjusted so as to result in dispersivity values that were consistent with the scale of the experiment and which were within range of values reported elsewhere in the literature. Permeabilities were chosen with the aid of *in situ* hydraulic conductivity measurements made at each site by Guelph permeameter. An attempt was made to minimize the magnitude of the dispersivity while maintaining the goodness-of-fit. This addition of judgement and utilization of existing data improved the uniqueness of the curve fits and allowed for results into which a much higher degree of confidence could be placed.

In the form that was available, CHAMP did not explicitly evaluate the dispersive fluxes separately from those due purely to molecular diffusion, but rather treated them together through one lumped parameter, the apparent dispersion coefficient, D_h. Therefore, dispersivities (α_l) were calculated assuming a linear relationship between D_h and v on the basis of the following expression, which is discussed in a later section:

$$\alpha_l = \frac{(D_h - D_e)}{\bar{v}} \tag{4}$$

where the effective coefficient of molecular diffusion was taken to be 1×10^{-11} m^2/s. Since the average pore water velocity was not constant over the course of the experiment, due to the variable nature of the fluid potential boundary conditions, an effective average pore water velocity, $\bar{v}$, which represents the average value over time of the linear pore velocity, is used in (4). This results in an approximation to the actual α_l, however, since the actual variation of pore water velocity was $\approx \pm 50\%$ of $\bar{v}$, at each site during the course of the experiment, this is felt to be acceptable. D_h was treated as a constant, even though in reality it may have varied.

It should be noted that throughout this paper, the parameter k or *intrinsic permeability* is used to describe the conductance property of the porous medium. k is a property only of the porous medium and has
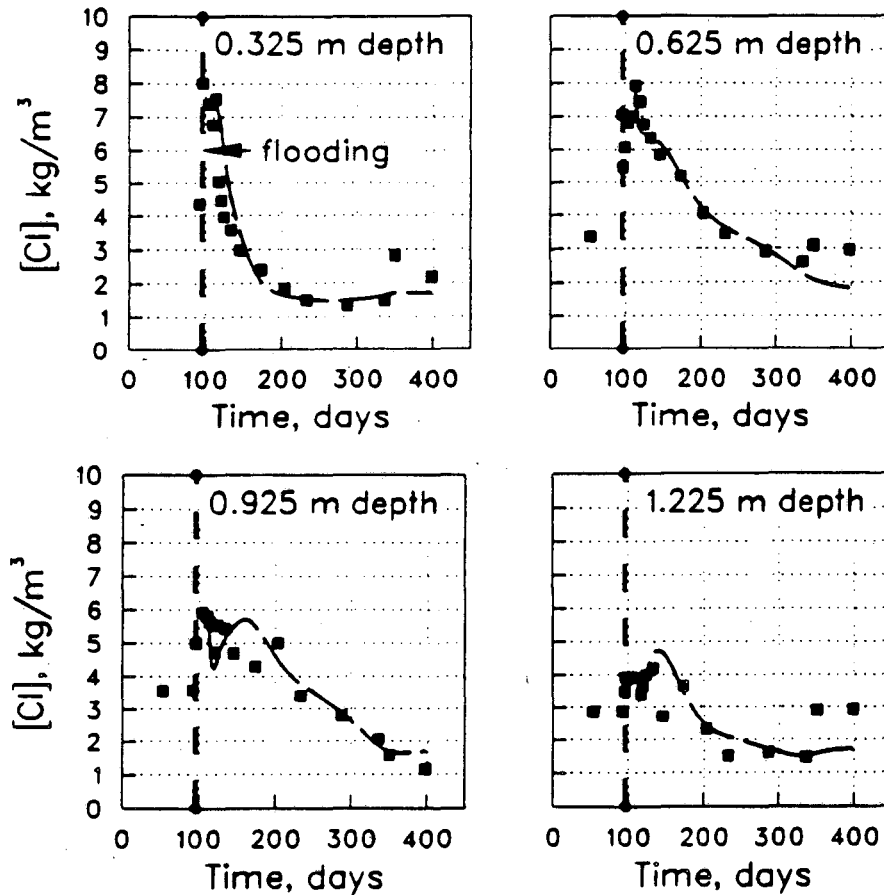
Figure 4. History-matches of modeled chloride response (solid curve) to observed breakthrough data (boxes) at depths of .325, .625, .925 and 1.225 m at site UZ-8

dimensions of L^2. The more commonly used expression K or *hydraulic conductivity* $(L \cdot T^{-1})$ is a function of the fluid as well as the medium. Hydraulic conductivity is related to the permeability by the relation:

$$K = \frac{k \rho g}{\mu} \qquad (5)$$

where ρ is the fluid density $(M \cdot L^{-3})$, g the acceleration of gravity $(L \cdot T^2)$, and μ is the fluid viscosity $(L \cdot T \cdot M^{-1})$. In a water-saturated soil at ambient temperatures, the conversion between the two parameters is easily made by K (m/s) $\approx 10^7 \cdot k$ (m^2).

RESULTS AND DISCUSSION

k and D_h

A summary of properties determined in the modeling effort is presented in Table 1 including values of k, D_h, v, and α_l. The arithmetic mean average pore water velocity of all 40 locations is 1.13 m/yr (3.7 ft/yr)

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varying from a low, based on plot averages, of 0.3 m/yr (1 ft/yr) to 3.11 m/yr (10.2 ft/yr). For k an arithmetic mean value of 2.6 x 10^{-14} m^2 is calculated. This value of k corresponds to a saturated hydraulic conductivity of 8 m/yr (26 ft/yr). Average k values calculated in this manner at each site are within an order of magnitude, both above and below, of *in situ k* measurements made by Guelph permeameter prior to flooding *(LBL,* 1987) and are within the range of values calculated from a series of ring infiltrometer measurements *(Luthin,* 1966).

Table 1. *Summary of Parameters Determined*							
Site	Depth, m	pore velocity, m/s	k, m^2	ln(k)	D_h, m^2/s	ln(D_h)	α_l, m
UZ-1	.175	0.186 x 10^{-7}	1.1 x 10^{-14}	-32.14	0.50 x 10^{-9}	-21.42	0.03
	.325	0.506 x 10^{-7}	3.0 x 10^{-14}	-31.14	0.50 x 10^{-9}	-21.42	0.05
	.475	0.169 x 10^{-6}	10.0 x 10^{-14}	-29.93	1.00 x 10^{-9}	-20.72	0.01
	.625	0.843 x 10^{-8}	0.5 x 10^{-14}	-32.93	0.50 x 10^{-9}	-21.42	0.06
	.775	0.413 x 10^{-9}	0.025 x 10^{-14}	-35.93	0.01 x 10^{-9}	-25.33	0.001
	.925	0.338 x 10^{-8}	0.2 x 10^{-14}	-33.85	0.20 x 10^{-9}	-22.33	0.06
	1.075	0.169 x 10^{-8}	0.1 x 10^{-14}	-34.54	0.10 x 10^{-9}	-23.03	0.05
	1.225	0.338 x 10^{-8}	0.1 x 10^{-14}	-34.54	0.50 x 10^{-9}	-21.42	0.06
UZ-3	.175	0.241 x 10^{-7}	0.70 x 10^{-14}	-32.59	2.0 x 10^{-9}	-20.03	0.08
	.325	0.138 x 10^{-7}	0.40 x 10^{-14}	-33.15	0.5 x 10^{-9}	-21.42	0.04
	.475	0.138 x 10^{-7}	0.40 x 10^{-14}	-33.15	2.0 x 10^{-9}	-20.03	0.14
	.625	0.863 x 10^{-9}	0.025 x 10^{-14}	-35.93	0.1 x 10^{-9}	-23.03	0.10
	.775	0.207 x 10^{-7}	0.60 x 10^{-14}	-32.75	4.0 x 10^{-9}	-19.34	0.19
	.925	0.259 x 10^{-7}	0.75 x 10^{-14}	-32.52	2.5 x 10^{-9}	-19.81	0.10
	1.075	0.345 x 10^{-7}	1.00 x 10^{-14}	-32.24	8.0 x 10^{-9}	-18.64	0.23
	1.225	0.259 x 10^{-7}	0.75 x 10^{-14}	-32.52	9.0 x 10^{-9}	-18.53	0.35
UZ-5	.175	0.177 x 10^{-7}	1.00 x 10^{-14}	-32.24	0.75 x 10^{-9}	-21.01	0.04
	.325	0.160 x 10^{-7}	0.90 x 10^{-14}	-32.34	0.90 x 10^{-9}	-20.83	0.06
	.475	0.177 x 10^{-7}	1.00 x 10^{-14}	-32.24	1.20 x 10^{-9}	-20.54	0.07
	.625	0.532 x 10^{-8}	0.30 x 10^{-14}	-33.44	0.10 x 10^{-9}	-23.03	0.02
	.775	0.222 x 10^{-7}	1.25 x 10^{-14}	-32.01	1.00 x 10^{-9}	-20.72	0.05
	.925	0.479 x 10^{-7}	2.70 x 10^{-14}	-31.24	1.30 x 10^{-9}	-20.46	0.03
	1.075	0.222 x 10^{-7}	1.25 x 10^{-14}	-32.01	0.60 x 10^{-9}	-21.23	0.03
	1.225	0.177 x 10^{-8}	0.10 x 10^{-14}	-34.54	0.10 x 10^{-9}	-23.03	0.05
UZ-6	.175	0.561 x 10^{-8}	2.5 x 10^{-14}	-31.32	0.8 x 10^{-9}	-20.95	0.14
	.325	0.225 x 10^{-7}	10.0 x 10^{-14}	-29.93	3.3 x 10^{-9}	-19.53	0.15
	.475	0.224 x 10^{-7}	10.0 x 10^{-14}	-29.93	10.0 x 10^{-9}	-18.42	0.44
	.625	0.168 x 10^{-7}	7.5 x 10^{-14}	-30.22	8.0 x 10^{-9}	-18.64	0.47
	.775	0.112 x 10^{-8}	0.5 x 10^{-14}	-32.93	0.5 x 10^{-9}	-21.42	0.44
	.925	0.225 x 10^{-8}	1.0 x 10^{-14}	-32.24	1.0 x 10^{-9}	-20.72	0.44
	1.075	0.202 x 10^{-8}	0.9 x 10^{-14}	-32.34	1.0 x 10^{-9}	-20.72	0.49
	1.225	0.225 x 10^{-8}	1.0 x 10^{-14}	-32.24	1.0 x 10^{-9}	-20.72	0.44
UZ-8	.175	0.376 x 10^{-7}	2. x 10^{-14}	-31.54	3.0 x 10^{-9}	-19.62	0.08
	.325	0.940 x 10^{-7}	5. x 10^{-14}	-30.63	15.0 x 10^{-9}	-18.01	0.16
	.475	0.244 x 10^{-6}	13. x 10^{-14}	-29.67	30.0 x 10^{-9}	-17.32	0.12
	.625	0.564 x 10^{-7}	3. x 10^{-14}	-31.14	10.0 x 10^{-9}	-18.42	0.18
	.775	0.376 x 10^{-7}	2. x 10^{-14}	-31.54	8.0 x 10^{-9}	-18.64	0.21
	.925	0.940 x 10^{-7}	5. x 10^{-14}	-30.63	10.0 x 10^{-9}	-18.42	0.11
	1.075	0.376 x 10^{-7}	2. x 10^{-14}	-31.54	10.0 x 10^{-9}	-18.42	0.27
	1.225	0.188 x 10^{-6}	10. x 10^{-14}	-29.93	40.0 x 10^{-9}	-17.03	0.21

A high degree of spatial variability is evident throughout the field. Permeabilities pond-wide vary by nearly 3 orders of magnitude from a high of 10×10^{-14} m^2 to a low of 0.025×10^{-14} m^2 while apparent dispersion coefficients fluctuate similarly. Within plots, heterogeneity is not as pronounced yet it is still exhibited to a significant extent. Values of k determined at site UZ-1 suggest that pore water velocities at one location in the plot are 100 times the pore water velocities at locations positioned just a meter laterally away. At other sites as well, one to nearly two orders of magnitude is a typical range over which k and D_h are shown to vary.

To determine the form of the population density function that best describes the distribution of k and D_h, the method as presented in *Warrick and Nielsen* (1980), has been applied to the data where fractile diagrams are generated based on the normal density function. The 40 values of k and D_h are listed in ascending order from $i = 1$ to $i = 40$ and the cumulative distribution function, P(x), is calculated as $i/40$. Corresponding values of the probability units, $(x - \mu)\sigma^{-1}$, where x represents the actual value of k and D_h, μ is the mean value of x, and σ is the standard deviation, are then obtained from tabular values of the cumulative normal distribution. This procedure is also performed in the same fashion using natural logarithms of x where μ and σ are now the mean and standard deviation of ln(x). The linearity of the ln(k) plot in Figure 5 demonstrates that a log-normal distribution best describes the permeability variations. A similar result is obtained with D_h.
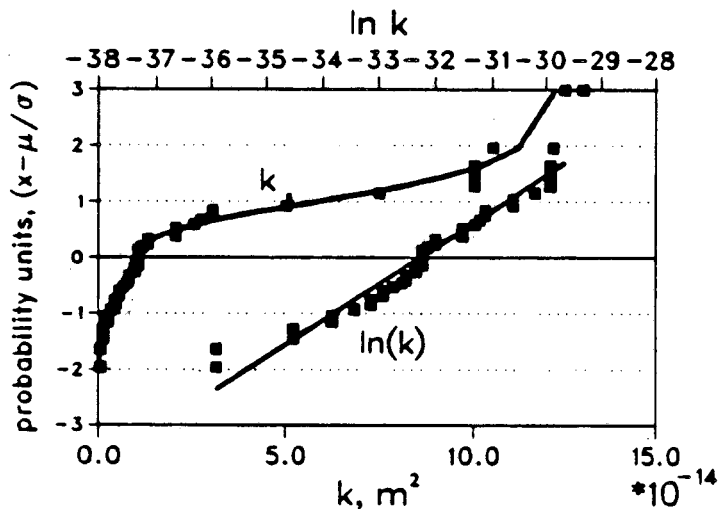

Figure 5. The linearity of the ln(k) figure suggests that the distribution of k is best described by a log-normal density function.

In Figure 6 we see the frequency of occurrence of the observed permeability values, k, with the theoretical relative-frequency curve based on fitting the 40 samples to the frequency density function for a log-normal distribution:

$$L(x;\mu;\sigma) = \frac{1}{\sigma\sqrt{2\pi}}e^{\frac{-(\ln(x)-\mu)^2}{2\sigma^2}} \qquad (6)$$

The idealized distribution is an approximation and does not exactly match the observed values. A chi-square goodness-of-fit test has been applied to both the k and D_h distributions to determine the agreement between the observed and the theoretical log-normal distribution. k and D_h both pass the test at the 5% significance level suggesting that, from the basis of this test, there is no reason to reject the hypothesis of a log-normally distributed population. It may be possible, however, to also consider other distributions i.e. the Gamma distribution.

In a log-normal distribution the mean is defined as $\mu_1 = e^{(\mu+.5\sigma^2)}$, and the variance as $\sigma_1^2 = e^{(\sigma^2+2\mu)}(e^{\sigma^2}-1)$ where μ and σ are based on the set $\ln(x)$ *(Biggar and Nielsen, 1976)*. For k, we have a mean value of 3.2×10^{-14} m^2 with a standard deviation of 9.14×10^{-14}. The arithmetic mean k calculated above is 20% lower than this value. For D_h, a mean value of 6.41×10^{-9} m^2/s is calculated with a standard deviation of 28.3 $\times 10^{-9}$. The coefficient of variance (CV) is a parameter often used as a measure of relative variability and is defined as:

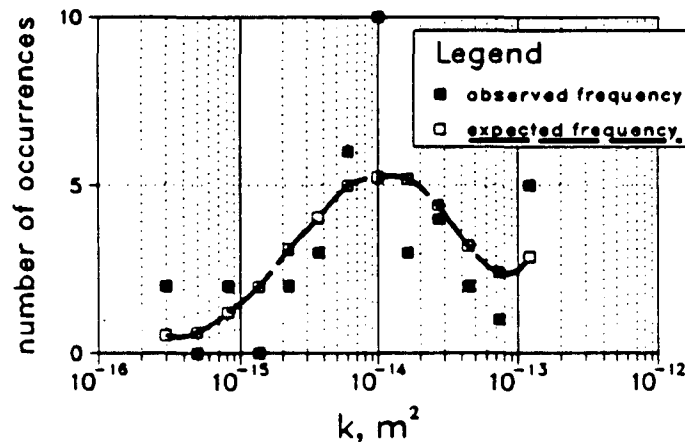$$CV = \frac{\sigma_1}{\mu_1}\cdot 100\% \qquad (7)$$

Figure 6. Frequency distribution of the observed values of permeability and the theoretical values based on a log-normal distribution

For k and D_h the CV values are both relatively high, 290% and 440% respectively, suggestive of a large degree of variability. For comparison, CV values for some soil parameters, i.e. bulk density, are often below 10% *(Warrick and Nielsen,* 1980).

In Figure 7, we see the effect of sample number on the measure of uncertainty by plotting number of samples vs the 95% confidence interval for k. This analysis assumes a measure of the sample mean and variance and can be calculated as,

$$-\mu_1 - t_{\frac{\alpha}{2}(n-1)} \frac{\sigma_1}{\sqrt{n}} \leq \mu_1 \leq \mu_1 + t_{\frac{\alpha}{2}(n-1)} \frac{\sigma_1}{\sqrt{n}} \qquad (8)$$

where μ_1 and σ_1 are calculated as above. The expression, $t_{\alpha/2(n-1)}$, refers to the t distribution with n-1 degrees of freedom at the $1-\alpha$ confidence interval. The figure indicates that to obtain an estimate of k within an order of magnitude of the true mean, approximately 10 measurements would be required, within ±100% 50 measurements would be needed; 150 measurements would estimate k within ±50% of its true value. A similar calculation performed on D_h indicates that 20 measurements would yield an estimate within an order of magnitude, 100 would be required to be within ±100% and 350 would produce an estimate within ±50% of the true mean.
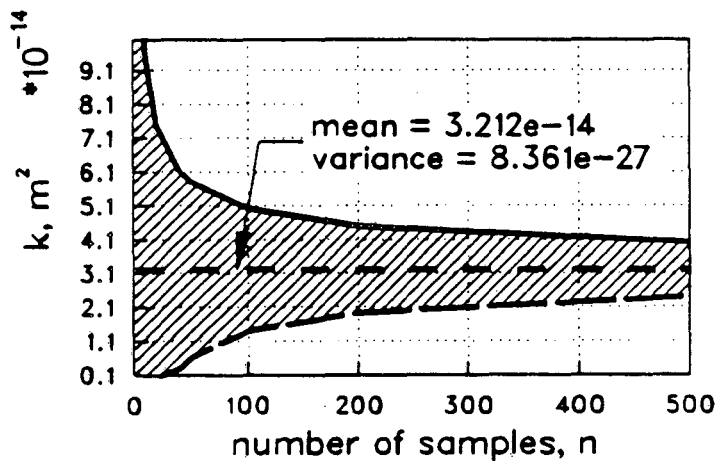

Figure 7. The effect of sample number on the accuracy of the mean k estimation. The shaded area represents the 95% confidence interval.

The significance of variability cannot be overlooked in the prediction of solute fluxes at this and other sites. In the data presented we have seen that fluid velocities can vary by orders of magnitude within the confines of small field plots. The extent that this degree of heterogeneity extends deeper into the soil profile is not known, however, certainly an aware-

ness must exist in data collection and analysis that the heterogeneous soil profile is a composite of numerous flow paths a large number of which have the ability to transmit solutes many times more rapidly than the mean fluid velocity.

Longitudinal Dispersivities

Longitudinal dispersivities determined through the use of CHAMP are presented in Table 1. They range from a low value of ≈ 0.1 cm to 49 cm. Dispersivity values obtained from laboratory column experiments on undisturbed cores of unconsolidated material generally fall in the range of 0.01 to 2 cm *(Freeze and Cherry*, 1979), considerably smaller than the values reported here. This tendency has been reported elsewhere *(Fried*, 1975; *Cherry et al.*, 1975; *Bredehoeft et al.*, 1976; *Anderson*, 1979; and *Biggar and Nielsen*, 1980) and can be attributed to several factors. Field-scale heterogeneity is often on a scale greater that that which can be conveniently included in a sample. Microscopic pore geometry variations, the type of heterogeneity that would be exhibited in a small sample, occur to such a completely random extent as to make only a minimal contribution to dispersion, however, large scale textural variability, layering, fingering, lateral discontinuities, and other types of major field structural heterogeneities often lead to fluid velocities which become highly spatially variable. The greater advective variability of the fluid stream in the field over that found in relatively small uniform laboratory samples will be exhibited in greater apparent dispersivity. Also, diffusion into immobile phases is not accounted for in deterministic treatments. This contribution to the apparent dispersion coefficient may be small in laboratory columns, but in the field it may account for the major portion of D_h *(Davidson et al.*, 1983).

In Figure 8, we see values of dispersivity plotted vs depth (travel distance) at one of the monitoring sites - UZ-8. While the trend is not without exception, what is evident at this site, and in general, at the other four, is an increase in dispersivity with increasing scale of observation. At the shallower depths, dispersivities tend to be relatively smaller, while the largest values tend to be located at the deeper depths. Scale dependent dispersivity is a result of processes similar to those discussed above, i.e soil structural variability. As the scale of the observation is increased, the likelihood is greater that soil variability will be encountered. Also, greater travel distances allow for the effects of soil variability to act for longer periods of time on the solute distribution, thereby leading to a more dispersed solute plume. The trend towards increasing α_l with increased travel distance is consistent with other field observations *(Gelhar et al.*, 1985). No correlation was observed, however, between α_l, and D_h or v.

Numerous investigators have studied the theoretical relationship between apparent dispersion coefficient, D_h, average pore water velocity, v, molecular diffusion, D_o, and other characteristics of porous media.

Harleman and Rumer (1962), and *Biggar and Nielsen* (1976) have suggested the following relationship:

$$D_h = D_e + \alpha v^n \qquad (9)$$

where α and n are constants to determined from data. Laboratory studies have indicated though that for practical purposes n can be taken as unity, thereby reducing (9) to a linear equation:

$$D_h = \tau D_o + \alpha_l v \qquad (10)$$

where α_l is designated the longitudinal dispersivity (L). D_o is the coefficient of molecular diffusion in pure water, and τ is an empirical, dimensionless quantity related to the tortuosity of the medium. In Figure 9, all 40 values of v are plotted vs D_h. It appears that on the log-log axes the relation is approximately linear suggesting that D_h does exhibit a linear relationship with v and that for this field soil (10) is a valid expression. *Biggar and Nielsen* (1976), also demonstrated an approximately linear correlation between D_h and v, however, the fluid velocities were one to two orders of magnitude greater than those in this study. *Kirda et al.* (1973), in a study that involved chloride displacement through columns of sieved and packed sandy loam observed that at pore water velocities less than $\approx 1.7 \times 10^{-6}$ m/s the apparent dispersion coefficients were no longer velocity dependent and were essentially equal to the effective diffusion coefficient. Fluid velocities in the present study were significantly below this limit, and yet a similar functional relationship with velocity is still demonstrated. The greater degree of soil structural heterogeneity present in the field soil may help to explain this difference. It is also interesting to note that with only 40 samples in the present study (correlation coefficient of 0.81), the linear functional relationship appears to be demonstrated equally well as in *Biggar and Nielsen* (1976) with 359 samples (correlation coefficient of 0.79).
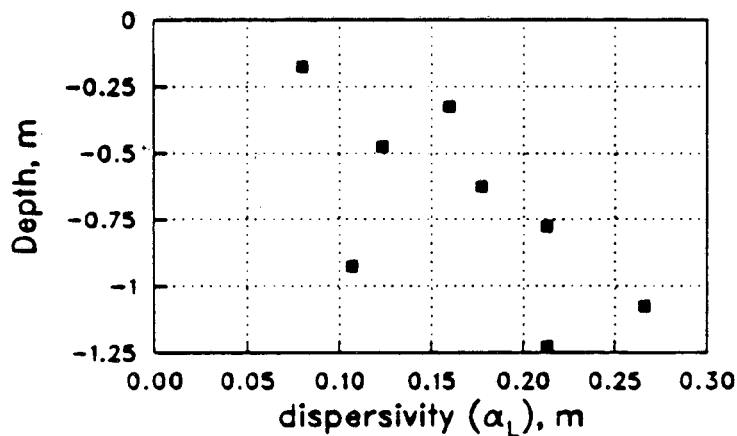

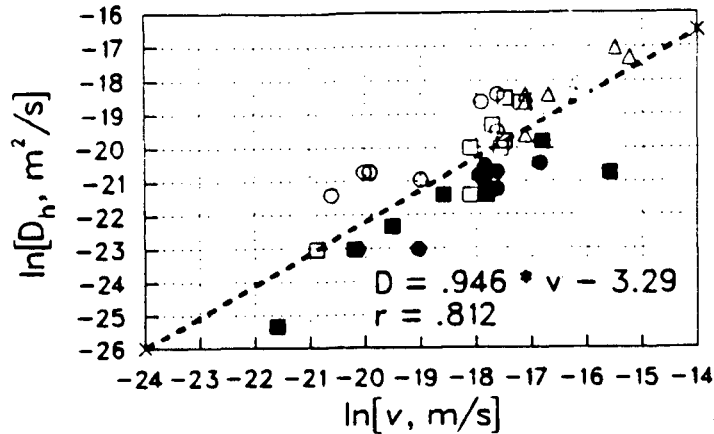Figure 8. Travel distance vs longitudinal dispersivity for site UZ-8

Figure 9. A functional relationship is demonstrated between apparent dispersion coefficient, D_h, and average pore water velocity, v. Differing symbol types represent individual plots.

CONCLUSION

The usefulness of a numerical model for solving the advection-dispersion equation has been demonstrated in the point estimation of soil hydraulic properties under transient flow conditions. Reasonable estimates of the soil properties were obtained without the use of an artificially introduced tracer or the manipulation of boundary and initial conditions. A high degree of spatial variability of water and solute transport parameters in a field soil has been exhibited, and the frequency distribution has been shown to be log-normal. Recognition of the appropriate sample distribution can be important in mean parameter estimation, and a need has been demonstrated for a consideration of the chance of extreme transport behavior. Dispersivities were calculated and presented in the spirit of supplementing the sparse existing database. α_l was shown to increase in a general sense with depth, but not to correlate with any other subsurface parameter. D_h and v were shown to be related in an approximately linear fashion, even though v was quite small.

ACKNOWLEDGEMENT

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