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12 ABSTRACT (PURPOSE, METHOD, RESULTS, CONCLUSIONS)

Spatial variability of saturated hydraulic conductivity is examined to assess the effect of uncertainty in leaching of pesticides from heterogeneous soils. Saturated hydraulic conductivity, an important soil parameter that controls the transport of pesticides in soils, is assumed to be composed of a homogeneous mean value and a perturbation caused by the spatial variability of soil properties producing a stochastic process in the mean flow direction. The spatial heterogeneity of porous soils is characterized by the variance and the correlation scale of the saturated hydraulic conductivity in the transport domain. In the first part of the study, numerical experiments are used to investigate the development of scale-dependent macrodispersivity in the unsaturated heterogeneous soils. In the second part of the study, the significance of the variance on the spatial and temporal distribution of tracer spreading is demonstrated for Hawaii Oxic soils. The significance of variance regarding the spatial and temporal distribution of tracer concentrations is demonstrated using solute breakthrough curves at various depths in the soil profile. Macrodispersivity values in heterogeneous soils are proportional to the variance at smaller travel distances and converge to the same value at larger travel distances. For greater correlational distances, a faster breakthrough of solutes at various depths was observed.

AUTHORS:

Dr. Clark C.K. Liu
Professor
Department of Civil Engineering
University of Hawaii at Manoa
2540 Dole Street
Honolulu, Hawaii 96822
Tel.: 808/956-7658

Dr. Keith Loague
Assistant Professor of Soil and
Wildland Hydrology
Department of Soil Science
108 Hilgard Hall
University of California
Berkeley, California 94720
Tel.: 415/643-5327

Dr. Ali Azimi-Zonooz
Imperial Irrigation District
Water Resources Unit
Imperial, California 92251
Tel.: 619/339-9110

Mr. Jing-Song Feng
Graduate Student
Department of Civil Engineering
University of Hawaii at Manoa
2540 Dole Street
Honolulu, Hawaii 96822

SIMULATION OF SOLUTE TRANSPORT IN HETEROGENEOUS SOILS
VOLUME II: Numerical Experiments

Clark C.K. Liu
Keith Loague
Ali Azimi-Zonooz
Jing-Song Feng

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WATER RESOURCES RESEARCH CENTER
University of Hawaii at Manoa
Honolulu, Hawaii 96822

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INTRODUCTION

Groundwater contamination from surface application of chemicals and land disposal of hazardous wastes is one of the most serious hazards to the Earth's hydrologic environment. Lack of information on contaminant transport in the unsaturated portion of the Earth's crust, the zone that separates freshwater aquifers from surface pollutants, has precluded the development of an accurate and efficient method of predicting the extent and timing of groundwater pollution from various forms and amounts of waste inputs. Understanding the natural heterogeneity of the spatial properties of porous formations and the uncertainties in the physical, chemical, and biological transformations that various pollutants encounter in their path through unsaturated porous media requires more research. This is illustrated in Figure 1, which shows the effect of heterogeneity of the porous media properties on the vertical transport of ethylene dibromide (EDB) in Hawai'i's soils. The concentration values are for soil samples collected three weeks after uniform application at four separate locations in the same field block down to a depth of 2.4 m. The unequal vertical transport of tracer due to the random nature of the porous media properties raises the question of how to effectively simulate the field transport processes in heterogeneous soils. The main aim of this study is to evaluate the effect of such heterogeneity on the dispersion of contaminants in unsaturated soils by the use of stochastic mathematical models.

The complexity of the mathematical models that incorporate the natural processes in the transport of residual chemicals depends on the importance of each process in that unique hydrogeologic environment, represented as parameters in the mathematical structure of the models. Mathematical models that incorporate the transport mechanisms within the soil volume in the form of differential equations are classified as physically based approaches. Their uses are often limited because of the difficulties in solving the interrelated problems of parameter estimation, specification of system boundary conditions, and mathematical solution. An alternative approach for the prediction of residual chemicals in unsaturated soils is based on the systems theory, which usually does not require an intimate knowledge of the detailed transport mechanisms within the soil system. By following a systems approach, the dynamic relations between pollutants at the soil surface and their subsequent downward movement are represented by system response functions. The main advantage of the system modeling approach for prediction of contaminant transport through soils is its superior computational efficiency and limited data requirements. However, a thorough evaluation of the approach must be performed and compared to a physically based approach before direct application to field problems is possible. Mathematical solute transport models can further be classified as deterministic models, which assumes the system operates in such a way that a set of uniquely

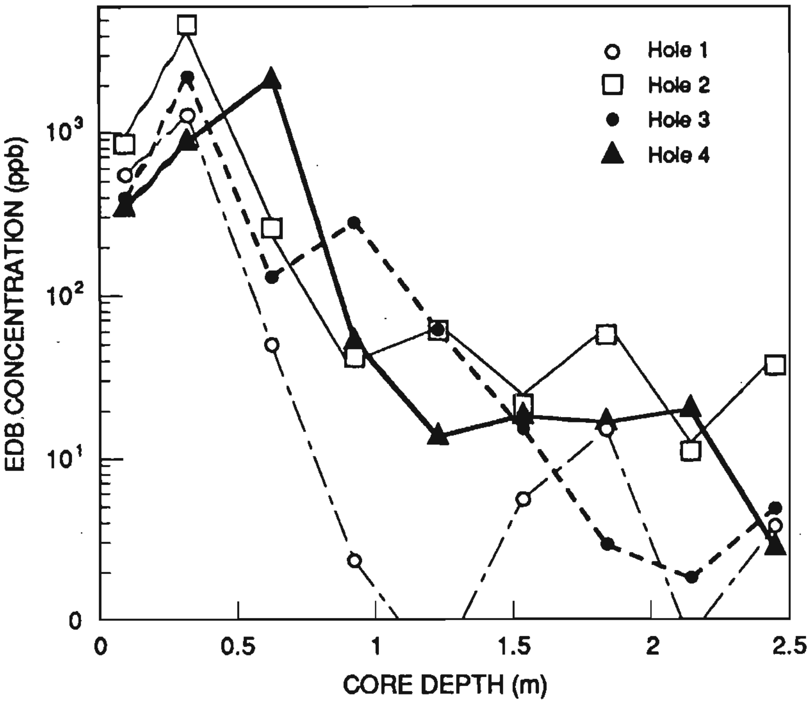


Figure 1. Ethylene dibromide (EDB) residual concentration in soil samples collected on 9 August 1983 at Del Monte Field No. 2

definable outcomes is associated with a given input event, or as stochastic models, which assume that the system input, output, or the system itself is uncertain and defined by the laws of probabilities.

Stochastic Physically Based Modeling Approach

The most widely used approach for simulating solute transport in field soils is based on deterministic, physically based models, which assume that the soil-solute system is homogeneous and operates in such a way that a set of uniquely definable output concentrations can result from given input concentration levels. The main problem with this approach is that the spatial variability of soil properties not considered in the structure of the model may introduce significant errors into the quantitative characterizations of mass transport phenomena. Stochastic physically based models, however, assume that the soil properties vary spatially, and this inherent variability is the cause of uncertainty in predicting contaminant transport in porous media. Under this assumption, the investigator may proceed to evaluate the distribution of output concentration values for a given set of randomly distributed input spatial parameters.

Examples of such studies include the study by Biggar and Nielsen (1976), who used a Monte Carlo technique to generate random pore water velocity and a diffusion coefficient to evaluate the solute travel times for spatially variable soils. This study found that the predicted solute concentrations are significantly different for heterogeneous soils, and the consideration of variability in convective velocities, rather than the diffusion coefficient, is significant in the prediction of spatially variable solute fluxes. Studies by Dagan and Bresler (1979), Bresler and Dagan (1979, 1981), Warrick and Amoozegar-Fard (1979), Luxmoore and Sharma (1980), and Amoozegar-Fard, Nielsen, and Warrick (1982) have reached similar conclusions. These studies, rather than making an attempt to represent the soil spatial variability in detail, have proposed approximate procedures for describing flow and solute transport under high transverse and longitudinal soil variability based on the scaling theory. Simulations are performed by obtaining a set of scaling factors for infiltration throughout a field, which may use scaled forms of the advection-dispersion equation (Warrick and Amoozegar-Fard 1979) or combine water infiltration and soil transport variability together with a probability model (Dagan and Bresler 1979). These studies have led to the general belief that mass transport phenomena in heterogeneous soils can only be described with mathematical techniques of random processes.

Research in subsurface mass transport and dispersion in heterogeneous porous media has shown that under field conditions, the dispersion coefficient parameter, which describes the degree of mixing and spread of contaminants, is a scale-dependent process (Konikow and Bredehoeft 1974; Fried 1975). A lack of correct understanding of this scale dependence may limit the accurate predictive capability of models based on the classic advection-dispersion equation. Scale dependence of macrodispersivity has generally been attributed to the local variations in the distribution of hydraulic conductivity. Gelhar, Gutjahr, and Naff (1979) analyzed the longitudinal dispersion produced as a result of the spatial variability of hydraulic conductivity in stratified aquifers. The stochastic differential equations describing the mass transport process were solved using spectral techniques. The result of the analysis showed that longitudinal dispersivity produced by the heterogeneity of the porous media grows with travel distance, reaches an asymptotic constant value, and is dependent on the statistical properties of the medium. Other studies (Gelhar and Axness 1983; Dagan 1988) have also demonstrated that the scale-dependent dispersivity produced as a result of the heterogeneity of the porous medium increases with travel distance and reaches an asymptotic constant value. Dagan (1988) estimated that the travel distance required for a contaminant plume to reach an asymptotic value is tens of times greater than the correlation length of the saturated hydraulic conductivity in the mean flow direction.

The stochastic approaches for explaining contaminant transport in heterogeneous porous media generally rely on the assumption that the spatial distribution of concentration values as random processes possesses a finite correlation scale and is statistically homogeneous and ergodic. An alternative approach proposed by Wheatcraft and Tyler (1988) makes use of the principle of self-similarity and fractal geometry to explain scale dependence of dispersivity in a heterogeneous medium. This type of approach assumes that the dispersion phenomena exhibit a pattern that is independent of the scale of observation and thus has a very large correlation distance. This study, by comparing field dispersivity with fractal models, demonstrated that the dispersion process may be explained in porous media represented by a set of fractal stream tubes.

Stochastic System Modeling Approach

The interpretation of contaminant transport in heterogeneous soils can be alternatively viewed in the context of systems analysis. The theory of systems analysis is based on the assumption that the output from a given soil-solute system represents a unique response to a given input. The relations between contaminant concentration levels at the soil surface and their subsequent downward movement at various depths is described by the convolution integral, which relates input/output to the system response in the time domain. A system model can be stochastic (Distefano 1974) if its response function takes the form of a probability density function describing the system's spatial variability. The major advantage of a system model is that in cases when the dynamical structure of the system is unknown or not at all understood, the impulse response function can be constructed from the observed time series.

One approach to solute transport modeling in soils (Jury 1982) makes use of the convolution equation, with a log-normal probability density function of the velocity as the model's impulse response function, to predict the output solute concentration levels at various depths in the soil profile. In this study, comparisons between field-measured and predicted bromide concentration distributions showed agreement. In subsequent studies (Jury, Sposito, and White 1986; White et al. 1986; and Sposito et al. 1986), the Jury transfer function model was generalized to predict the movement of a solute that may undergo physical, chemical, and biological transformations as it moves down a soil column in which the water travel may vary in both space and time. The model's impulse response function in this case is referred to as the solute-lifetime density function, which is consistent with the law of mass balance in the soil profile. Liu (1988) investigated the conjunctive use of the physically based and linear system solute transport modeling approaches for predicting chloride concentration in the upper soil zone. He showed that the dispersion coefficient in a physically based advection-dispersion model is not constant and grows linearly as a function of travel distance.

OBJECTIVES

As part of the overall objective of this study, a physically based stochastic approach is used to investigate the effect of soil heterogeneity on solute dispersion in unsaturated soils. The analyses are performed by using synthetically generated random fields representing the variation of saturated hydraulic conductivity in a three-dimensional column of soil with its prespecified first- and second-order statistics. The specific objectives of the research are to:

1. Investigate the scale dependence of macrodispersivity in heterogeneous soils by simulating fluid flow and solute transport using a three-dimensional finite element model
2. Use the model to evaluate the effect of spatial heterogeneity of porous soils characterized by the variance and correlation scale of the random saturated hydraulic conductivity on solute dispersion and scale-dependent macrodispersivity in Hawaii Oxic soils
3. Propose and discuss the possible ways of incorporating the spatial variability of fluid flow and solute transport parameters in the impulse response function of a stochastic system model to increase the computational efficiency of chemical residual transport simulation in heterogeneous soils.

ANALYSIS OF MACRODISPERSION IN HETEROGENEOUS SOILS

Methodology

As a result of the natural soil-water processes, the hydrodynamics of contaminant migration through soils vary drastically through space. To account for this uncertainty in characterizing the soil heterogeneity, a physically based stochastic approach to soil-water flow and contaminant transport modeling is utilized in this research. The heterogeneity of saturated hydraulic conductivity, as the controlling parameter in the vertical transport of contaminants, is represented as a three-dimensional random field defined by a probability density function with log-normal distribution.

The analysis involves first solving the three-dimensional form of the partial differential equation for flow of water in unsaturated soils (Davis and Segol 1985):

$$\frac{\partial}{\partial x_i}\left[K^r(h)\,K^s_{ij}\,\frac{\partial h}{\partial x_j} + K^r(h)\,K^s_{ij}\right] = [C(h) + \beta S_s]\frac{\partial h}{\partial t} - Q\,, \qquad (1)$$

where i,j = 1,2,3

x_i, x_j = spatial coordinates

K^r = relative hydraulic conductivity
h = pressure head
K^s_{ij} = saturated hydraulic conductivity tensor
C = specific moisture capacity ($\partial\theta/\partial h$)
β = θ/ϕ
θ = volumetric water content
ϕ = porosity
S_s = specific storage
t = time
Q = source/sink term.

The assumptions for the fluid-flow component of the model are summarized in Table 1.

The partial differential equation governing dispersion of a conservative tracer in a three-dimensional flow field through soils is given as follows (Davis and Segol 1985):

$$\frac{\partial}{\partial x_i}\left[\theta \; D_{ij} \frac{\partial c}{\partial x_j}\right] - \frac{\partial(q_i c)}{\partial x_i} = \frac{\partial(\theta \; c)}{\partial t} + Qc_o \, , \tag{2}$$

where D_{ij} = hydrodynamic dispersion tensor
c = solute concentration

TABLE 1. ASSUMPTIONS USED IN FLUID-FLOW SIMULATIONS

No.	Assumptions	Rationale
1	Darcy approach to flow through a porous medium is valid.	Flow rate can be expressed by Darcy's law.
2	Hydraulic pressure head, water content are continuous.	Partial differential equation for flow can be established.
3	Principal direction of anisotropy coincides with the x, y, z coordinate axes. $K^s_{ij} = \begin{bmatrix} K_{xx} & 0 & 0 \\ 0 & K_{yy} & 0 \\ 0 & 0 & K_{zz} \end{bmatrix}$	The nine-component, second-order saturated hydraulic conductivity tensor is reduced to three components.
4	Fluid density is constant, based on a single fluid and isothermal flow.	Normally assumed for near-surface underground solute transport.
5	Saturated hydraulic conductivity is randomly distributed (a log-normal distribution is used), and its auto-correlation function is an exponential function.	The heterogeneous saturated hydraulic conductivity field can be simulated by a random generator.
6	Relationship between suction pressure, water content, and relative hydraulic conductivity is nonhysteretic.	Assumed for convenience.

TABLE 2. ASSUMPTIONS USED IN SOLUTE TRANSPORT SIMULATIONS

No.	Assumptions	Rationale
1	Local dispersion in porous material is Fickian and deterministic.	Assumed for convenience.
2	Dispersion in partially saturated media follows the theory developed for saturated flow.	Assumed for convenience.

q_i = mass average velocity
c_o = solute concentration in source/sink fluid.

The assumptions for the solute transport component of the model are summarized in Table 2. The unsaturated flow and solute transport computer model developed by Davis and Segol (1985) was used to investigate the tracer spreading resulting from the spatial variability of a saturated hydraulic conductivity field in a heterogeneous, three-dimensional column of soil. A three-dimensional model was used since simulation of solute spreading in all three dimensions is important in analyzing the macrodispersion process. The analyses are performed under the assumption that the scale of variations of the saturated hydraulic conductivity field is larger than the size of the representative elementary volume, which is taken as the unit mesh size in the finite element grid network.

The fluid flow and solute transport components of the computer model are coupled by the mass average fluid velocity, qi, which is determined using the following relationship:

$$q_i = -\left[K^r K^s_{ij} \frac{\partial h}{\partial x_j} + K^r K^s_{ij} \right] . \tag{3}$$

The dispersion coefficient, assuming that the effect of molecular diffusion is negligible, is given by:

$$D_{ij} = \alpha_l |V| + (\alpha_l - \alpha_t) \frac{V_i V_j}{|V|} , \tag{4}$$

where α_l = longitudinal local dispersivity
α_t = transverse local dispersivity
$|V|$ = magnitude of the pore water velocity vector
V_i = pore water velocity in the direction x_i (q_i/θ)
V_j = pore water velocity in the direction x_j (q_j/θ).

The parameters α_l and α_t control the solute spreading at a local scale. The phenomenon of the increased solute spreading in the mean flow direction as a result of heterogeneity of porous media is referred to as macrodispersion and is estimated under the assumption that the local dispersivity is finite by setting $\alpha_l = 0.01$ m and $\alpha_t = 0.001$ m in equation [4]. The magnitude of the macrodispersivity as a function of distance in the hypothetical soil profile was determined using a curve-fitting procedure associated with the tracer methods (Bear 1972), as follows:

$$\alpha_L = X/8\,[\,(t_{0.84} - t_{0.16})/t_{0.5})\,]^2, \tag{5}$$

where α_L = macrodispersivity
$t_{0.84}$ = time when 84% of solute passed depth X
$t_{0.16}$ = time when 16% of solute passed depth X
$t_{0.5}$ = time when 50% of solute passed depth X.

Under natural conditions, the transport properties of soils vary from profile to profile, thus producing a complex dispersive mixing that can be analyzed only by means of the theory of spatial stochastic processes. In this study, we are assuming that the randomness of the spatial transport properties in the soils is reduced to that of the saturated hydraulic conductivity field, which requires its joint probability density function to be known. The saturated hydraulic conductivity field for a single column of soil represents only a single realization of the random process, from which the joint distribution of the random field cannot be inferred. One needs to invoke the statistical homogeneity and the ergodicity assumptions to infer the statistical moments of the random saturated hydraulic conductivity field from a single realization. The assumption of statistical homogeneity assumes that the first- and second-order statistics are invariant under translation and rotation. The ergodic hypothesis assumes that the behavior of a single realization of the saturated hydraulic conductivity field is represented by the ensemble average over a large number of realizations with the same statistical moments. Since the distribution of the random saturated hydraulic conductivity field is assumed log-normal, the natural log of the observations is normally distributed. Under the normality assumption, the joint probability density function can be completely characterized by the first two moments. It is also assumed that the log-conductivity field is described by an exponential covariance function. Under these assumptions, the mean and the covariance function for the log-conductivity field are as follows:

$$E\,[K_n] = E\,[\ln K_l] = \mu_n \tag{6a}$$

$$\mathrm{Cov}\,(K_{ni}\,, K_{nj}) = \sigma_n^2\, e^{-x_{ij}/\lambda_n} \tag{6b}$$

where E[ ] = expectation
K_n = second-order homogeneous and isotropic random process representing the log-conductivity

K_l = random process representing the saturated hydraulic conductivity assigned to K_{11}^2, K_{22}^2, and K_{33}^2 in equation [1]

μ_n = log-conductivity mean

Cov[ ] = covariance

σ_n^2 = log-conductivity variance

x_{ij} = distance between K_{ni} and K_{nj}

λ_n = log-conductivity field correlation length.

The random conductivity field is therefore statistically characterized by μ_n, σ_n^2, and λ_n. Specification of these parameters allows one to use a physically based stochastic model for the transport of contaminants in heterogeneous soils.

To maintain the statistics of the original random process representing the saturated hydraulic conductivity field without introducing bias into their estimates, the statistical parameters of the distribution of K_n are first computed using the relationships given by Vanmarcke (1983), as follows:

$$\mu_n = \ln(\mu_l) - \sigma_n^2 / 2 \tag{7a}$$

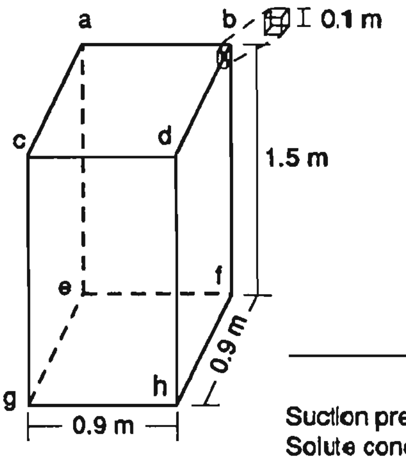
$$\sigma_n^2 = \ln\left(\frac{\sigma_l^2}{\mu_l^2} + 1\right) \tag{7b}$$

$$\rho_n = \frac{\ln\left[1 + \rho_l\left(e^{\sigma_n^2} - 1\right)\right]}{\sigma_n^2}, \tag{7c}$$

where ρ_n and ρ_l are the lag-one correlation coefficients of the normal and log-normally distributed random processes, respectively.

Obtaining the sample mean, variance, and correlation coefficient of the corresponding normally distributed random process allows one to generate correlated synthetic realizations of the three-dimensional log-conductivity field using the turning bands random field generator. After the inverse transformation $K_l = \exp(K_n)$, the saturated hydraulic conductivity field is entered into the physically based three-dimensional flow and solute transport model with prespecified initial and boundary conditions. The algorithm for a three-dimensional turning band method of generating random fields, developed by Tompson, Ababou, and Gelhar (1987), was used.

The dispersion of a conservative tracer originating from the soil surface was simulated in a three-dimensional spatial domain, which represents a hypothetical column of soil. The boundary and initial conditions and the size of the soil column, as well as the spatial increments of the cubical finite element grid network, are shown in Figure 2. The region of interest for the



BOUNDARY	FLOW MODEL	SOLUTE TRANSPORT MODEL
abcd	Constant flux*	Constant concentration†
abef	No flow	No flow
dbhf	No flow	No flow
cdgh	No flow	No flow
cage	No flow	No flow
efgh	Water table	Outflow flux

INITIAL CONDITIONS

Suction pressure: no-flow initial condition, $P(x,y,z,0) = -1 - z$.

Solute concentrations: constant input at top surface, $C(x,y,0,0) = C_0$, $C(x,y,z,0) = 0$.

*$Q = 1.0 \times 10^{-4}$ cm/s

†$C_0 = 1.0$

Figure 2. System boundary and initial conditions of hypothetical soil column

numerical experiments is 0.81 m^3, which has the dimensions 0.9 × 0.9 × 1.0 m (Tab. 3) and which represents a column of soil. The spatial increments of the elemental units are 0.1 × 0.1 × 0.05 m for the upper ten layers, and 0.1 × 0.1 × 0.1 m for the lower five layers. This grid-size scheme of the finite element mesh was selected based on the scale of the transport domain and on the storage limitation of the computer we used. Input data for the turning band random field generator are shown in Table 4. Saturated hydraulic conductivity is the only parameter that we considered varying spatially in the hypothetical soil column. The statistical characteristics of the ten realizations of the saturated hydraulic conductivity are given in Table 5. The input parameters for the fluid flow and solute transport components of the model simulations performed in this part of the study are given in Table 6.

As a continuation of the study of scale-dependent macrodispersivity in heterogeneous soils, a larger column of soil was analyzed. The extended soil column's dimensions were 1.2 × 1.2 × 2.0 m; and the dimensions of the finite elements were 0.1 × 0.1 × 0.05 m for the upper ten layers, and 0.1 × 0.1 × 0.1 m for the bottom fifteen layers. Four separate cases for the estimated spatial means and variances of the saturated hydraulic conductivity of Hawaii Oxic soils (Green et al. 1982) from two locations were analyzed. The data from saturated hydraulic conductivity measurements presented by Green et al. (1982) were found to have a similar mean but different variances. The mean and variance values for the soil from the first location were, respectively, $5.183\,6 \times 10^{-2}$ m/hr and $47.791\,0 \times 10^{-4}$ m^2/hr^2; and those for the soil from the second location were, respectively, $5.051\,1 \times 10^{-2}$ m/hr and $10.719\,7 \times 10^{-4}$ m^2/hr^2.

TABLE 3. BASE CASE MESH

LAYER	DIMENSIONS (m)			GRID SPACING (m)			NO. OF NODES	NO. OF ELEMENTS
	x	y	z	x	y	z		
1	0.90	0.90	0.50	0.10	0.10	0.05	1 100	810
2	0.90	0.90	0.90	0.10	0.10	0.10	600	405

NOTE: Half-band width for fluid flow = 111; half-band width for solute transport = 221.

TABLE 4. STATISTICAL CHARACTERISTICS OF INPUT DATA FOR TURNING BANDS RANDOM GENERATOR

	DIRECTION		
	x	y	z
Number of points	9	9	20
Nodal spacing (m)	0.10	0.10	0.05
Correlation length (m)	0.10	0.10	0.10
KG = exp (mean of ln Ks) (m/s)			$0.501\,2 \times 10^{-5}$
σ_f = standard deviation of ln K_s			0.5
Number of lines			100
Nodal spacing along each line (m)			0.062 8
Maximum normalized spectral frequency			100
Normalized spectral frequency increment			0.5
Number of Monte Carlo runs			10
Starting seed for random numbers			32 621
Maximum computed lag			8
Lower histogram limit			-3.0
Upper histogram limit			3.0
Number of histogram increments			20

For the first two cases that were analyzed, the saturated hydraulic conductivity field had the mean and variance values of the first location, with correlation length values of 0.1 m and 0.5 m, respectively. For the last two cases, the saturated hydraulic conductivity field had the mean and variance values of the second location, with the same correlation length values, 0.1 m and 0.5 m, respectively. The main purpose of this part of the analysis was to examine the effect of the two combinations of the variance and correlation length values on solute dispersion specifically for the soil-water parameters theorized for Hawaii Oxic soils.

TABLE 5. STATISTICAL CHARACTERISTICS OF 10 REALIZATIONS GENERATED WITH TURNING BANDS RANDOM GENERATOR

Realization No.	$E[K_s]$	K_G ($\times 10^{-6}$ m/s)	σ_{K_s}	σ_f	λ_x (m)	λ_y (m)	λ_z (m)
1	5.024	4.445	2.645	0.495	0.093	0.121	0.101
2	6.819	6.089	3.439	0.476	0.085	0.096	0.103
3	5.669	5.018	2.981	0.494	0.100	0.086	0.115
4	5.158	5.310	2.769	0.468	0.107	0.093	0.092
5	5.871	5.310	2.769	0.448	0.100	0.113	0.085
6	5.355	4.826	2.576	0.456	0.114	0.100	0.117
7	5.739	5.072	3.038	0.497	0.114	0.097	0.148
8	5.572	5.024	2.672	0.455	0.104	0.097	0.107
9	5.958	5.323	2.995	0.475	0.097	0.095	0.105
10	5.211	4.629	2.693	0.487	0.085	0.118	0.105

Note: Realizations 9, 3, 7 were selected as base cases 1, 2, 3.

Note: λ_x = correlation length of log-conductivity in x direction.
λ_y = correlation length of log-conductivity in y direction.
λ_z = correlation length of log-conductivity in z direction.

TABLE 6. INPUT PARAMETERS FOR FLUID AND SOLUTE TRANSPORT SIMULATIONS

Parameters	Value	Reference	Confidence
Soil porosity	0.47	Jensen and Hanks 1967	H
Molecular dispersion coefficient	2.2×10^{-2} m^2/s	Davis and Segol 1985	M
Minimum allowable capillary pressure	-2.6 m	Jensen and Hanks 1967; Davis and Segol 1985	M
Maximum allowable infiltration and evaporation flux	2.083×10^{-5} m/s	Davis and Segol 1985	M
Longitudinal local dispersivity	0.01 m	Gelhar, Gutjahr, and Naff 1979	M
Transverse local dispersivity	0.001 m	Gelhar, Gutjahr, and Naff 1979	M

Note: Infiltration rate is 7.2×10^{-7} m/s.

Results of Numerical Experiments

Ten three-dimensional realizations of the saturated hydraulic conductivity were generated using the turning bands method. Three of the realizations in which the original statistics were best preserved were selected as the hypothetical realities representing the heterogeneous soil columns that were used in the numerical experiments. Examples of the saturated hydraulic conductivity variability in these three hypothetical soil columns are shown in Figures 3 through 5.

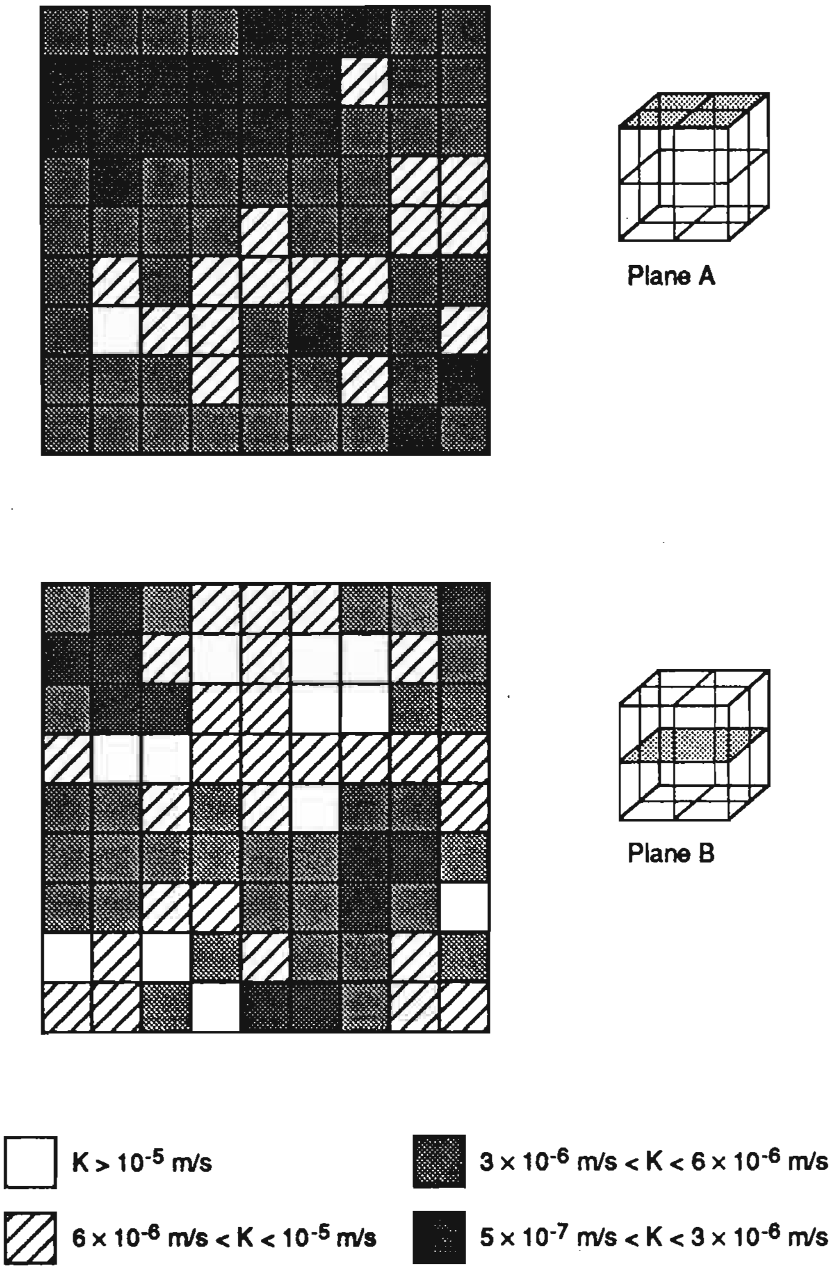


Figure 3. Hydraulic conductivity variations for horizontal and vertical cross sections, case 1 hypothetical soil column

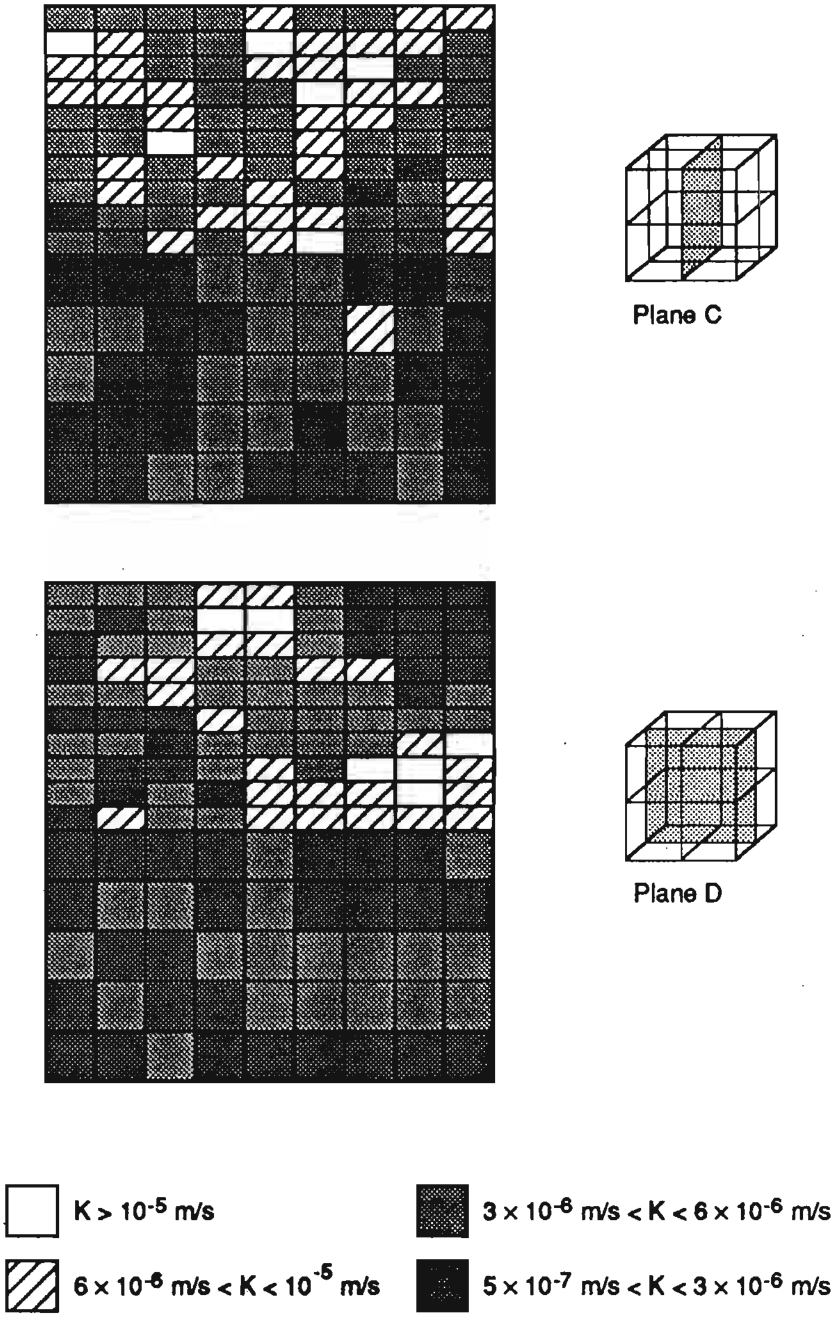


Figure 3.—*Continued*

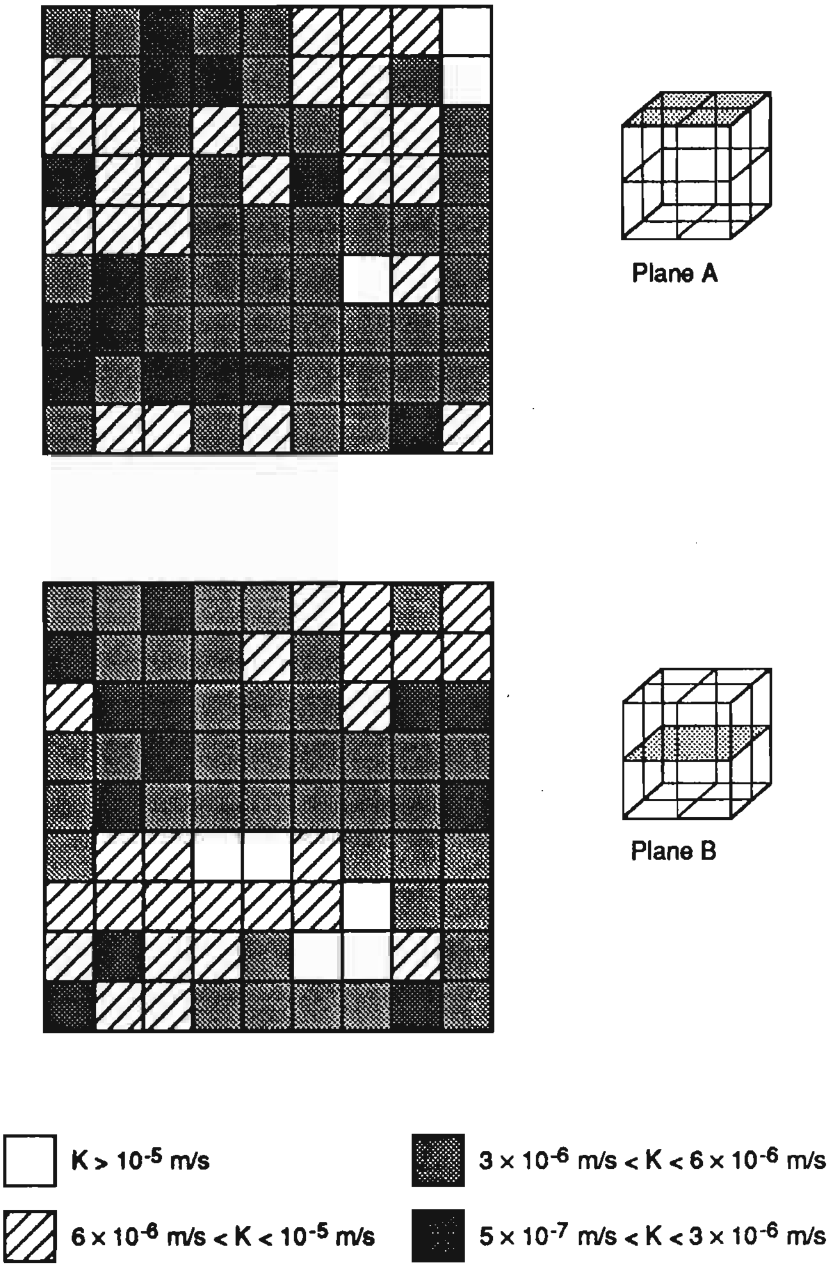
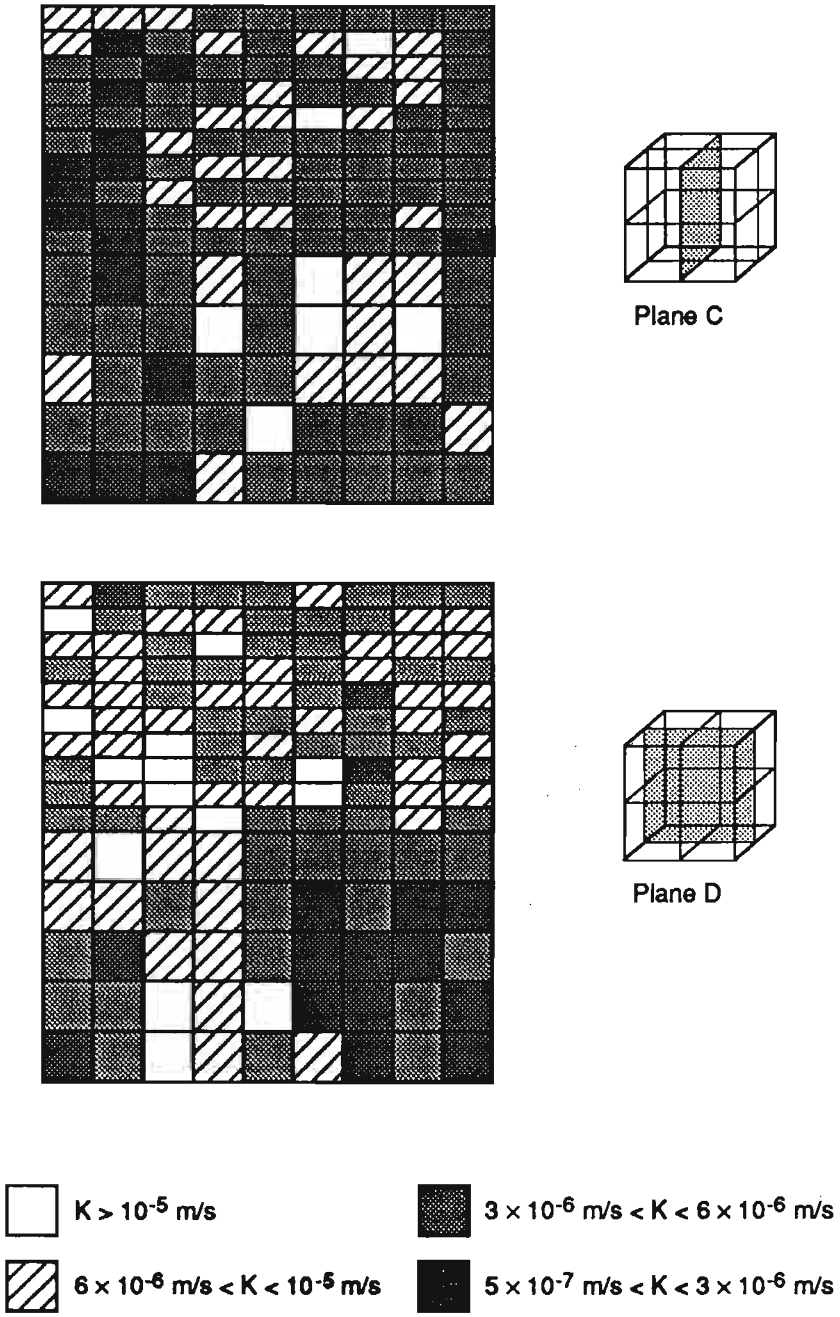


Figure 4. Hydraulic conductivity variations for horizontal and vertical cross sections, case 2 hypothetical soil column



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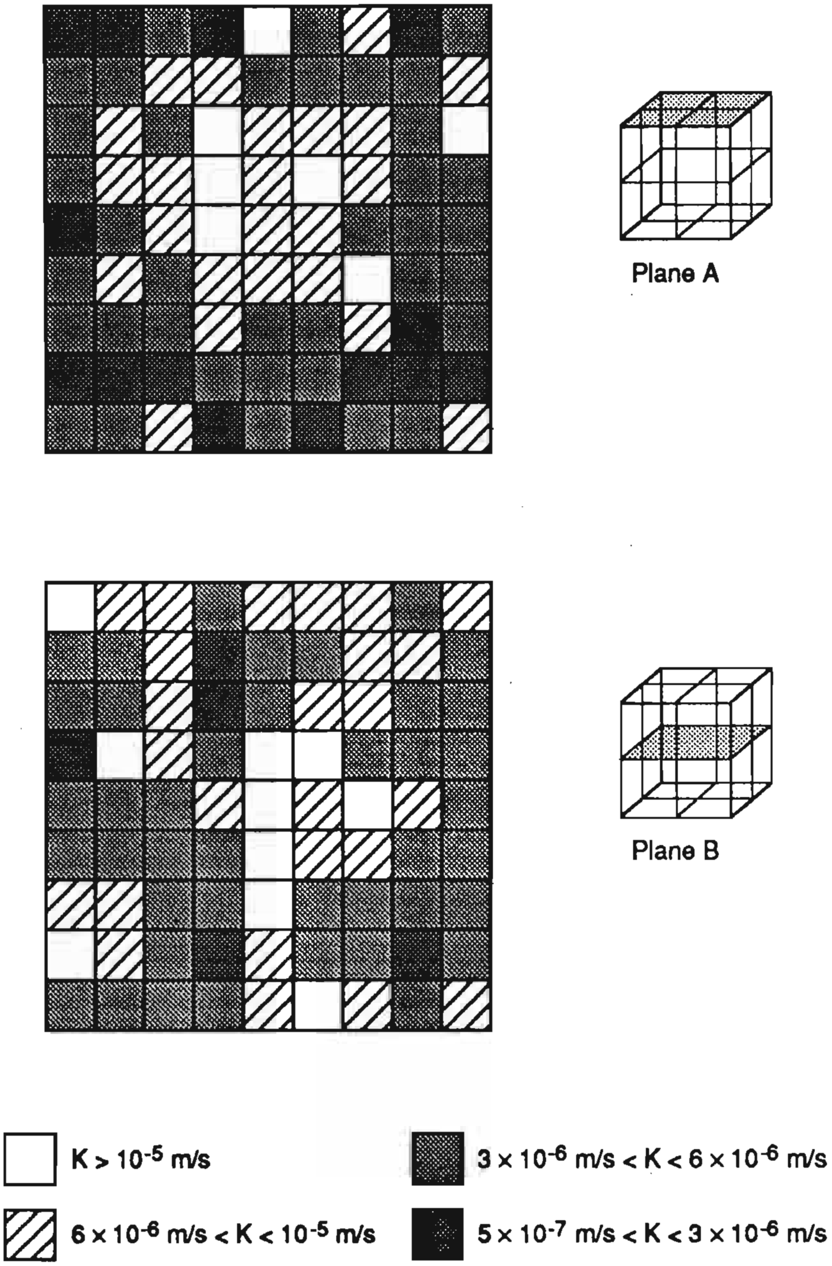


Figure 5. Hydraulic conductivity variations for horizontal and vertical cross sections, case 3 hypothetical soil column

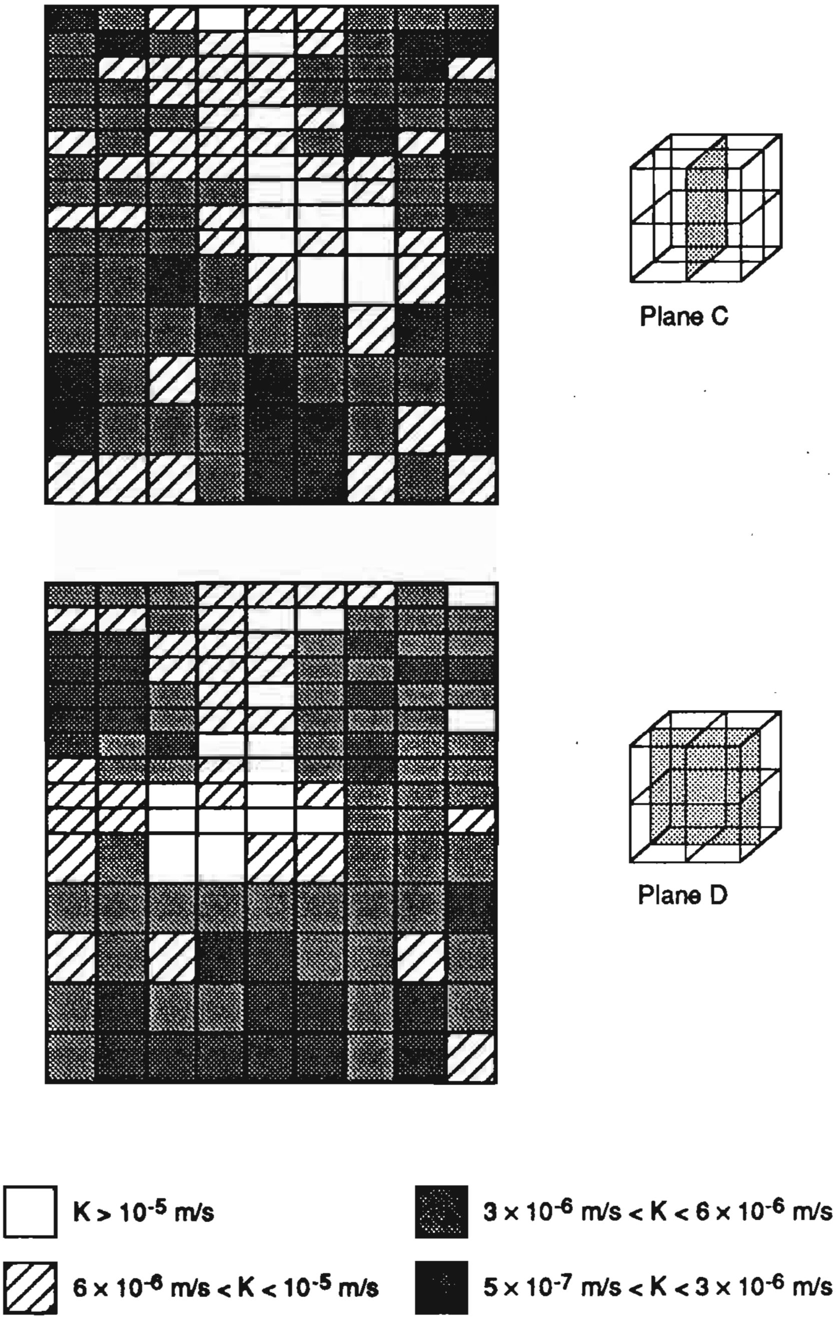


Figure 5.—*Continued*

Simulation results reveal that soil heterogeneity produced no noticeable effect on the simulated average pressure heads along the various soil columns at the end of the 8-day simulation period. Variances of lateral pressure head distribution at any horizontal plane in the heterogeneous soil, however, decrease gradually from a high value of 2.1 on the surface to a low of 0.1 at the bottom of the column (Fig. 6). Figure 7 shows that the variances of the pressure head distribution at any given depth increased with time and reached constant values at the end of the 8-day period. At that time, a large portion of the column was saturated and flow was in a steady state.

Heterogeneity produces significant lateral variations in downward flow velocities, which can be characterized by their probability distribution. The probability density function of ln V_Z (natural log of the velocity in the vertical direction) at several depths and at the end of the eight-day simulation period is plotted and shown in Figure 8. Theoretical log-normal plots of downward velocity with the same mean and variance are also shown in these figures. The closeness between the probability density function and the theoretical log-normal plots indicates that for a heterogeneous soil with log-normally distributed hydraulic conductivity, the downward velocity is also log-normally distributed. Figure 9 presents the changes in the areal-averaged ln V_Z and the variances with soil depth. These curves indicate that the mean and the variance of ln V_Z increase with travel distance and approach a constant value at travel distances of 0.2 m and 0.3 m, respectively.

Solute concentration distributions at several soil depths at the end of the 8-day period are shown in contour plots in Figure 10. These contour plots indicate that the solute plume moved downward rather irregularly in the heterogeneous soil column. If the areal average of these solute concentrations is plotted with respect to time, we obtain the solute breakthrough curves, shown in Figure 11. Although the solute distribution at any depth is quite irregular, the breakthrough curves turn out to be rather smooth. The breakthrough curves for a comparable homogeneous soil column with the same mean saturated hydraulic conductivity and mean local dispersivity were also calculated and are shown in Figure 11. Comparison of these two sets of breakthrough curves indicates that the longitudinal mixing of a solute is more effective in a heterogeneous soil than in a homogeneous soil and, furthermore, that this difference becomes more pronounced as the travel distance increases.

The phenomenon of increased longitudinal spreading of solute in a heterogeneous porous medium is referred to as macrodispersion (Gelhar, Gutjahr, and Naff 1979). Values of macrodispersivity are plotted as a function of dimensionless travel distance and are shown in Figure 12. This figure shows that macrodispersivity increases with travel distance. The effective dispersivity of our experimental soil column was estimated to be 0.01 m at the 0.2-m soil depth and 0.02 m at the 1-m depth. These values are more than ten times greater than the

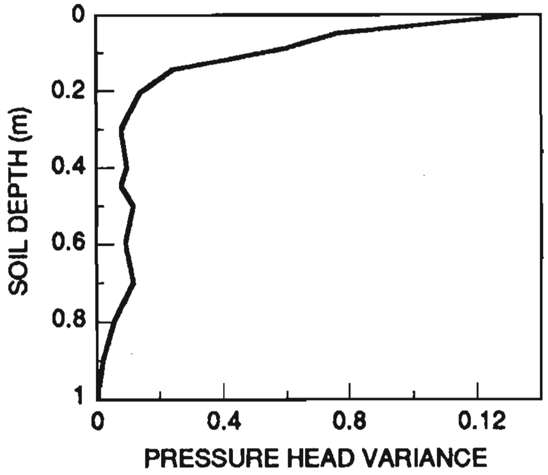


Figure 6. Variances of areal pressure head along soil profile in heterogeneous soil column

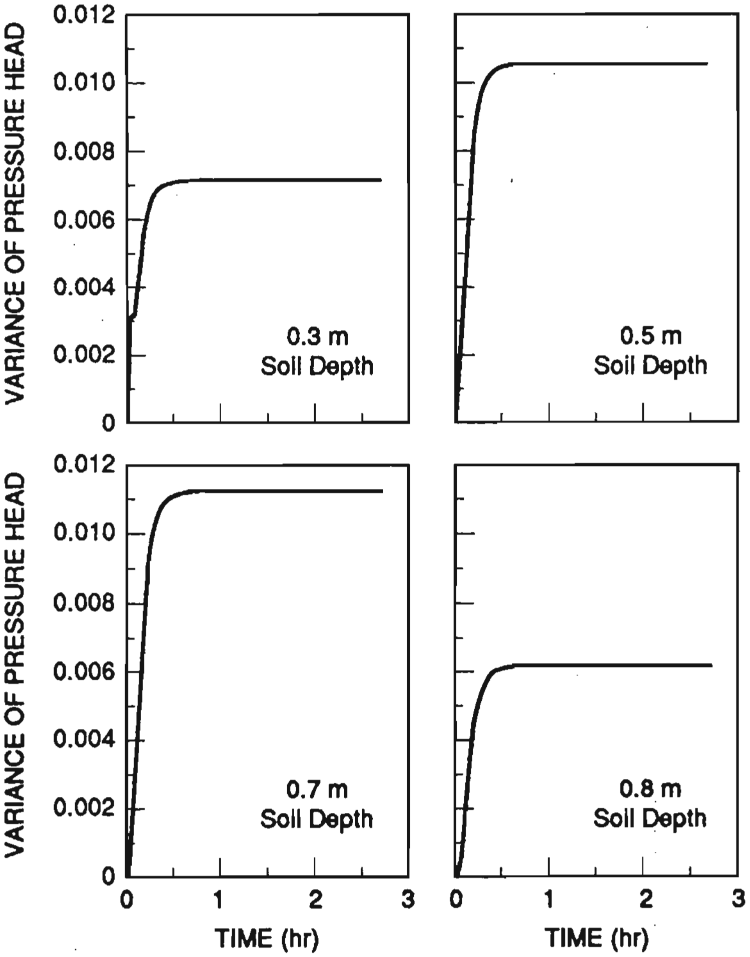


Figure 7. Changes of variances of pressure head at selected soil depths over time

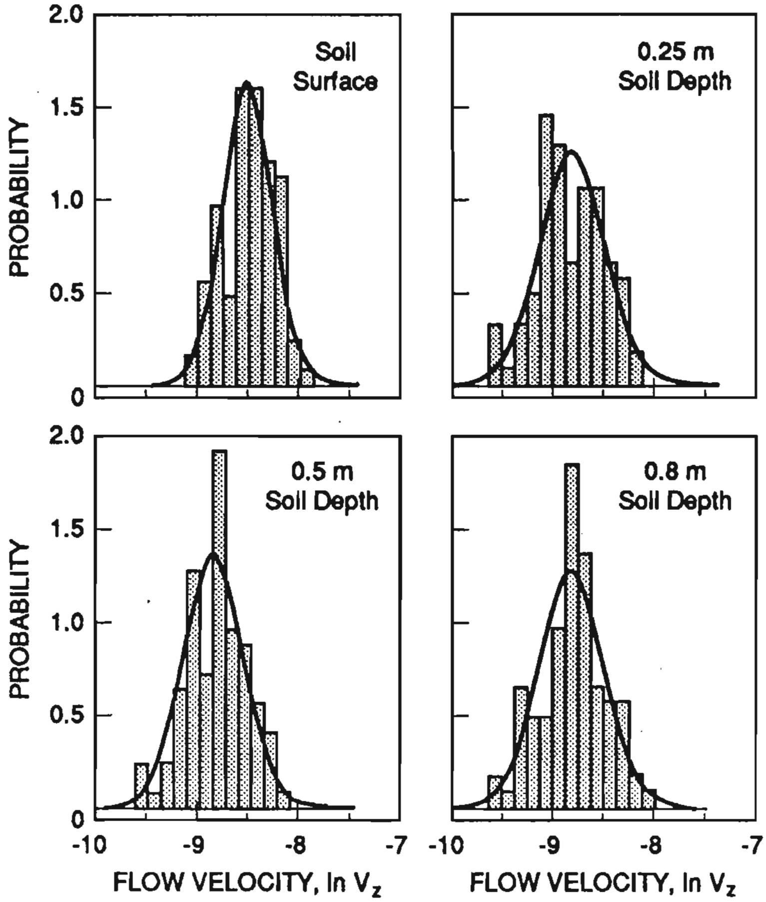


Figure 8. Probability density functions of logarithmic flow velocity (ln V_2) at selected soil depths, case 1 hypothetical soil column

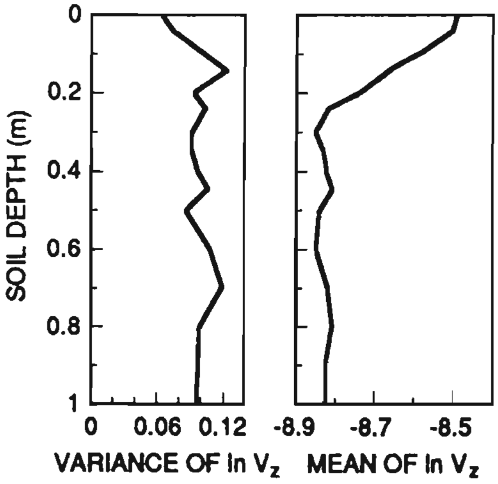


Figure 9. Changes in mean and variances of logarithmic downward flow velocity (ln V_2) at end of 8-day simulation period, case 1 hypothetical soil column

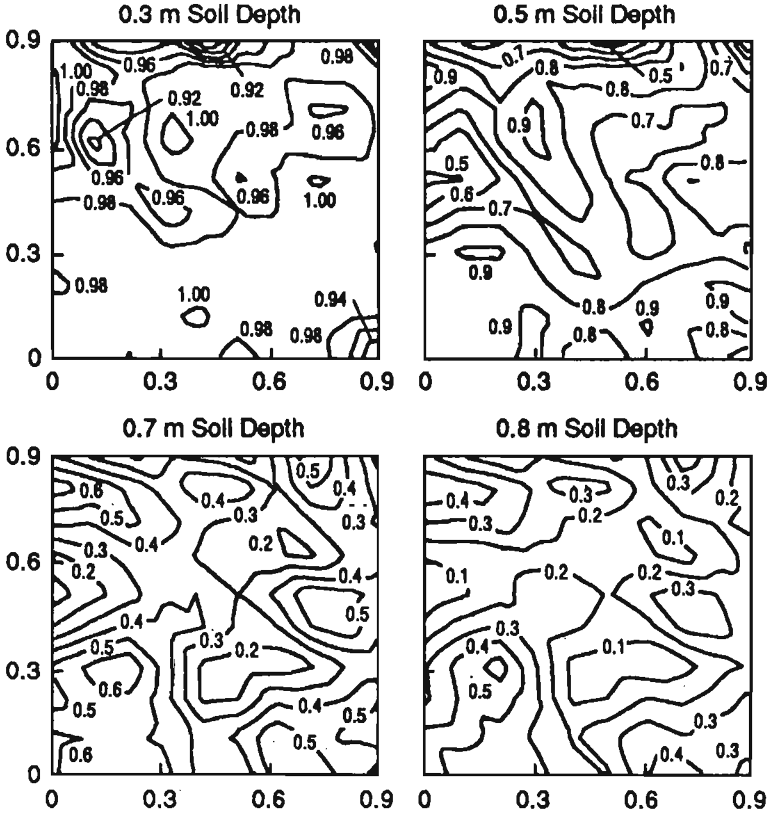


Figure 10. Solute concentration contours (C/C_0) at four soil depths at end of 8-day simulation period, case 1 hypothetical soil column

value of 0.001 m, which was from a tracer test for the laboratory sand (Chung et al. 1982). These values, however, are much smaller than field values reported in previous studies of regional groundwater flow and transport (Voss and Souza 1987). This feature of the numerical results can be mainly attributed to the small size of the soil column used in our numerical experiments. The dispersivity value was still increasing at a travel distance of 1 m, the point at which the front had already reached the bottom of the soil column (Fig. 12). Earlier studies (Gelhar and Axness 1983; Dagan 1988) indicated that the dispersivity produced by the heterogeneity of a porous medium increases with travel distance and reaches an asymptotic constant value. The travel distance required for a tracer plume to reach the asymptotic macrodispersivity was estimated to be tens of times greater than horizontal correlation length, which is 0.1 m in this part of the numerical experiments. Thus, it would take a tracer plume 1 to 10 m to have a constant macrodispersivity. Generally, in the study of solute transport through unsaturated soils, one would deal with the preasymptotic region.

Before the macrodispersivity becomes a constant, the solute dispersion in a heterogeneous soil is not a Fickian process. In our numerical experiments, the longitudinal and lateral

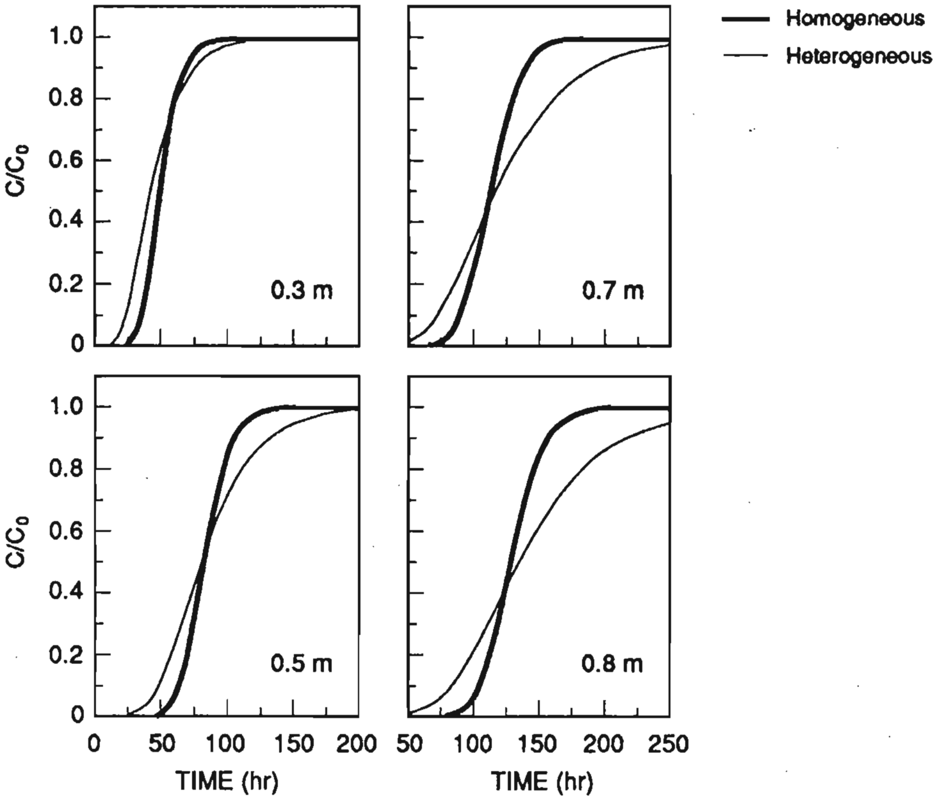


Figure 11. Simulated breakthrough curves for homogeneous and heterogeneous soil columns at selected soil depths, case 1 hypothetical soil column

correlation lengths were given the same value. Based on the study of time-dependent macrodispersion in saturated porous media by Dagan (1988), it appears that macrodispersivity changes with respect to dimensionless travel distance. Figure 12 also shows the curve of macrodispersivity plotted against travel distance, as calculated by Dagan's equation. These results indicate that our experimental results are consistent with those predicted by Dagan's equation.

Figure 13 shows the simulated concentration breakthrough curves for the lower variance in the saturated hydraulic conductivity case and the two correlation length values at various depths for the extended soil column case, and compares them with the homogeneous case. For the lower correlation length value, the tracer spreading consistently increases to the depth of 1.4 m. The tracer spreading for the homogeneous saturated hydraulic conductivity and the higher correlation length cases are very close to the depth of 1.4 m. Below 1.4 m, the tracer spreading for the homogeneous case becomes larger than the higher correlation length case. This behavior of the tracer spreading for the homogeneous saturated hydraulic conductivity can be mainly

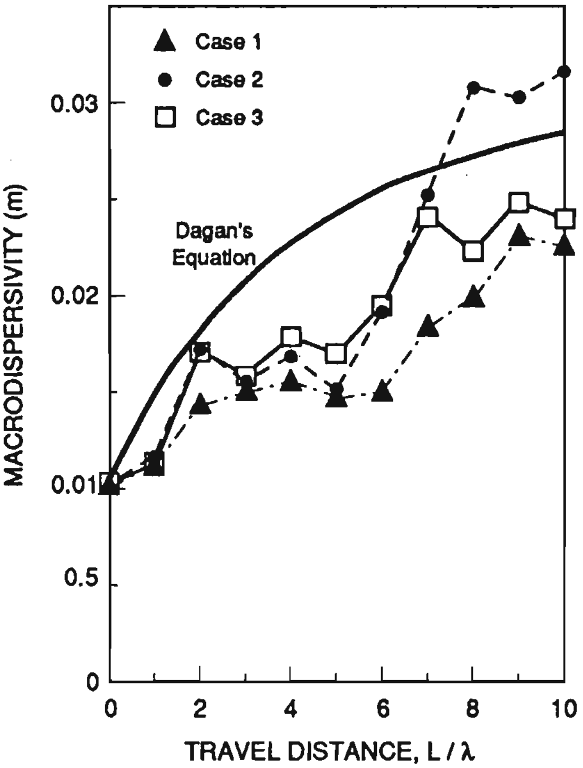


Figure 12. Development of macrodispersivity in heterogeneous soil determined by numerical experiments and Dagan's 1988 equation

attributed to the additional numerical dispersion in the solution of the advection-dispersion equation, which increases below the depth of 1.4 m.

Figure 14 illustrates the solute breakthrough curves for the higher variance case with two different values of correlation length and compares them with the homogeneous case. In this case, the solute spreading is consistently the largest to the depth of 1.9 m for the higher correlation length value, followed by the lower correlation length value and the homogeneous case. The differences in the solute spreading increase to the depth of 1.4 m and then begin to converge.

Figure 15 compares the solute breakthrough curves among the homogeneous case in saturated hydraulic conductivity with the low and the high values of saturated hydraulic conductivity variance when the correlation length is 0.1 m. In this case, the tracer spreading is largest for the higher saturated hydraulic conductivity variance to the depth of 0.6 m. Between this depth and the depth of 1.4 m, the tracer spreading of the two variance levels is very close, and significantly different from the homogeneous saturated hydraulic conductivity case.

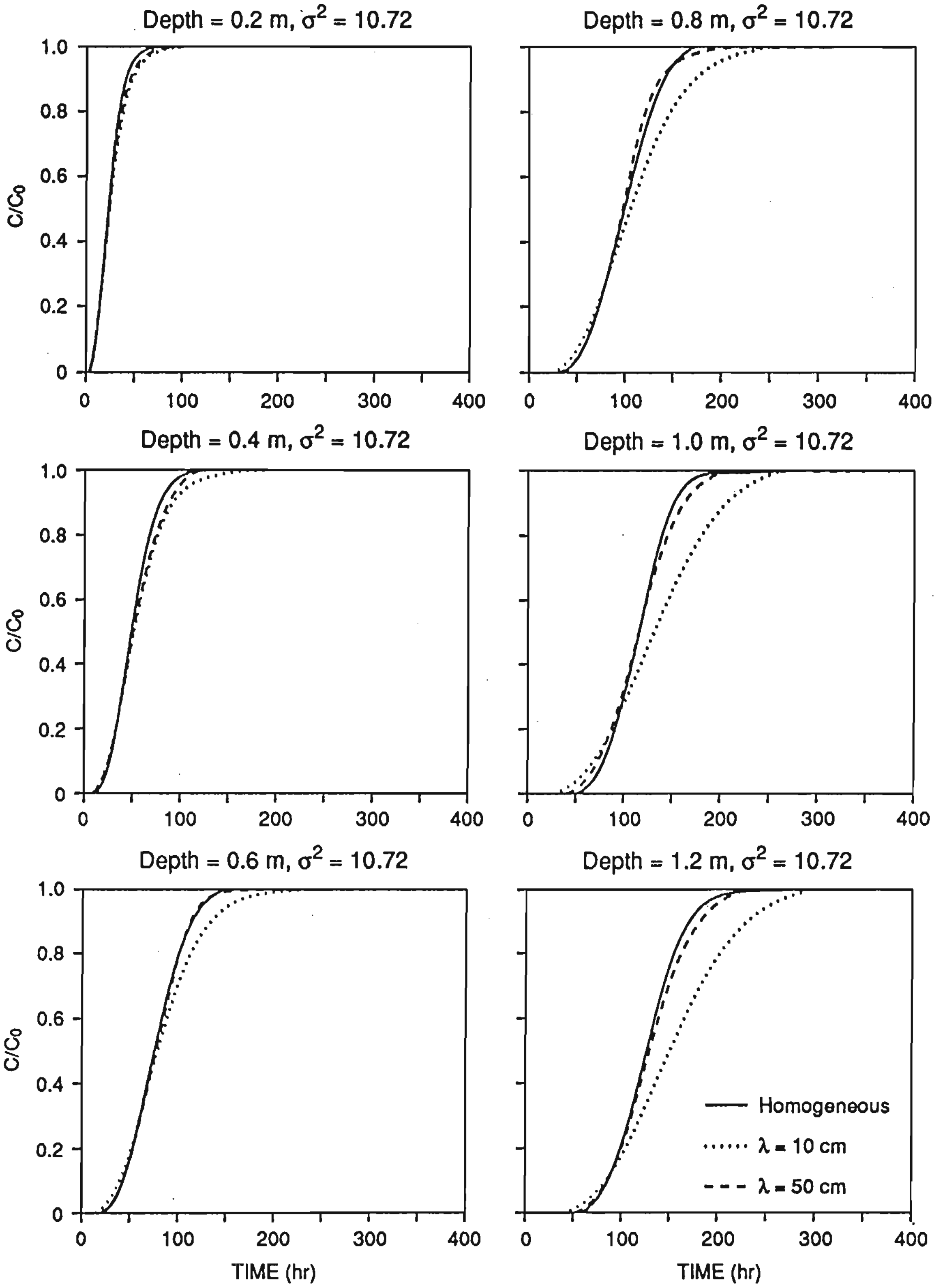


Figure 13. Simulated concentration breakthrough curves, log-conductivity variance value of 10.72

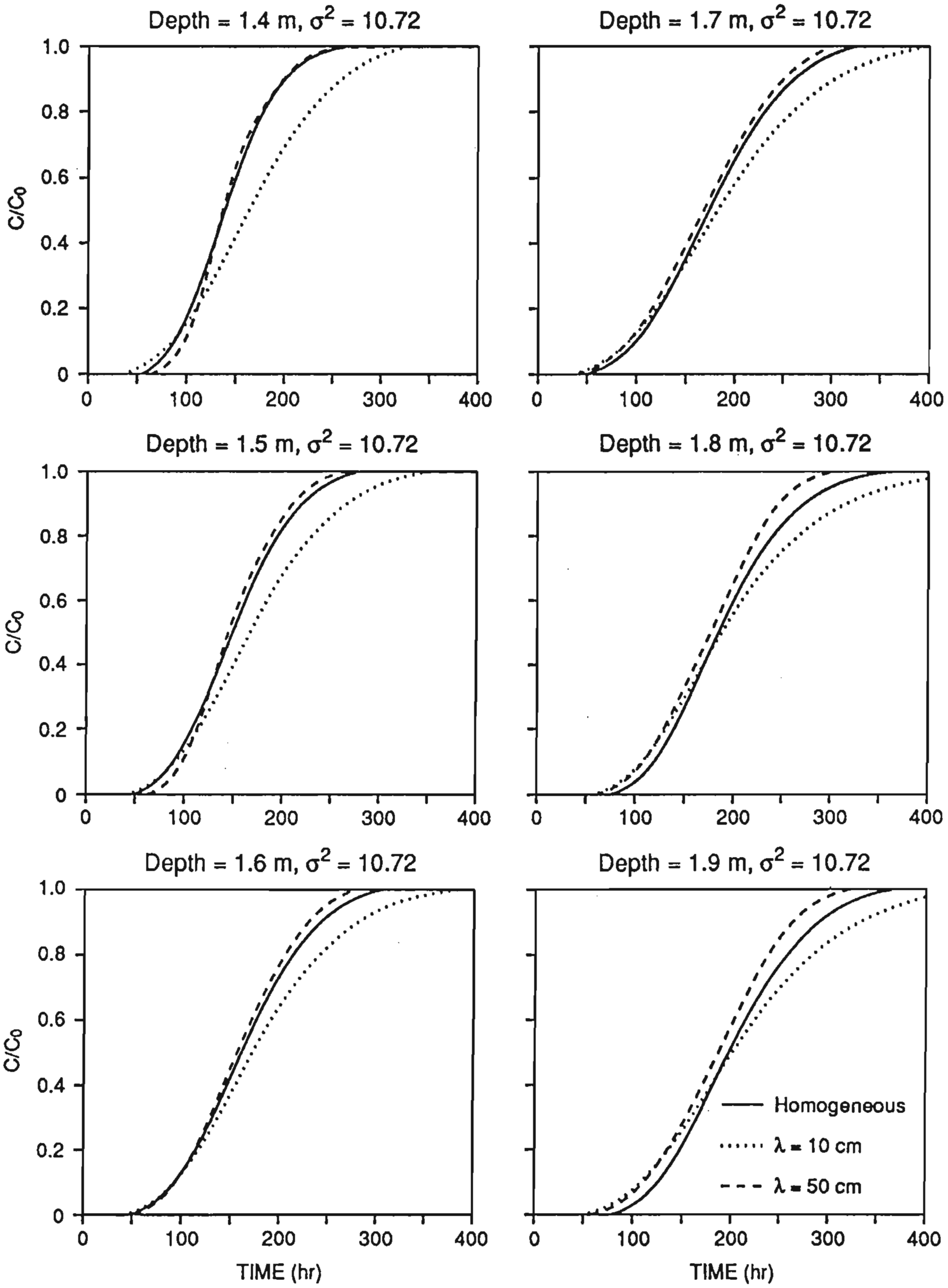


Figure 13.—*Continued*

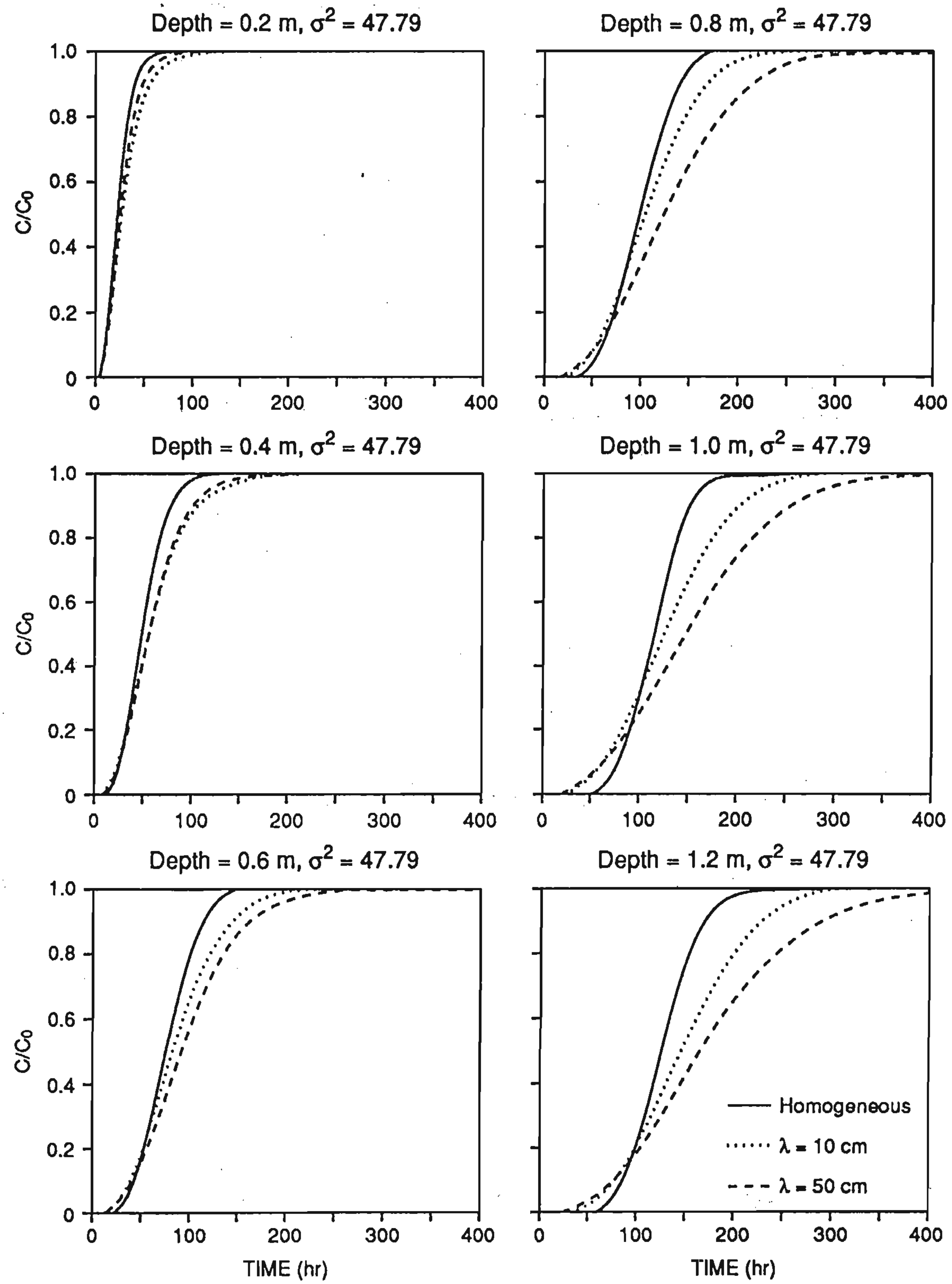
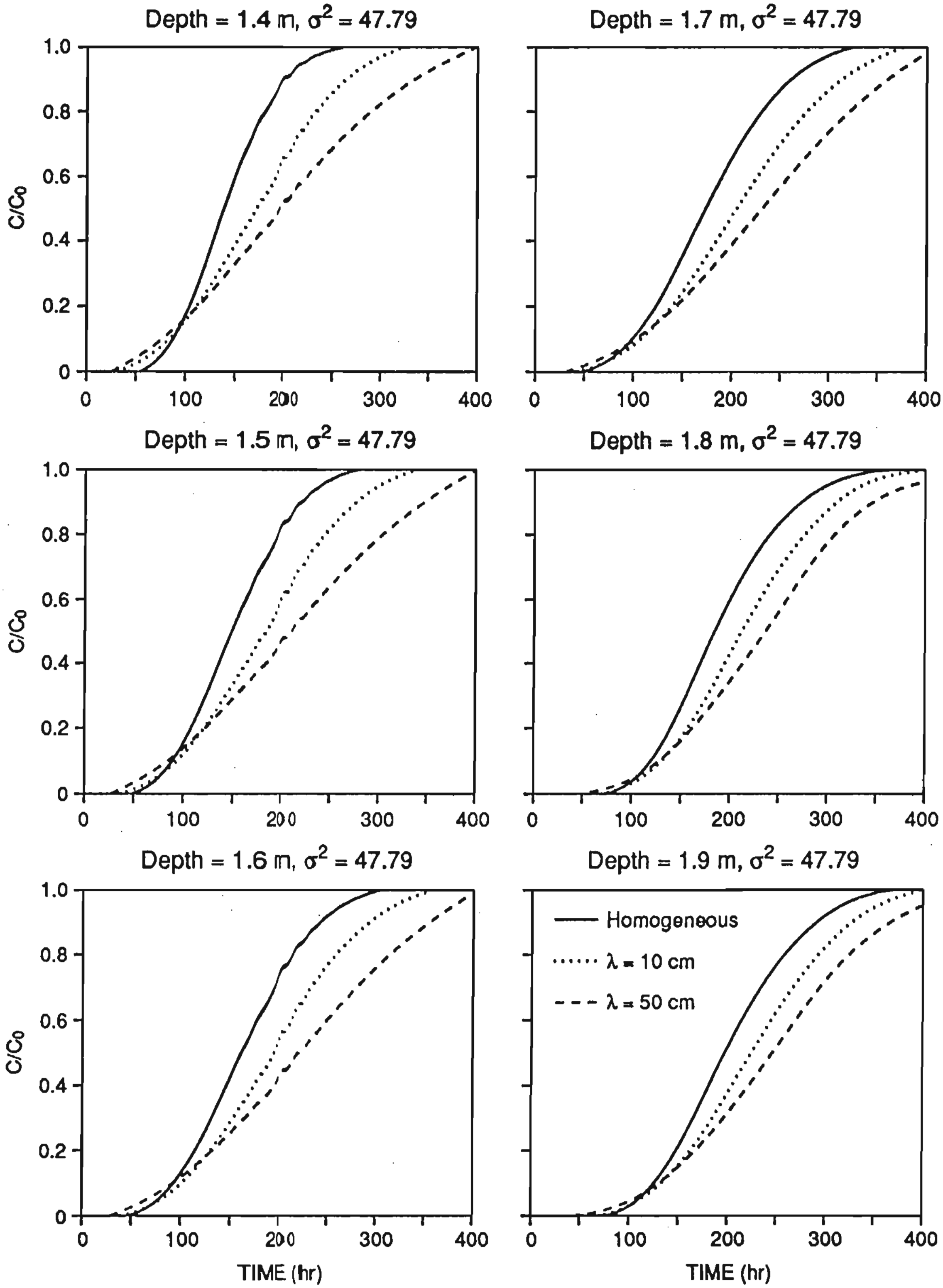


Figure 14. Simulated concentration breakthrough curves, log-conductivity variance value of 47.79



Depth = 1.4 m, $\sigma^2 = 47.79$

Depth = 1.7 m, $\sigma^2 = 47.79$

Depth = 1.5 m, $\sigma^2 = 47.79$

Depth = 1.8 m, $\sigma^2 = 47.79$

Depth = 1.6 m, $\sigma^2 = 47.79$

Depth = 1.9 m, $\sigma^2 = 47.79$

Figure 14.—*Continued*

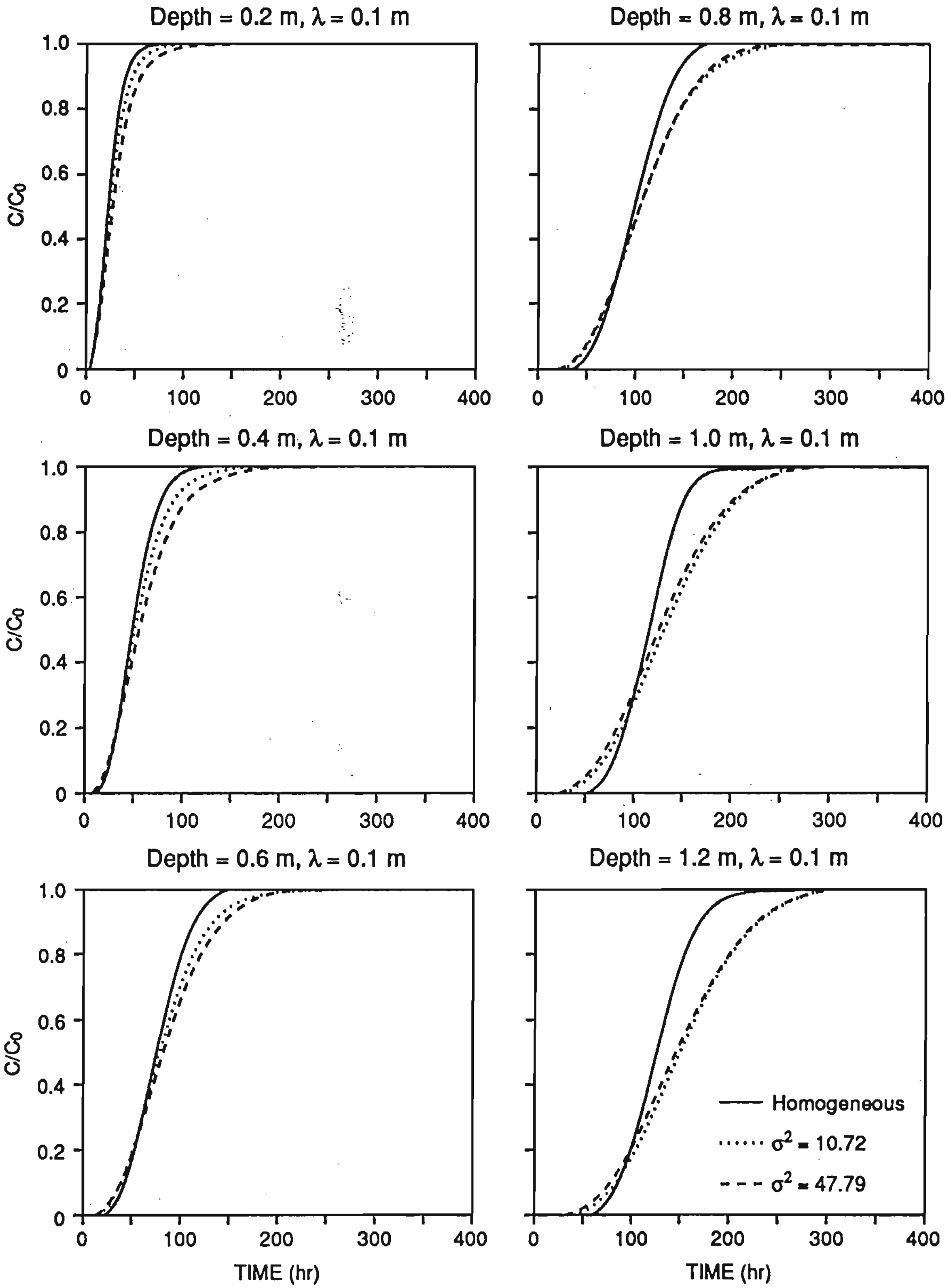


Figure 15. Simulated concentration breakthrough curves, log-hydraulic field correlation length of 0.1 m

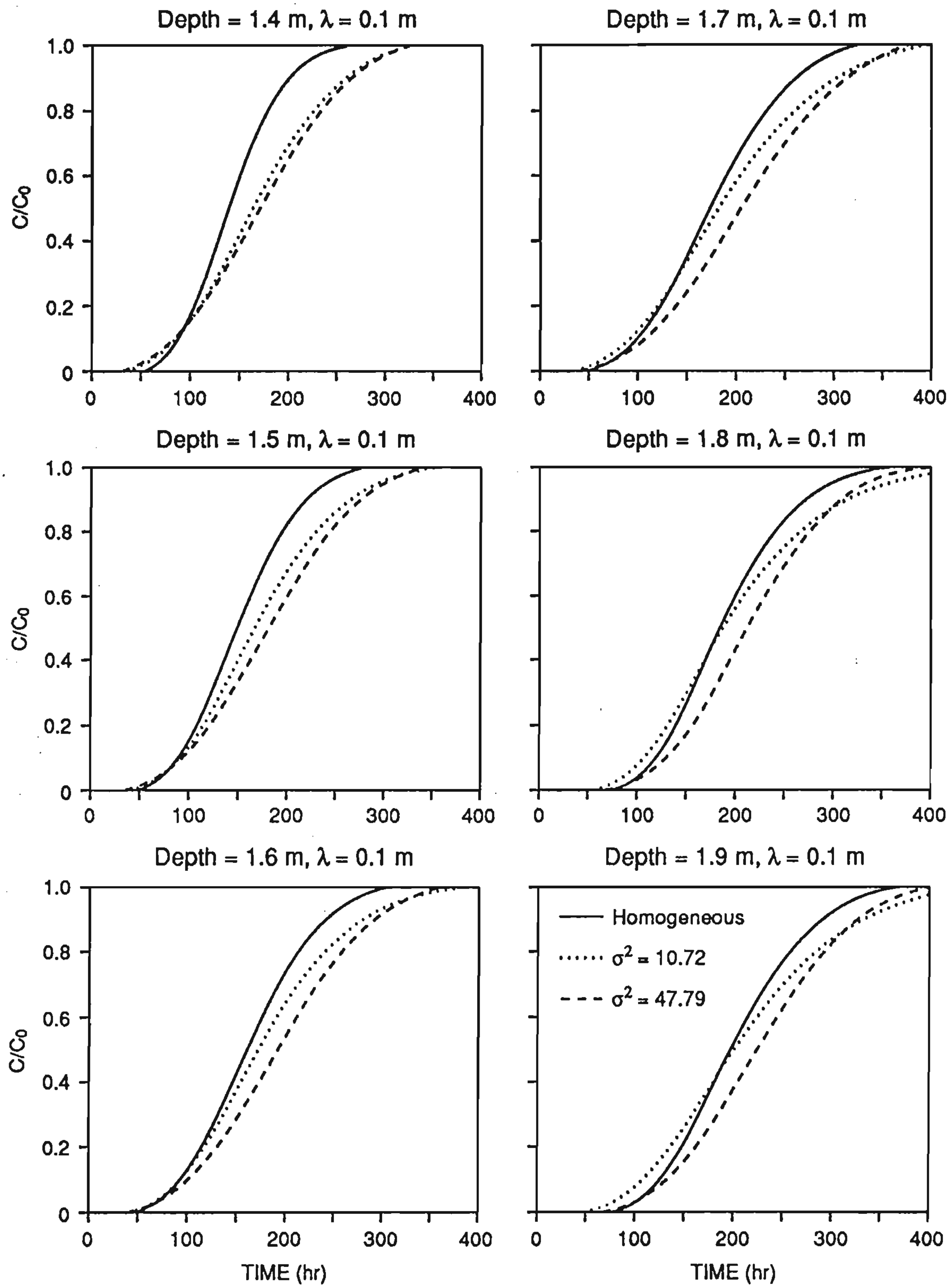


Figure 15.—*Continued*

However, below the depth of 1.4 m, as was observed in the previous cases, the differences in the breakthrough curves begin to decrease to the depth of 1.9 m.

Figure 16 is an illustration of the solute breakthrough curves for the two different values of variance: when the correlation of length value is 0.5 m, and that of the homogeneous saturated hydraulic conductivity cases. In this case, the solute spreading is highest for the larger variance case at all depths and consistently increases to the depth of 1.4 m. As can be inferred from these plots, the differences between the homogeneous and the lower variance cases are insignificant to the depth of 1.7 m. However, at 1.8- and 1.9-m depths, the solute spreading becomes slightly larger in the homogeneous case. This again is caused by an excessive numerical dispersion that is in the solution of the advection-dispersion equation for the homogeneous case. Below 1.4 m, the differences between all cases begin to decrease to the depth of 1.9 m.

Figure 17 shows the curves of the macrodispersivity plotted against the normalized travel distance (D/λ) for the two values of correlation length and the two different variance levels. The scale dependence of macrodispersivity from all these curves can be seen. When the correlation length is lower ($\lambda = 0.1$ m), the macrodispersivity values for the two variance levels generally show similar values up to the normalized travel distance of about 10. However, between D/λ of 11 and 20, the macrodispersivity begins to increase in the lower variance case. For the higher correlation length value ($\lambda = 0.5$ m), the macrodispersivity curves for the two variance levels are similar up to $D/\lambda = 1$. Between distances of 1 and 4 m, macrodispersivity is higher for the larger variance.

STOCHASTIC ANALYSIS OF SOLUTE DISPERSION IN HAWAII OXIC SOILS

The application of pesticides for control of nematodes in Hawai'i's pineapple fields has been discovered to be a major source of groundwater pollution here. Groundwater comprises 85% of the total potable water use on the island of O'ahu, and the discovery of trace amounts of organic chemicals in several municipal water wells and their eventual closure have raised some serious concerns about the protection of public health (Lau and Mink 1987; Oki and Giambelluca 1987). EDB (ethylene dibromide) and DBCP (dibromochloropropane), the two most widely used pesticides in the past, are known to be carcinogenic and their use has been discontinued. TCP (trichloropropane), a third type of commonly used pesticide, has a chemical structure similar to that of DBCP and is still in use. Recent field investigations by Wong (1983) and Peterson et al. (1985) have shown that EDB, DBCP, and TCP can be found at considerable

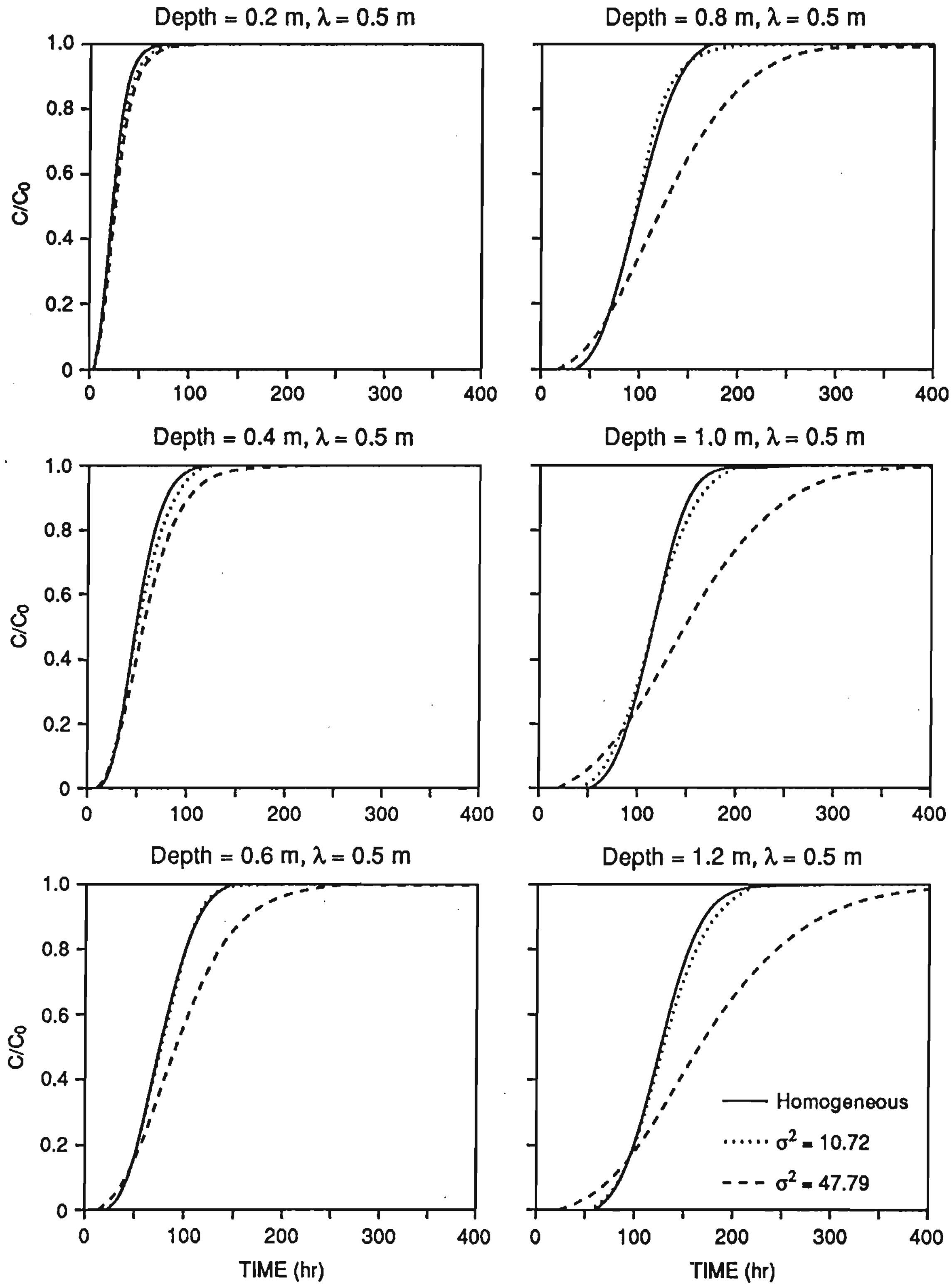


Figure 16. Simulated concentration breakthrough curves, log-hydraulic field correlation length of 0.5 m

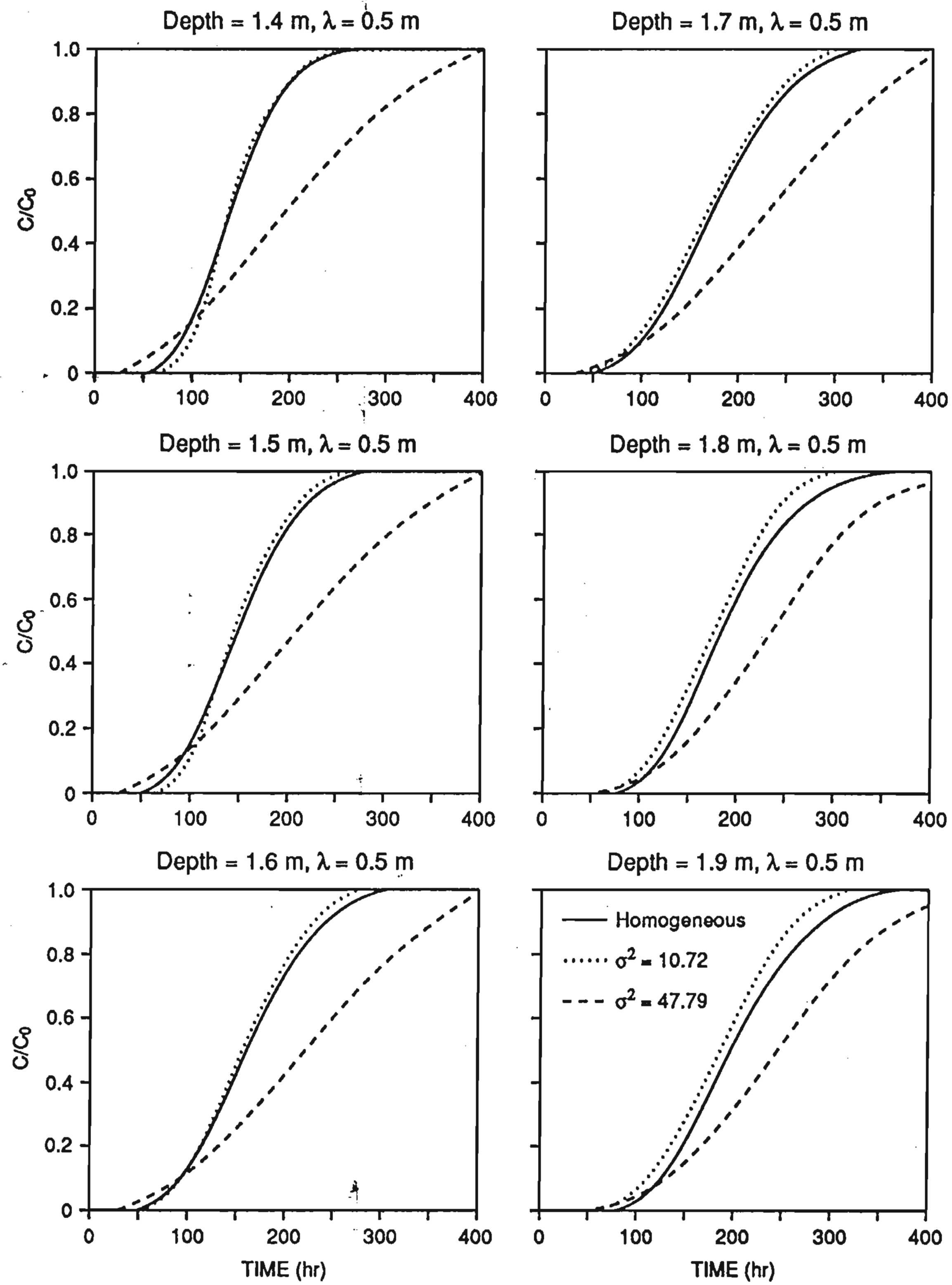


Figure 16.—*Continued*

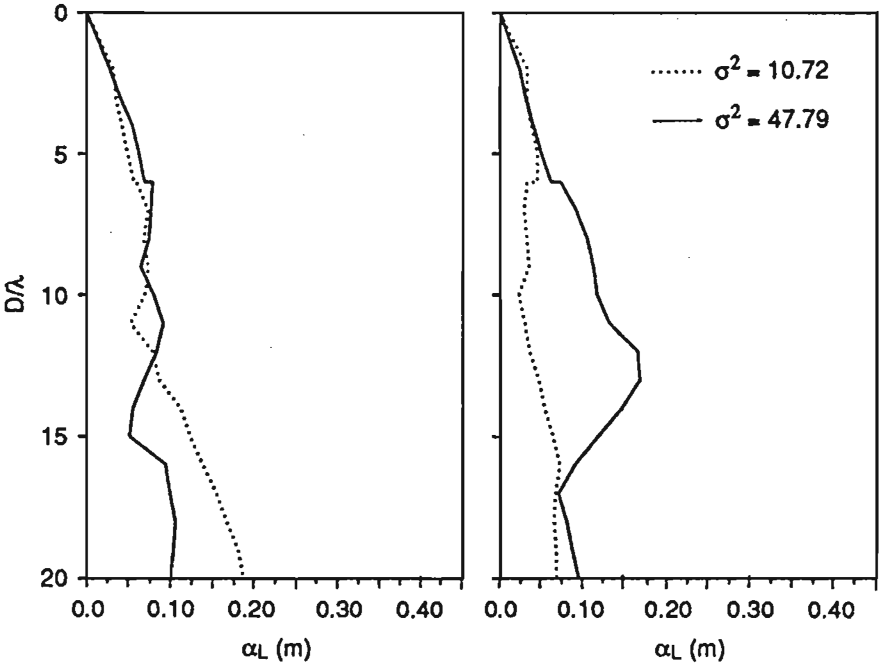


Figure 17. Development of macrodispersivity in heterogeneous soil with different variances and correlation lengths

depths below cultivated fields and pose a serious threat to the quality of groundwater resources.

Among various strategies that have been proposed for the protection of water supplies is the need for better understanding of the potential of residual pollutants to leach from topsoils into the groundwater. Knowledge of the transport patterns of pollutants in soils can aid in better forecasting the extent, timing, and potential of groundwater pollution from surface application of pesticides and accidental spills. The present study deals primarily with spatial heterogeneity of the hydrodynamic properties of a soil-solute system that determine contaminant transport in the soil taxonomic group classified as Hawaii Oxic soils. The shaded area on the map in Figure 18 shows the where Oxic soils are found on the island of O'ahu. These soils are principally derived from basaltic rocks of alluvium and are composed of kaolinite and the oxides iron and aluminum. They are highly structured and thus quite permeable and generally well drained (Green et al. 1982). Most of the area covered with Oxic soils is in pineapple cultivation, so pesticides have been used extensively on the cultivated fields within this region for the past three decades.

This part of the study is based on the fact that porous soils under field conditions are naturally heterogeneous, their hydraulic properties varying substantially in short distances as contaminant residuals migrate downward within the soil. An understanding of the effects of

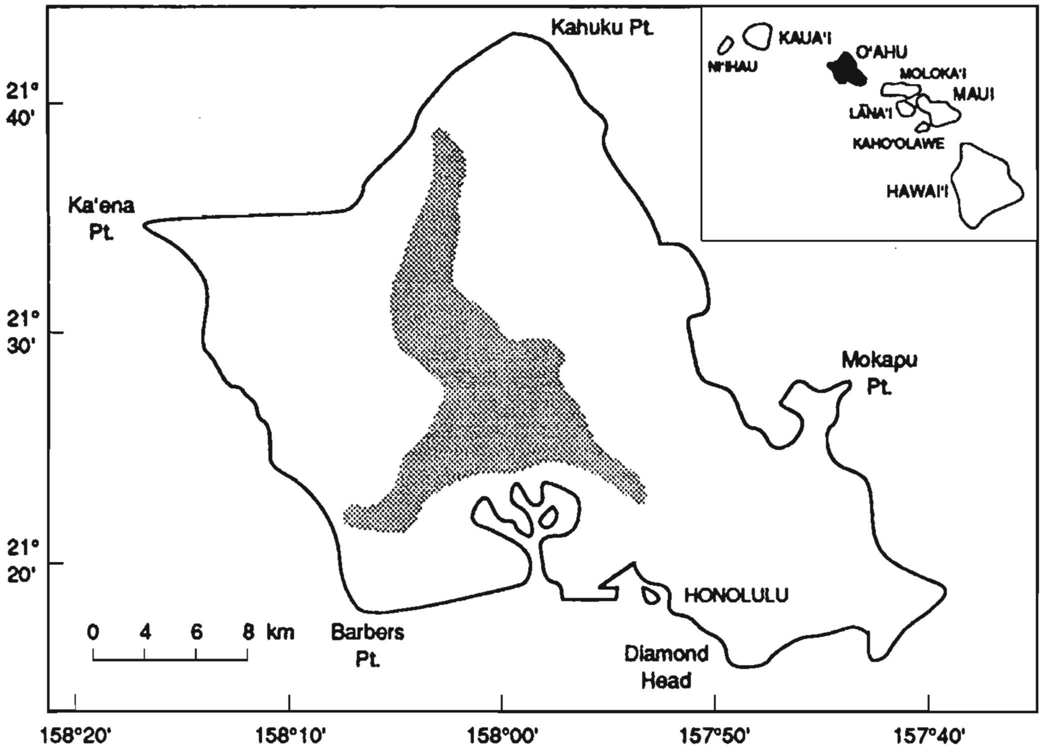


Figure 18. Areal extent of Oxic soils, O'ahu, Hawai'i

this small-scale heterogeneity on the macroscopic dispersion of contaminants in topsoils is the main focus of this project.

The main problem in dealing with soil heterogeneity is evaluating the uncertainty of predicting contaminant transport in heterogeneous soils. The data bases one usually has access to are inadequate to describe the spatial variability of soil structure in detail. Furthermore, treatment of such problems deterministically introduces large errors into the prediction of contaminant transport. These errors mainly arise from lack of knowledge on the spatial variability of hydraulic properties. The effect of this uncertainty on predicting contaminant spreading and migration patterns in the vadose zone must be quantified before any decisions regarding timing and extent of groundwater pollution from surface application of pesticides can be made.

In this regard, the parameter of particular importance is the spatial variability of saturated hydraulic conductivity. Saturated hydraulic conductivity is treated as a three-dimensional stochastic process in the solution of the physically based flow and solute transport equations. The physically based stochastic approach generally consists of two steps. The first operation involves generation of multiple realizations of the random saturated hydraulic conductivity field from statistical parameters inferred from field data. In the second operation, each realization,

TABLE 7. SATURATED CONDUCTIVITY STATISTICS

Location	Mean ($\times 10^{-2}$ m/hr)	Variance ($\times 10^{-4}$ m^2/hr^2)
1	5.183 6	47.791 0
2	5.051 1	10.719 7

which is an equally likely representation of actual soil heterogeneity, is entered into the unsaturated flow and solute transport model to simulate the transient migration of the contaminants in a soil column. Using such an approach, a controlled numerical experiment was carried out under field conditions: evaluated was the effect of two observed saturated hydraulic conductivity variance levels on the development of macrodispersivity in an unsaturated, heterogeneous, Hawaii Oxic soil column. The resulting solute concentration patterns were also compared with simulated concentration distribution in a column of soil with a homogeneous saturated hydraulic conductivity value. The analyses were further extended to evaluate the effect of correlation length of the random conductivity field on the solute dispersion along the flow path in the hypothetical column of soil.

Experimental Design

Stochastic analyses of solute dispersion were performed for two different saturated hydraulic conductivity variance levels estimated from the core Hawaii Oxic soil samples. The dispersion of a conservative tracer originating from the soil surface was simulated in a three-dimensional spatial domain, which represents a hypothetical column of soil. The boundary and initial conditions and the size of the soil column, as well as the spatial increments of the cubical finite element grid network, were similar (Fig. 2), except that $Q = 1.0 \times 10^{-4}$ m^3/s and boundary bf was 1.5 m.

The soils data giving the spatial variance of the saturated hydraulic conductivity of Hawaii Oxic soils from two locations on O‘ahu were used (Green et al. 1982). The computed statistics of the saturated hydraulic conductivity measurements are given in Table 7. Soil spatial variability of the two soil groups is represented by the estimates of their respective variances. The data for the two soil groups show the same mean but different variances, which makes them particularly useful for studying spatial variability.

A total of 200 realizations of the saturated hydraulic conductivity field for each variance level and the mean given in Table 7 were generated, and a convergence test was performed to determine the number of realizations needed to satisfy the ergodic hypothesis. A correlation length equal to the unit mesh size ($\lambda_l = 0.1$ m) in the finite element grid network was used in

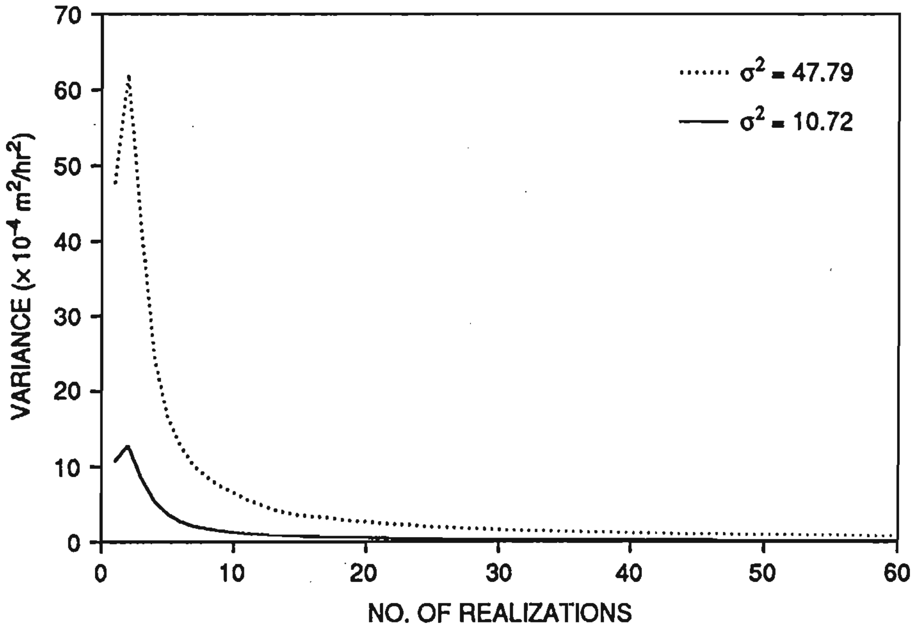


Figure 19. Variance of ensemble mean vs. number of realizations for each variance level

generating the random saturated hydraulic conductivity field. The results of the convergence test were given as a plot of the variance of ensemble mean against the number of realizations for each variance level (Fig. 19). Figure 19 illustrates that for larger variances, 30 realizations of the random conductivity field produce an ensemble mean variance that is sufficiently close to zero. Based on these results, a total of 30 realizations of the random conductivity field from each variance level was selected for the numerical experiments.

Results of Numerical Experiments

Figure 20 shows the simulated concentration breakthrough curves for the smaller variance (σ_f^2 = 10.72 × 10^{-4} m^2/hr^2) over the entire ensemble of saturated hydraulic conductivity realizations, indicated by the scatter plot, and for the flow field with a homogeneous mean value in saturated hydraulic conductivity (5.05 × 10^{-2} m/hr) at various depths in the soil profile. These results show that the spreading of the tracer increases in a heterogeneous soil as the contaminant plume, which has an inflow concentration of unity, moves down the soil profile. As expected, the solute dispersion is much less extensive for the soil with a uniform saturated hydraulic conductivity field. A similar solute dispersion behavior can be observed for the larger variance in saturated hydraulic conductivity (σ_f^2 = 47.79 × 10^{-4} m^2/hr^2) (see Fig. 21). However, for the larger variance, the solute spreading becomes more significant than for the smaller variance at a depth of 0.4 m. At depths below 0.8 m, the two variance levels of

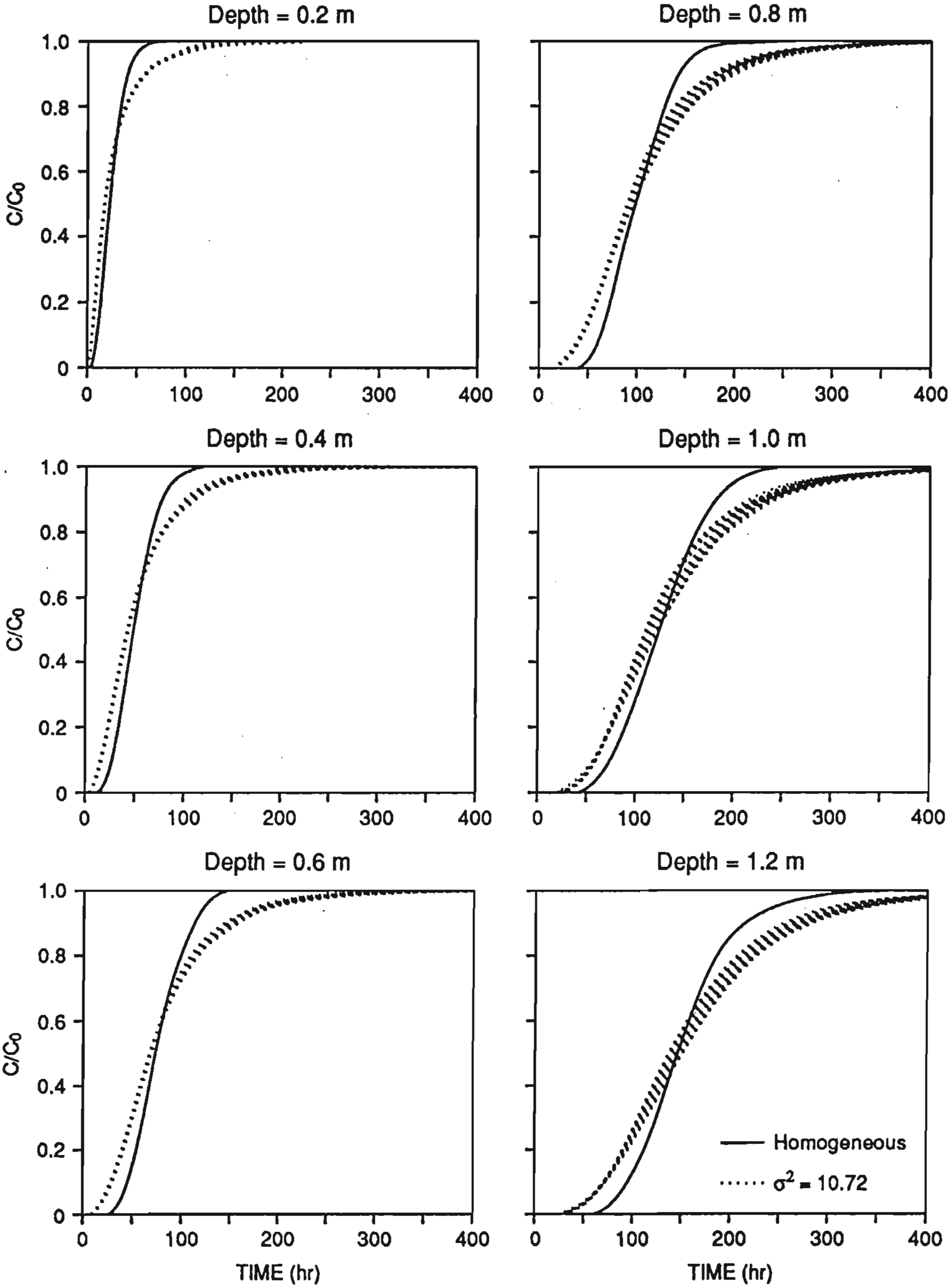


Figure 20. Simulated concentration breakthrough curves over entire ensemble of saturated hydraulic conductivity realizations, log-conductivity variance value of 10.72

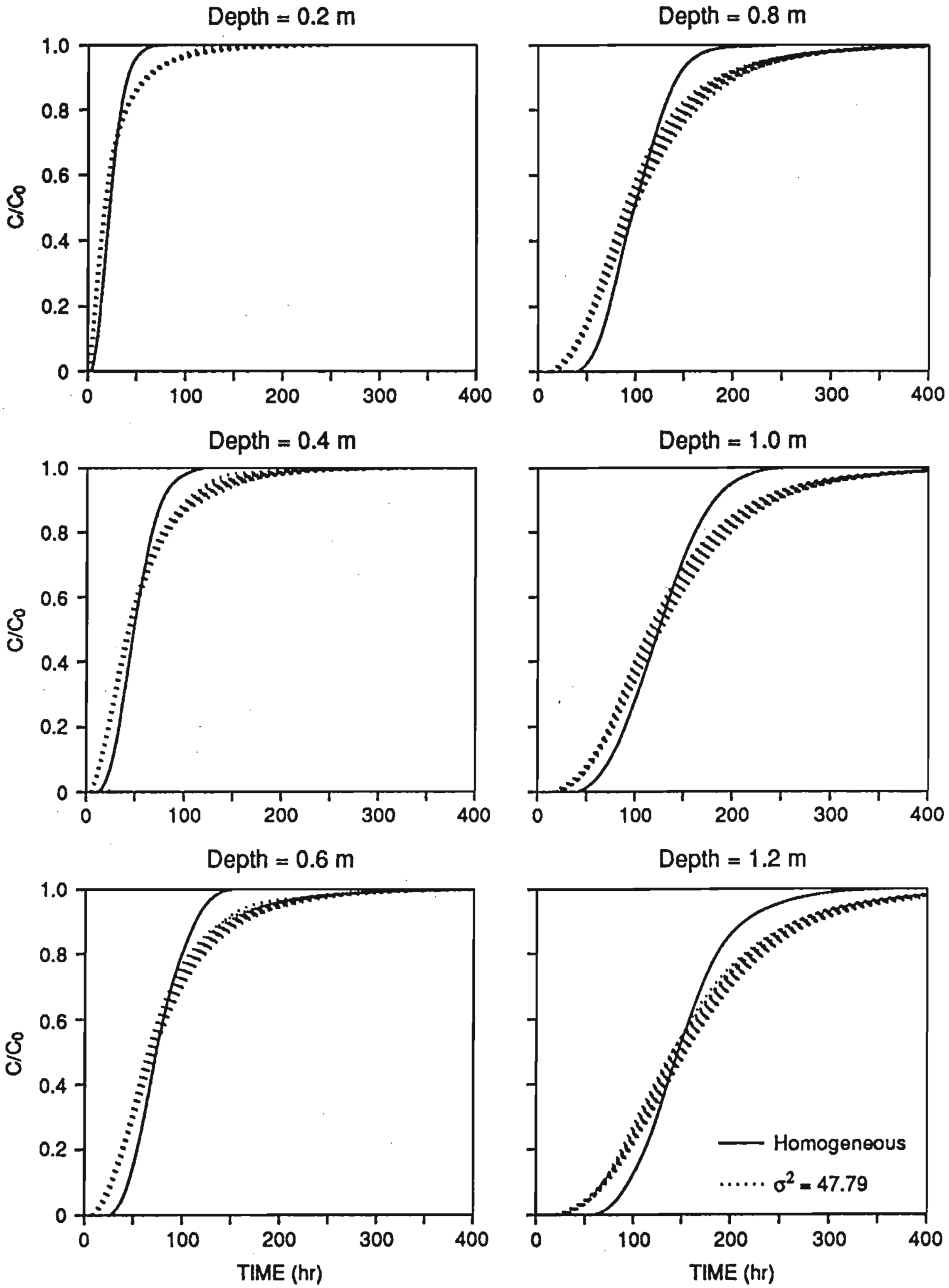


Figure 21. Simulated concentration breakthrough curves over entire ensemble of saturated hydraulic conductivity realizations, log-conductivity variance value of 47.79

saturated hydraulic conductivity generally correlate with very similar solute dispersion behavior.

Figure 22 shows the mean values of the solute breakthrough concentration curves over the ensemble of realizations for both variance levels and for the uniform flow field with the same mean. The two variance levels in the saturated hydraulic conductivity field generally produce very similar solute dispersion in the mean, which is significantly different from the uniform flow field. As the solute plume migrates down the soil profile, the solute dispersion for the larger variance becomes slightly greater than for the smaller variance. The higher dispersion levels for these two cases are mainly the result of the velocity variations induced by the heterogeneity of saturated hydraulic conductivity in the soil profile.

Figures 23 and 24 give examples of spatial variability in the distribution of velocity in the z and x directions, respectively, for the three cases. The velocity distribution in the z and x directions are uniform for the flow field with homogeneous saturated hydraulic conductivity. The variability in the spatial distribution of velocity in the z and x directions becomes much more significant for the smaller variance ($\sigma_f^2 = 10.72 \times 10^{-4}$ m^2/hr^2) and for the larger variance ($\sigma_f^2 = 47.79 \times 10^{-4}$ m^2/hr^2) of the saturated hydraulic conductivity. The increases in the longitudinal spread of the contaminant plume that were observed in the solute breakthrough curves are mainly caused by the lateral and longitudinal variations in the velocity distributions, as depicted in these figures.

Figures 25 shows the box-whisker plots of the vertical variability in the spatial distribution of concentration values in the soil profile after simulation times of 20, 138, and 246 hr, respectively. These plots indicate that the variability in the distribution of tracer concentration is much larger in heterogeneous soils than in a homogeneous soil with the same mean saturated hydraulic conductivity. The dispersion of tracer concentrations is also more pronounced in soils with a higher saturated hydraulic conductivity variance. The variability in the vertical direction decreases as the tracer, which has an inflow concentration of unity, moves down the soil profile.

The values of macrodispersivity over the entire ensemble of realizations of the saturated hydraulic conductivity field for the two variance levels were plotted as a function of travel distance (Fig. 26). In the case of heterogeneous soil with a larger saturated hydraulic conductivity variance, larger macrodispersivity values were observed at shorter travel distances, as compared with the smaller variance. However, at greater travel distances, the macrodispersivity values of both variance levels seem to narrow to the same value.

Figure 27 compares the concentration breakthrough curves at various depths in the soil profile for the two variance levels and for five different correlation lengths. Variations in correlation lengths seem to have a more pronounced effect on the differences in the

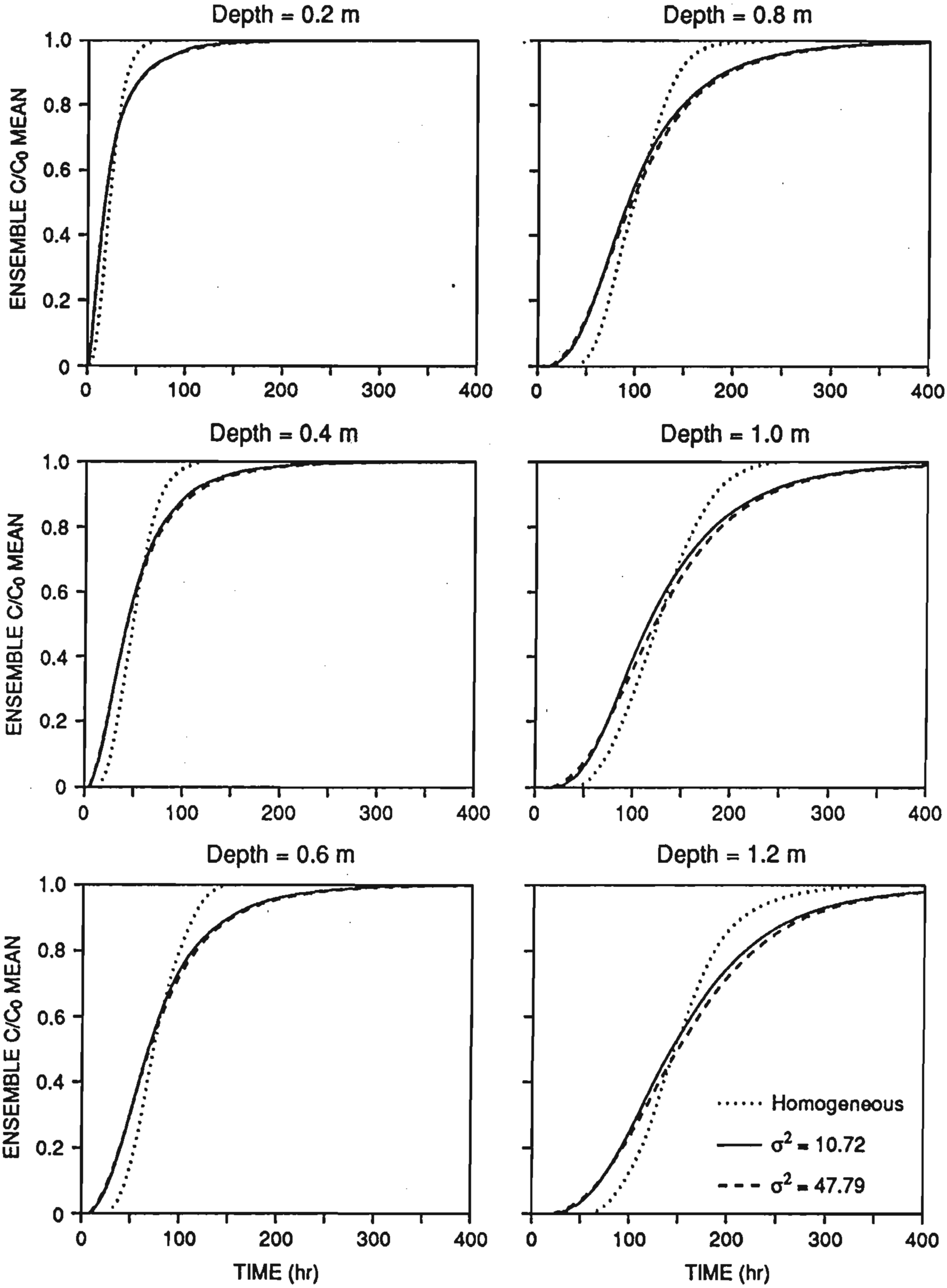


Figure 22. Mean values of solute breakthrough concentration curves over ensemble of realizations

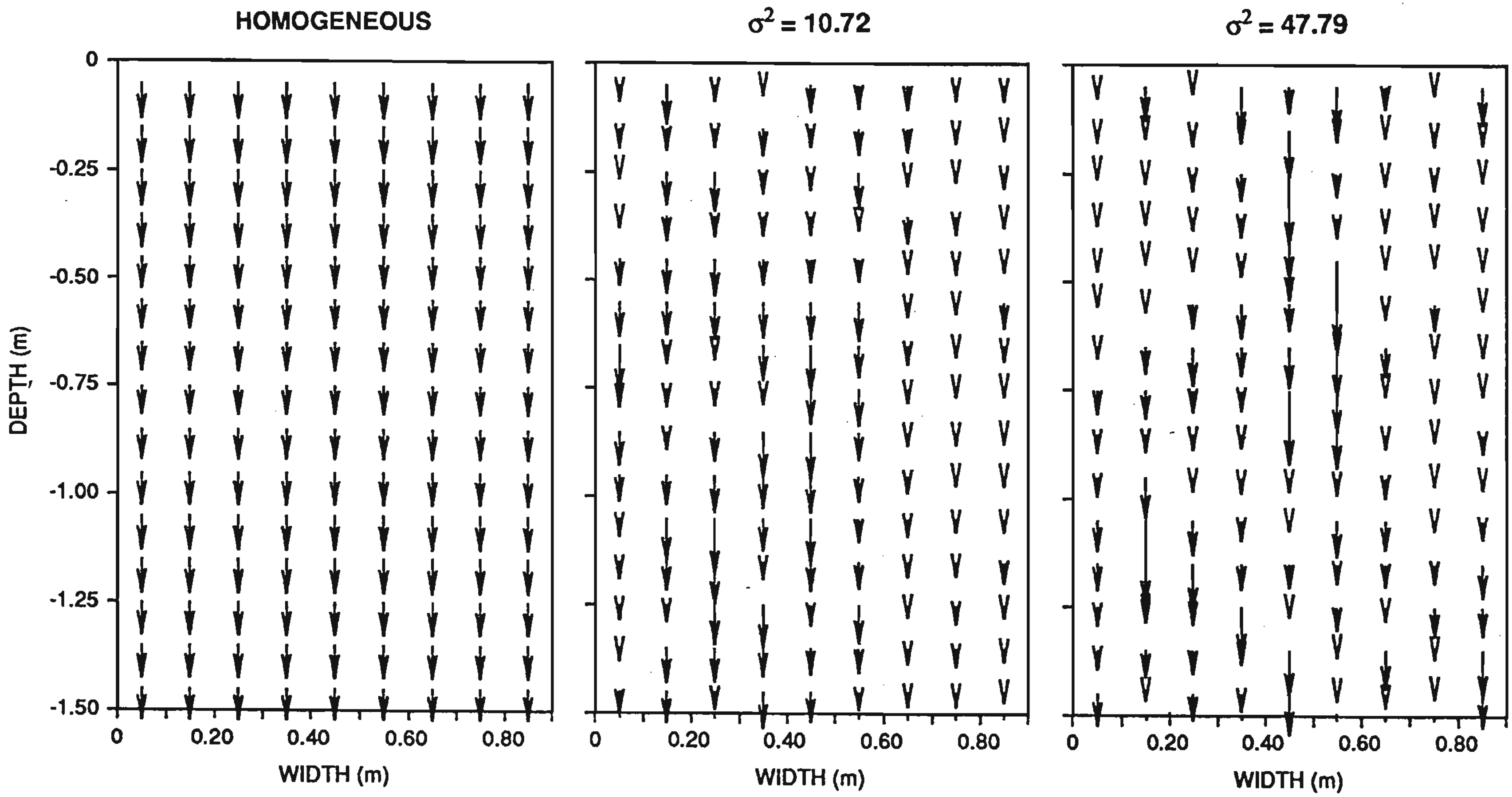


Figure 23. Spatial variability of velocity along principal flow direction

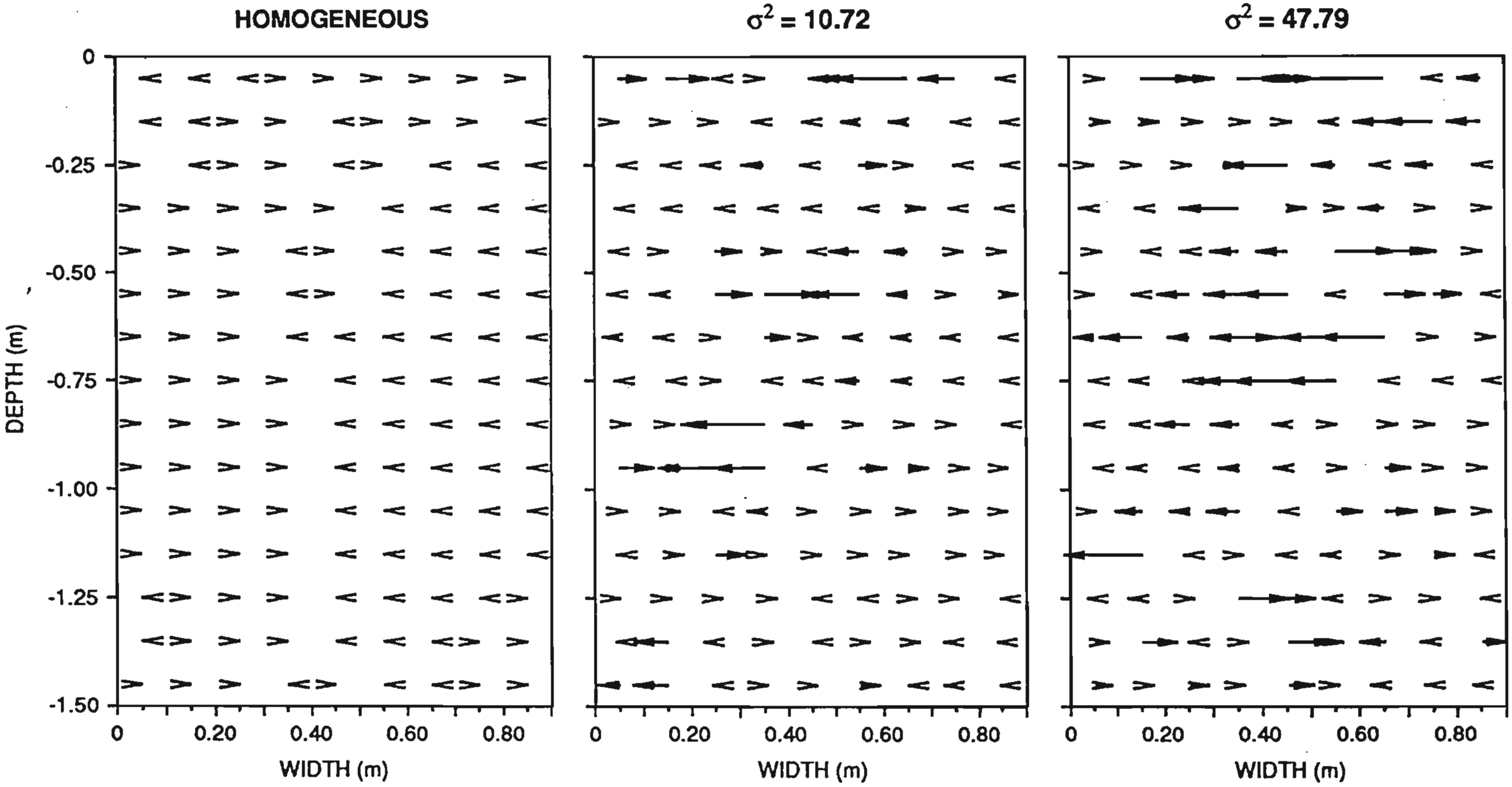


Figure 24. Spatial variability of lateral velocity

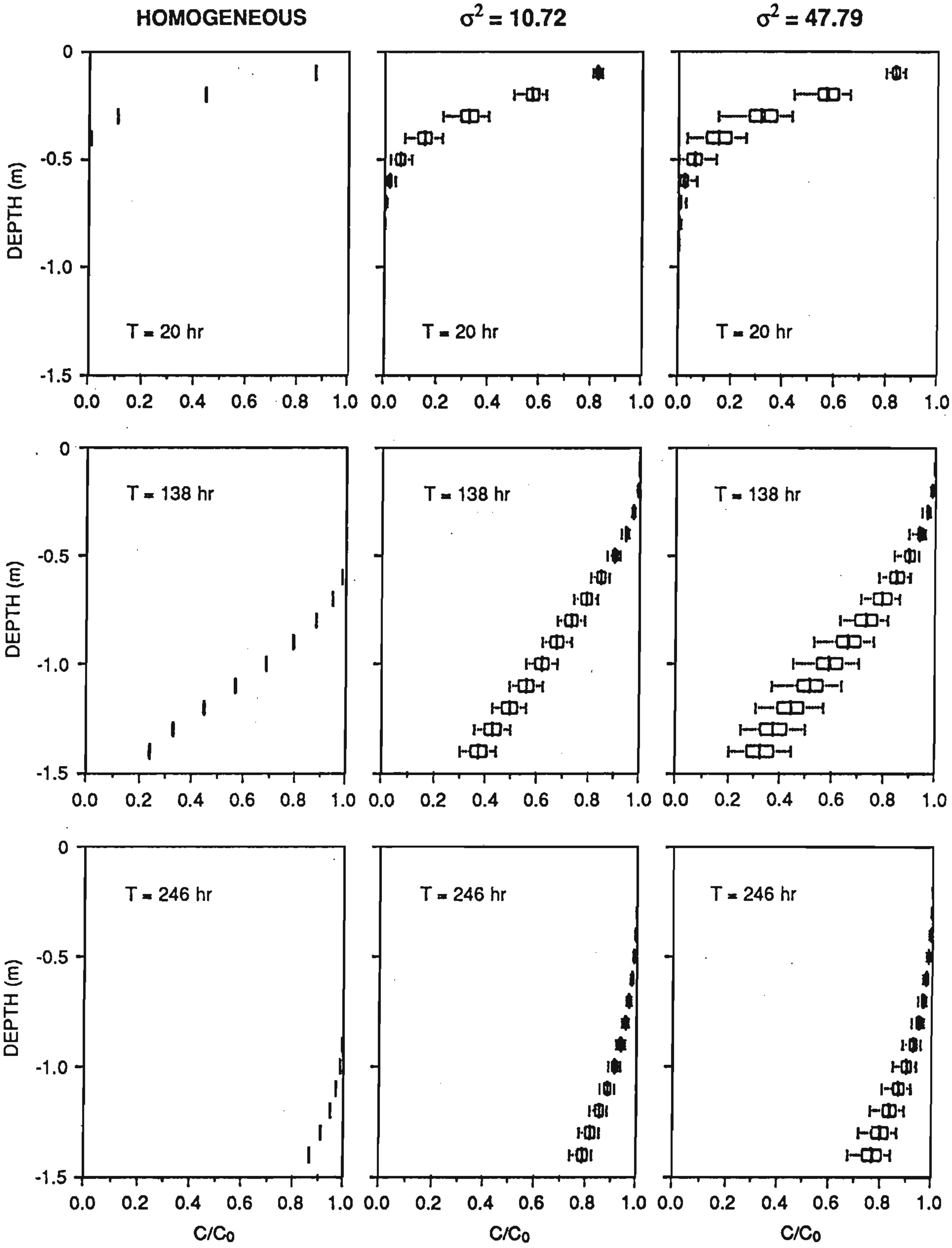


Figure 25. Box-whisker plots of vertical variability in spatial distribution of solute concentration after simulation times of 20, 138, and 246 hr

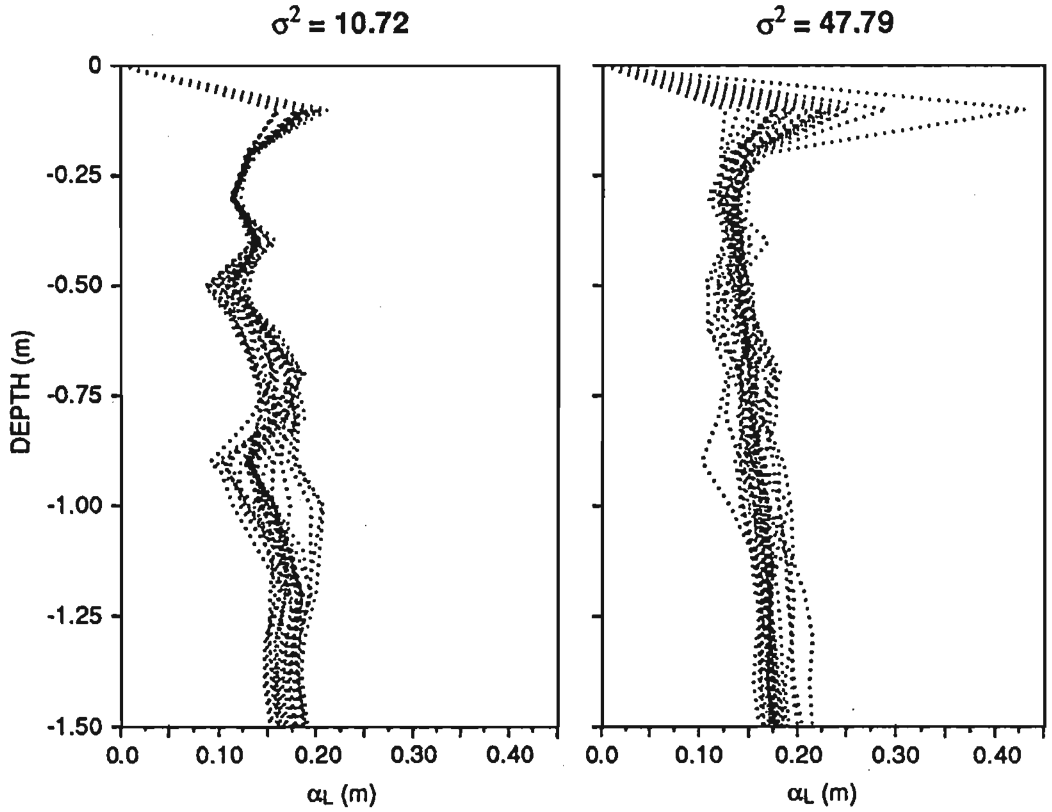


Figure 26. Development of macrodispersivity vs. travel distance over entire ensemble of realizations of saturated hydraulic conductivity field for variances of 10.72 and 47.79

breakthrough curves in the smaller variance case. As the correlation length increases, the solute spreading seems to occur faster as the contaminant plume travels down the soil profile. The same trend can be observed in the larger variance case. However, in this case, the differences in the solute breakthrough curves are much smaller.

SUMMARY AND CONCLUSIONS

The transport of solutes through unsaturated porous media traditionally has been investigated in terms of physically based mathematical models, which are based on the theory of dispersion. Just as with groundwater, the value of effective dispersivity is difficult to determine, and sometimes even the fundamental assumption of the Fickian diffusion process is questionable. Stochastic analysis of the variability of hydraulic conductivity in saturated heterogeneous porous media has been conducted by several researchers (Gelhar and Axness 1983; Dagan 1988). In these studies, the spatial variations of hydraulic conductivity of a heterogeneous

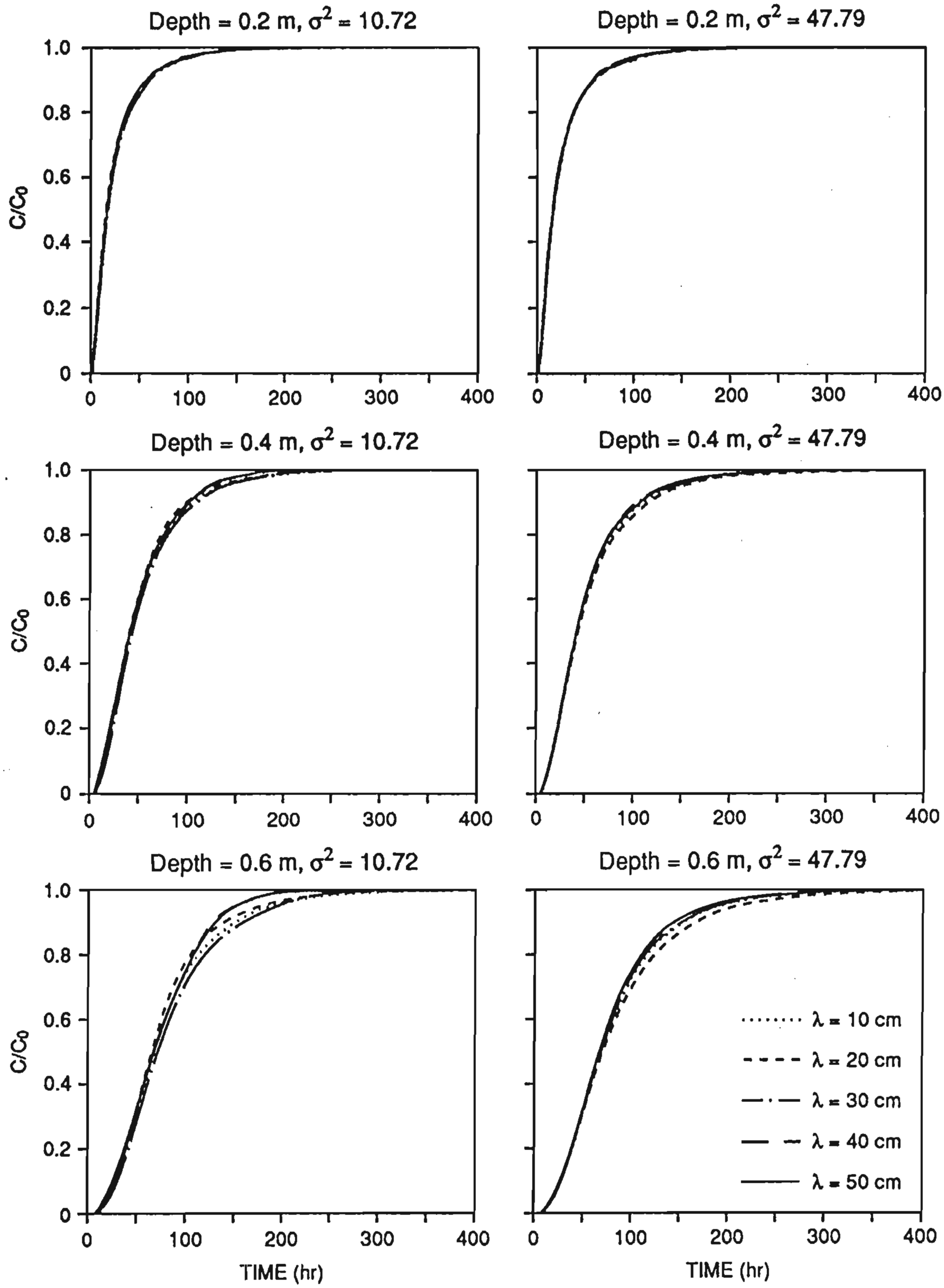


Figure 27. Simulated concentration breakthrough curves down soil profile for different log-conductivity variance levels and correlation lengths

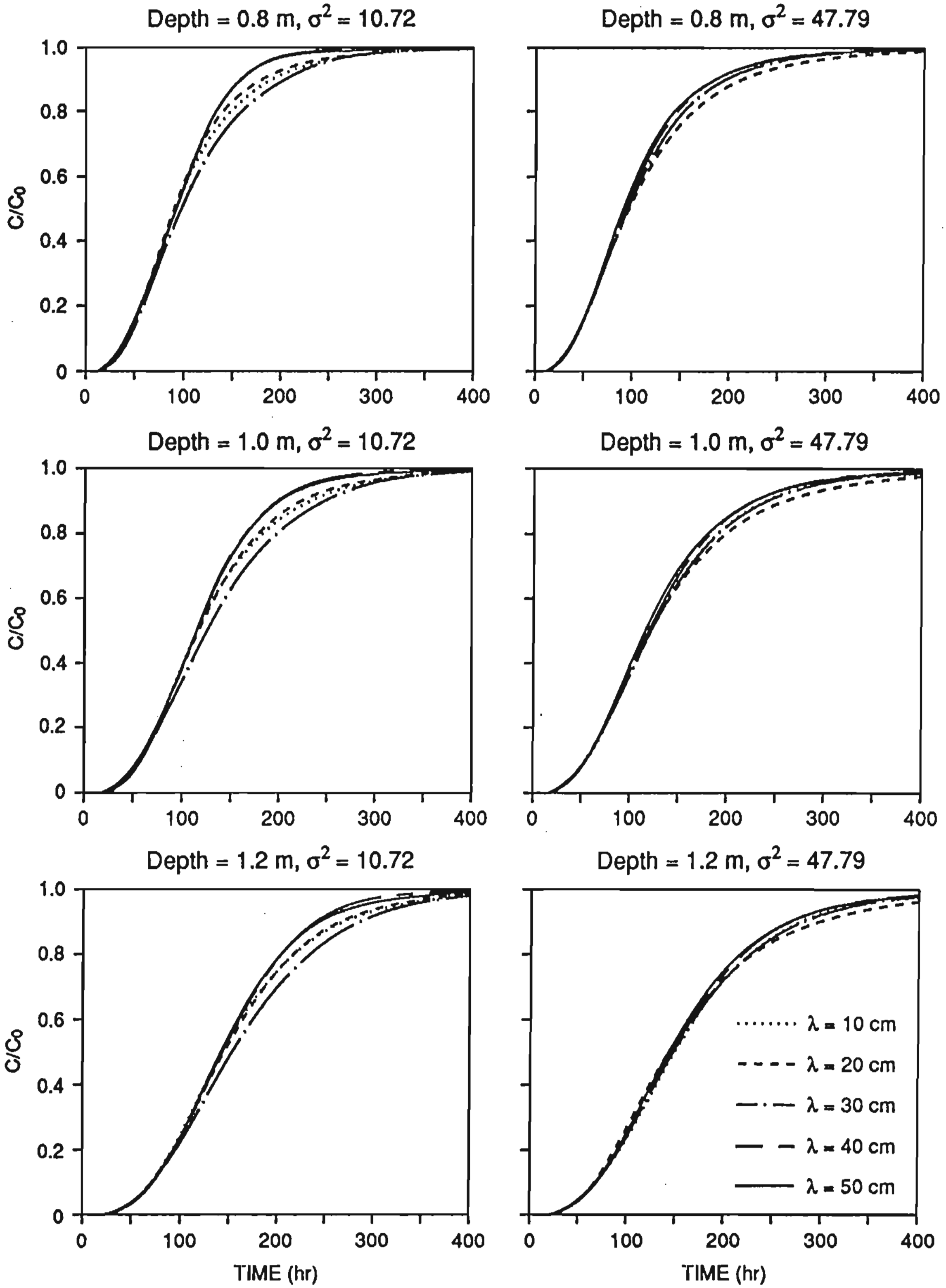


Figure 27.—*Continued*

porous medium (assumed to be a random process) were incorporated into the dispersion concept. The objective was to allow the use of a conventional advection-dispersion equation to simulate the mean transport of solute. The researchers found that the dispersivity associated with the simulation of solute transport through the heterogeneous porous media, called macrodispersivity, is much larger than that associated with the homogeneous media. In a study of heterogeneous soil, the equation could be applied to a homogeneous soil if the macrodispersivity of a particular heterogeneous soil could be estimated.

Macrodispersivity was also found to be scale-dependent for it initially increases as a linear function of travel distance. Later, the relation between macrodispersivity and travel distance becomes nonlinear, and eventually the macrodispersivity value approaches an asymptotic constant . Therefore, the mean solute transport can be considered a Fickian process only after macrodispersivity reaches a constant value, after a long period of travel. Dagan (1988) showed that, for an isotropic three-dimensional heterogeneous soil, the distance a solute plume travels before it spreads in true Fickian manner is about fifty times the log hydraulic conductivity scale. The typical value of log-conductivity correlation length is 1 m (Dagan 1986); and thus, a solute plume must travel about 50 m before the mean transport process becomes Fickian. Research on stochastic subsurface hydrology in the last decade has produced equations for the determination of asymptotic dispersivity, which can be used in the mathematical simulation of solute transport in large regional aquifers. But for the simulation of solute transport through unsaturated soils, where the region of interest is often as short as a few meters, one would more likely deal with macrodispersion in the linear or nonlinear development phases. In a short travel distance, macrodispersivity increases linearly with distance. This study estimated that in a three-dimensional isotropic heterogeneous soil, the length of the linear growth phase is approximately 0.2 times the correlation length.

The linear growth phase corresponds to the advection period of the longitudinal dispersion of solute in a shear flow, first shown by Taylor (1959) in his analysis of the spread of solutes flowing through a pipe. Taylor (1959) found that, for solute transport in a shear flow, the advection-dispersion equation with a constant dispersion coefficient can be applied only after a simple balance between longitudinal advective solute transport and lateral diffusive transport is established. Shortly after a plume of contaminated water is introduced into a flow field, however, the spread of solute in the plume is influenced mainly by the distribution of advective velocity. This initial phase of solute spreading and mixing is usually called the advection period. Taylor's concept was later applied by Mercado (1967) to advective horizontal displacement of solutes through a stratified aquifer, Mercado showing that dispersivity increases with travel distance.

Analysis of the macrodispersion of the column of soil with the dimensions 1.2 × 1.2 × 2.0 m revealed that the combined effect of the soil saturated hydraulic conductivity variance and the correlation length may have a considerable influence on the dispersive behavior of a conservative tracer in heterogeneous soils. As inferred from the results of the solute breakthrough curves and scale-dependent macrodispersivity, there are small differences in macrodispersivity values up to a normalized travel distance (D/λ) of 10 when the correlation length is low ($\lambda = 0.1$ m). In contrast, in the case of the larger correlation length ($\lambda = 0.5$ m), macrodispersivity values are similar up to $D/\lambda = 1$. Beyond this value, macrodispersivity values increase in the larger variance case.

The variability of spatial and temporal distribution of contaminant transport as affected by the spatial heterogeneity of saturated hydraulic conductivity was demonstrated for Hawaii Oxic soils. Our analysis showed that, in the presence of soil heterogeneity (described by the saturated hydraulic conductivity variance) and a finite local dispersivity, the tracer spreading in the mean flow direction, as depicted by the solute breakthrough curves, is controlled by the fluctuations in the velocity distribution. Contaminant transport simulations indicate that tracer spreading is much more significant in heterogeneous soils than in a homogeneous soil with the same mean. Furthermore, large errors in the prediction of contaminant plume concentrations may result from the uniformity assumption of saturated hydraulic conductivity in the soil profile. The errors would mainly result from a lack of knowledge of the spatial variability of the saturated hydraulic conductivity in soils. However, the mean solute breakthrough concentration curves over the ensemble of saturated hydraulic conductivity realizations for the two variance levels at various depths were not significantly different.

The spatial variability in tracer concentrations, as depicted by the box-whisker plots, is greater for the soil with larger saturated hydraulic conductivity variance. This is a direct result of the relative magnitude of the longitudinal and lateral variations in the spatial distribution of velocity in the soil profile. Spatial variability decreases as the contaminant, which has an inflow concentration of unity, travels down the soil profile.

Analysis of macrodispersion, as influenced by the variance of the saturated hydraulic conductivity, showed that the larger variance results in larger macrodispersivity values at shallow depths in the hypothetical soil column. The macrodispersivity values seem to converge to the same constant value at greater depths for both variance levels as the travel distance of the contaminant plume increases.

The analysis shows that macrodispersion in Hawaii Oxic soils with a finite local dispersivity does not appear to be a scale-dependent process: macrodispersivity converges to a constant value (about 0.15 m) and remains constant down to a depth of 1.5 m. However, the estimated macrodispersivity values are clearly influenced by the limited size of the soil column and the boundary effects in the transport domain.

Analysis of the effect of correlation length on the solute spreading shows that increasing correlation length generally produces a faster breakthrough of solutes at various depths in the soil profile. For the smaller saturated hydraulic conductivity variance ($\sigma_f^2 = 10.72 \times 10^{-4}$ m^2/hr^2), the larger correlation length values ($\lambda_l = 0.4$–0.5 m) resulted in the largest tracer spreading, followed by the smaller correlation length values ($\lambda_l = 0.1$–0.2 m). The intermediate correlation length value ($\lambda_l = 0.3$ m) produced the smallest tracer spreading. In the larger variance case ($\sigma_f^2 = 47.79 \times 10^{-4}$ m^2/hr^2), the differences in tracer spreading for different values of correlation lengths were smaller. In this case, the correlation length value $\lambda_l = 0.2$ m resulted in the smallest tracer spreading, while values of 0.3 m and 0.1 m had similar effects on solute dispersion, and values of 0.4 m and 0.5 m produced the fastest breakthrough of solute plume at various depths in the hypothetical soil column. These observations can be attributed to an existing nonlinear relationship between the heterogeneity scale and the dispersivity values in the soil column.

The solution of the physically based equation showed that the spatial variance and correlation structure of the saturated hydraulic conductivity distribution are important parameters in the prediction of contaminant spreading in Hawaii Oxic soils. Another important factor identified was that at smaller variance values, different correlation lengths had a more pronounced effect on the dispersion of the contaminant plume in the soil profile. Thus, the ratio of correlation length to the variance, as the parameter controlling the heterogeneity scale (Dagan 1986), is an important factor in predicting the dispersion of contaminant plumes.

In our study, the Monte Carlo analysis was applied to a soil-solute system boundary value problem to analyze the effect of spatial variability of hydraulic conductivity on solute dispersion. The analysis was performed by generating realizations of the saturated hydraulic conductivity field, assuming each realization was an equally likely representation of actual soil heterogeneity. The major limitations of this technique, however, are that it has a high computer cost, it may produce erroneous results because of numerical dispersion errors, and deterministic boundary conditions affect the solution due to the statistical nonhomogeneities at the system's boundaries. Application of the spectral analysis approach (Gelhar, Gutjahr, and Naff 1979) eliminates numerical errors, due to the analytic nature of solution, and is applicable to infinite domains. In this approach, the variables in the partial differential equations are written in as expressions of a mean and a perturbation. The Fourier-Stieltjes integral is then used to transform the governing equations to the spectral domain, where a solution can be obtained.

FUTURE APPLICATION: EXTENSION TO STOCHASTIC SYSTEM MODELING APPROACH

Perhaps the most important finding of this study is that the spatial variability of hydraulic conductivity must be considered in the modeling of solute transport in unsaturated soils. Stochastic solute transport modeling approaches provide the means of handling the spatial variability in model parameters, assuming that they are realizations of a random process with some known probability density function. To apply this approach to field problems requires that observations on hydraulic conductivity be made with sufficient spatial detail so that the statistical parameters of the model (i.e., the mean, variance, and correlation structure) reflect the intrinsic soil variability. However, such intensive data collection, necessary to maintain the desired accuracy of the modeling results, may be a very costly effort. An alternative approach that does not require a high-density data base is based on stochastic system modeling approaches, which assume that the exact spatial variability in the hydrodynamics of the system is unknowable and the output variations are constructed on the basis of hereditary processes (Distefano 1974). By taking this approach, the output concentration levels for given input concentration values are established by a stochastic transfer function model that describes the system spatial variability by use of a probability density function. As an extension of the work presented in this report, future research will include evaluation of stochastic system modeling approaches for the simulation of solute transport in heterogeneous soils. The advantage of the system modeling approach in the prediction of contaminant transport through soils is obvious: it has superior computational efficiency and limited data requirements. However, a thorough evaluation of the approach must be performed in comparison with a physically based approach before its direct application to field problems is possible.

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