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The Distributed Source Problem

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ABSTRACT

This report presents a new methodology to model the time and space evolution of groundwater variables in a system of aquifers when certain components of the model, such as the geohydrologic information, the boundary conditions, the magnitude and variability of the sources or physical parameters are uncertain and defined in stochastic terms. This facilitates a more realistic statistical representation of groundwater flow and groundwater pollution forecasting for either the saturated or the unsaturated zone. The method is based on applications of modern mathematics to the solution of the resulting stochastic transport equations. This procedure exhibits considerable advantages over the existing stochastic modeling techniques. In particular, the semigroup solutions are not restricted to small variances in the stochastic elements (perturbation techniques), unsteady dynamic conditions are specifically considered, time and space randomness may be considered in the sources, the boundary conditions or the parameters, and the methodology reflects a well-posed functional-analytic theory. Several basic example problems are presented in order to illustrate the application of the methodology to the modeling of complex spatially and temporally distributed sources of interest in engineering hydrology today. Further potential applications of the method are very promising, including the modeling of non-conservative contaminants in groundwater systems.

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LIST OF SYMBOLS

A A partial differential operator.

$A(\omega)$ A random operator.

B a Borel field.

C Contaminant concentration.

C_0 Initial concentration.

C_1, C_2 Contaminant Concentration.

$Cov\{.\}$ Covariance operator.

d^n $n-$ th ordinary derivative.

D^k $k-$ th partial weak derivative.

D Spatial domain. A partial differential operator. Dispersion Coefficient. Soil-water diffusivity.

D_1, D_2 Longitudinal and transversal dispersion coefficient, respectively.

$\overline{D}$ Mean dispersion coefficient or soil diffusivity.

D' Random part of dispersion coefficient.

$D^k f$ $k-$ th order derivative of f.

$E\{.\}$ Expectation operator.

$erf(\ )$ Error function.

$erfc(\ )$ Error function complement.

f A functional. A distribution.

$|\ f\ |$ Absolute value of f.

$\|\ f\ \|$ Norm of f.

$\|f\|_0$ "Zero" norm or L_2- norm of f.

$\|f\|_\Omega$ Norm of f in the sense of Hilbert space $L_2(\Omega)$.

$(f, g)_\Omega$ Inner product in the Hilbert space $L_2(\Omega)$ of random functions. It is also written as $E\{(f, g)\}$.

F A functional.

FC Field capacity.

g Forcing function, generally.

∂G The boundary of the G domain.

$g(x,t,\omega)$ Random forcing function, generally.

G Spatial domain in $\mathbb{R}^n$. Impulse response function.

h Piezometric head.

h_0 Initial piezometric head.

H Separable Hilbert space.

H_0^1 First - order Sobolev Space of first differentiable distributions with compact support.

$H^1(G)$ First order Sobolev space of all functions $f \in L_2(G)$ such that all the first partial derivatives belong to $L_2(G)$.

H^m $m-$ th order Sobolev space of second-order functions

H_0^m $m-$ th order Sobolev space with compact support.

I Identity operator.

i Subindex. Deep Percolation.

J_t A strongly continuous semigroup.

K Hydraulic conductivity.

ln Natural logarithm. L Aquifer length. Linear space.

$L_2(\Omega,P;H)$ Space of square-integrable random functions from $\Omega\times(.)$ into H.

L_2 Space of square-integrable distributions.

M Modal matrix.

min( ) Minimum operator.

N An integer. Number of storms in a period of time.

$p\{.\}$ Probability operator.

$P(.)$ A probability measure.

PET Potential evapotranspiration.

q Variance parameter.

$\hat{q}$ Estimate of parameter q.

Q A boundary operator.

R A random operator.

$sinh()$ Hyperbolic sine function.

S Specific storage. Spectral matrix.

t Time coordinate.

T Time domain. Aquifer transmissivity.

$\overline{T}$ Mean transmissivity.

U Vector of heads.

u_0 Initial condition of the system.

$u(t)$ State of the system at time t. Pore velocity.

$u(x,t,\omega)$ State of system at time t.

$u_0(x,\omega)$ Random initial condition.

v A function.

V A real separable Hilbert space. Steady state function.

V' The dual of V.

$V(x)$ Steady state function.

w White noise process.

x Spatial coordinate.

y Spatial coordinate.

Z Poisson sequence of pulses.

z Spatial coordinate.

β Brownian Motion process.

$\delta(\ )$ Dirac's delta function.

Σ Summation.

ω Sample elements of probability space Ω.

Ω Probability space.

Φ Deterministic component. First approxiamtion.

$\mathbb{R}$ One dimensional real space.

λ Eigenvalues. Boltzmann reduced variable.

∇ Gradient.

∇^2 Divergence.

θ Water content.

θ_0 Top boundary water content.

θ_{in} Initial water content.

ψ pressure head.

∂^n $n-$ th partial derivative.

π 3.1415...

$\mathbb{R}^n$ $n-$ th dimensional real space.

$\mathbb{R}$ One dimensional real space.

∂ Partial derivative.

σ^2 Variance.

$\subset$ Subset of.

∞ Infinity.

$\int$ integral operator

CHAPTER I - INTRODUCTION:

Modeling Non-Point Sources in Groundwater

We begin by stating the specific objectives of the research: (1) To derive a new mathematical modeling procedure to analyze and forecast distributed source problems in groundwater liquid and solid transport. (2) To develop new solutions of transport partial differential equations in porous media when the forcing functions, the parameters, the initial conditions and the boundary conditions are uncertain functions defined in stochastic terms.

Let us discuss first the relation between the research objectives and the current modeling needs of distributed source problems in groundwater. Practical engineering problems involving groundwater transport modeling today require the prediction of the time and space evolution of a principal contaminant in an aquifer due to a particular contamination source. The accurate forecast of the concentration magnitude facilitates the design of appropriate preventive or remedial measures. The time and space evolution of a contaminant plume in a system of aquifers is theoretically, and ideally, predicted by a solution of the advective-dispersive partial differential equation in porous media subject to an appropriate set of boundary conditions and source functions. Solving this equation for the concentration distribution subject to the several physical and chemical uncertainties in the phenomenon of mass transport in aquifers and the insufficiency of hydrogeological and hydrochemical information is one of the main difficulties in engineering hydrology today (Fried, 1975; Anderson, 1979; Simmons, 1982; Matheron and De Marsily, 1980; Dagan and Bresler, 1979). The literature reports the innaccuracy of deterministic models in predicting contamination in situations when the parameters, the boundary conditions, and the pollution sources are difficult to measure or when they vary erratically in space and time. Modeling of reactive transport poses serious difficulties to the hydrologic community because of the ina-

bility of deterministic functions to represent the wide spectrum of variability of a non-conservative contaminant. It has also been reported the large differences between laboratory-measured dispersion coefficients and the corresponding field scale values. This discrepancy tends to increase as time or distance from the source increases (Smith and Schwartz, 19080; Sudiky, 1986).

As a result of the above difficulties, some limited stochastic modeling techniques attempting to describe an uncertain quantity in stochastic terms have emerged (Tang et al., 1982; Schwartz, 1977; Gelhar et al., 1979; Simmons, 1982; Matheron and De Marsily, 1980; Sudiky and Cherry, 1979; Dagan, 1982; Gelhar and Axness, 1983; Dagan, 1984; Warren and Skiba, 1964; Winter et al., 1984). While these stochastic methods have provided insight on the phenomenon of mass transport in aquifers, several inconsistencies and deficiencies have been noted, which can be related to the limitations of the mathematical procedures employed (Smith and Schwartz, 1980).

The main limitation of the existing stochastic methods relates to the assumption of small randomness required by the perturbation expansion solutions. The existing methods can only handle randomness in one quantity, and as a result the hydraulic conductivity has been assumed as the only source of uncertainty. The effect of randomness in the time or spatial distribution of the sources, randomness in the boundary conditions, or the randomness in the environmental evolution of the system has not been studied. In some cases the applications are limited to steady state asymptotic conditions of the concentration field and the dynamic features of the system have not been considered (i.e, Gelhar and Axness, 1983). Some of the apparent stochasticity in the hydraulic conductivity may be generated by small scale measurement approaches, and their unavoidable errors, to large scale contaminant migration as may be seen in the recent field work (Sudiky, 1986). Some of the approaches use Montecarlo simulations, which are expensive and empirical (i.e., Smith and Scwartz, 1980). Some of the existing modeling methods only provide information about the concentration variance,

without a description of the form of sample functions, different correlation functions and higher order moments, which would give a better information of the stochastic properties of the concentration process. Finally, the existing methods are in a sense parameter estimation techniques rather than methods to obtain explicit solutions for engineering forecasting purposes.

There is a strong need for a general modeling methodology capable of predicting the stochastic properties of the concentration distribution, given the stochastic properties of the uncertain quantities. This methodology should be able to handle arbitrary large variances, randomness in any component of the differential equation, unsteady conditions, and be based on a well-posed mathematical theory. This general modeling procedure would allow engineers, designers and planers to obtain a broad picture of the concentration evolution by identifying the relative importance of the different uncertain quantities and forecasting the general properties of the concentration field in a more realistic statistical sense. It is the main purpose of the present research report to present such new general methodology.

The proposed methodology is based on the application of modern mathematics to the solution of stochastic transport equations (Bensoussan, 1977; Chow, 1979; Curtain and Falb, 1971; and Sawaragi et. al. 1978, among others). The solutions are obtained by blending some developments on the theory of stochastic partial differential equations in Hilbert spaces, the theory of stochastic evolution equations, and the theory of semigroups of operators with some classical results on the heat flow (diffusion) equation. These works have defined a functional-analytic framework to study many stochastic equations in mathematical physics. Applications of these concepts to the modeling of stochastic groundwater flow have generated important results (Serrano and Unny, 1987(2); Serrano and Unny, 1986; Serrano et al., 1985(1), 1985(2) and 1985(3)). It is the aim of the present research report to present a modeling procedure for the more complex cases of solid and liquid transport in the saturated and the unsaturated zone

when the parameters, the boundary conditions or the sources are uncertain non-point functions of space and time.

In what follows I assume that the advective-dispersive equation subject to some form of stochasticity is an appropriate form of modeling the dispersion phenomenon in porous media for certain regional-scale pollution problems. I do not discuss here the methods to derive transport equations, which are treated in detail elsewhere (i.e., Cushman, 1987). In chapter II a general mathematical statement of the distributed groundwater pollution modeling problem is made. The relevant functional-analytic results leading to a new general solution of the differential equations is presented. The emphasis is on applications and the description is concentrated on main results. Therefore, theoretical aspects of existence and uniqueness of solutions, topological properties of solutions spaces and theorems have been omitted. In chapter II several application cases of modeling groundwater transport subject to different forms of uncertainty are shown in detail. These applications are chosen to satisfy the current needs in groundwater modeling and to illustrate the potentiality of the method in more complex cases.

CHAPTER II - RESEARCH PROCEDURES:

Mathematical Statement and Solution of Distributed Groundwater Transport

We begin our analysis by considering the problem of contamination of a shallow phreatic aquifer due to an industrial waste disposal pond which fully penetrates the aquifer. Assume that the chloride concentration in the pond varies erratically with time because industrial discharges are made randomly in time, and it is therefore difficult to describe them in deterministic terms. The groundwater velocity has been found to be fairly uniform, but the measured values of the aquifer dispersion coefficient are far from being constant and measurement errors are important. Finally it is known from the geology of the area that the main contaminant may react in certain places because of local aquifer chemical constituents, and all attempts at finding a fixed reaction function have failed. The objective of the modeling tasks is to predict the migration of a main contaminant, such as the chloride concentration, along the main groundwater flow direction with the aim of closing the site if the concentration levels reach certain maximum permissible levels for some drinking water wells located some distance downstream.

The modeling problem of this realistic example poses serious difficulties because of the uncertain functions. We choose the advective-dispersive differential equation in a semi-infinite aquifer subject to a plane source at the origin and assume that it is valid for the problem in question. Assuming that the porous media is homogeneous and isotropic, and that the average groundwater velocity is constant throughout the length of the flow field, the differential equation is obtained after applying the divergence theorem to an integral equation statement of mass conservation in a control aquifer volume, and combining this with the equation of the Fick's first law (Hunt, 1983). Because we have the source, the dispersion coefficient and the reaction term as uncertain random functions, the concentration distribution will also be random:

$$\frac{\partial C}{\partial t} - D(t, \omega)\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} = g(x, t, \omega), \tag{II.1}$$

subject to

$$C(0, t) = k(t, \omega); \quad C(\infty, t) = 0; \quad C(x, 0) = f(x),$$

where $C(x, t, \omega)$ is the stochastic process representing the concentration of the principal contaminant in the fluid (mgr/lit); $D(t, \omega)$ is the random process representing the aquifer dispersion coefficient (m^2/day); u is the average pore velocity, that is the flux velocity divided by the average porosity of the media (m/day); x is the coordinate parallel to the flow; t is the time coordinate; $k(t, \omega)$ is the time-dependent concentration at the origin (mgr/lit); $f(x)$ is the initial concentration distribution across the aquifer (mgr/lit); and $g(x, t, \omega)$ is the stochastic function representing the reaction term. Assume that the stochastic components are well-behaved and obtained after repetitive sampling in the aquifer and the pond

The modeling problem reduces to the solution of eq.(II.1) subject to the known random functions g, k and D and the boundary and initial conditions. By a solution we mean finding expressions for sample functions and some of the moments of the concentration function which would better characterize the concentration distribution than a single deterministic function. However, one may soon realize that it is not possible to obtain a solution of eq.(II.1) using the current perturbation or hierarchy techniques because these methods do not allow more than one random process or large variances (Adomian, 1983). In the search of better methods, we propose to use existing results of modern mathematics which will allow us to solve more general and more complex problems than the one being described.

We now consider the general stochastic groundwater pollution model. For the sake of notational economy, rigorousness, flexibility and generality, let us write in abstract functional-analytical terms the general three-dimensional stochastic advective-dispersive equation in porous media as a stochastic evolution equation of the

form

$$\frac{\partial u}{\partial t}(x,\ t,\ \omega) + A(x,\ t,\ \omega)u = g(x,\ t,\ \omega), \qquad (x,\ t,\ \omega) \in G \times [0,\ T] \times \Omega \tag{II.2}$$

$$Q(x,\ t,\ \omega)u = F(\omega), \qquad (x,\ t,\ \omega) \in \partial G \times [0,\ T] \times \Omega$$

$$u(x,\ 0,\ \omega) = u_0(x,\ \omega), \qquad (x,\ \omega) \in G \times \Omega$$

where $u \in L^2(0,\ T;\ V)$ is the system output; $g \in L_2(\Omega,\ B,\ P)$ is a second order random forcing function; $G \subset \mathbb{R}^3$ is an open domain subset of the three-dimensional real space with boundary ∂G; $0 < T < \infty$; Q is a boundary operator; Ω is the basic probability sample space of elements ω; $L_2(\Omega,\ B,\ P) = L^2(\Omega)$ is the complete probability space of second-order random functions with probability measure P and B Borel field or class of ω sets; x represents three-dimensional spatial domain; A is an m-th order random partial differential operator in space $H^m(G)$ and it is given by

$$Au = \sum_{k\ ,\ l \leq m} (-1)^{\ k}\ D^k(p_{kl}(x,\ t,\ \omega)D^l u),$$

where D is differentiation; $p_{kl}(x,\ t,\ \omega)$ are randomly-valued stochastic processes representing the system parameters, which are assumed bounded and mean- squared continuous on $[0,\ T]$; m is the order of the space; the space

$$L^2(0,\ T;\ V) = \{f{:}[0,\ T] \longrightarrow V{:} \int_0^T \|f\|_V^2\ dt < \infty\},$$

for $0 < T < \infty$; $V = H^m$ is the Sobolev space of order m of $L^2(\Omega)$- valued functions; $V \subset H \subset V'$, V is dense in H, where $H = H^0$; the norm on V is denoted by $\|\ \ \|_V$; V' is the dual of V; $g \in L_2(0,\ T;\ V')$; and $u_0 \in H \times \Omega$ is the system initial condition. For a more complete description of the above definitions the reader is referred to the available functional-analytic literature (i.e., Griffel, 1981; Hutson and Pym, 1980; Oden, 1977; Showalter, 1977; Sawaragi et al., 1978; Bensoussan, 1977).

Theorems and proofs concerning the existence and uniqueness the solution to a system given by eq.(II.1) have been extensively treated in Sawaragi et al., 1978; Bensoussan, 1977; Chow, 1979; and Curtain and Falb, 1971, among others.

Randomness may enter the system given by eq.(II.2) in the following ways: (i) The random initial value problem, when u_0 is random. (ii) The random boundary value problem, when F is random. (iii) The random forcing problem when g is random. (iv) The random operator problem, when A or Q is random. (v) The random geometry problem. It is the task of the modeler to determine which of the above cases represent the field problem and what are the most important or dominant random processes since the higher the number of random components, the more complex the problem is. For cases (ii) and (iii) above, the operator A is deterministic and in many practical applications it is a time-independent operator. This situation will arise when the parameters are deterministic functions independent of time. For example let us assume that this is the case in eq.(II.2), that the only uncertainty is due to the forcing term, and that the boundary conditions are deterministic. We would then transform the functional spaces for u in eq.(II.2) into an equivalent one for v in which the system has homogeneous boundary conditions, and the solution of the resulting evolution equation would be

$$v(t) = J_t v_0 + \int_0^t J_{t-s} h(x, s, \omega) ds, \tag{II.3}$$

where $v \in L^2(0, T; V)$ is the system output; $V = H_0^m$ is a closed subspace of H^m; H_0^m is the closure of $C_0^\infty(G; L^2(\Omega))$ in H^m, that is, H_0^m is the m-th order Sobolev space of second-order random functions with compact support; $h(x, t, \omega)$ includes the function $g(x, t, \omega)$ and the appropriate function(s) resulting from the space transformation, including the boundary conditions; $v_0(x)$ includes $u_0(x)$; $J_t \in l(H, H)$ is the evolution operator associated with A (Custain and Pritchard, 1978; Ladas and Lakshmikantham, 1972; Butzer and Berens, 1967). If a transformation of spaces is not done, it is clear

that the operator must satisfy the prescribed boundary conditions. If the operator A is time independent and if the evolutional operator J_t in the Hilbert space H satisfies:

(i) $J_{t+s} = J_t J_s \geq 0$,

(ii) $J_0 = I$, where I is the identity operator, and

(iii) $\| J_t v - v \|_H \longrightarrow 0$ as $t \longrightarrow 0$ for all $v \in H$,

where $\| \quad \|$ denotes the norm, then J_t is said to be a strongly continuous semigroup. Properties (i) and (ii) above give the semigroup structure, whereas property (iii) is topological and defines the "strong continuity".

Theoretically, we may be interested in finding the joint distribution function of all orders that characterize the process v. This task is frequently too complicated and in many situations represents more than is needed. We often can consider simpler and necessarily less complete characterizations in the form of expectations, dispersions, covariances, joint moments, etc., which are called statistical measures. This view is supported by the fact that it is usually not feasible to collect enough field information to evaluate the joint probability density function of the input processes and the parameters. Therefore, from the practical point of view, it is possible to calculate only the first few low order moments of the solution process v. The first two moments give considerable information of the joint probability density function of v.

The mean value of v is given by

$$E\{v(x, t)\} = J_t v_0 + \int_0^t J_{t-s} E\{h(x, s, \omega)\} ds, \tag{II.4}$$

where $E\{\ \}$ denotes the expectation operator.

Now the second moment of v in eq.(II.3) is given by

$$E\{v(t_1)v(t_2)\} = E\{\ [J_{t_1} v_0 + \int_0^{t_1} J_{t_1-s} h(s) ds] \cdot [J_{t_2} v_0 + \int_0^{t_2} J_{t_2-\xi}\ h(\xi) d\xi]\ \}, \tag{II.5}$$

where ω has been omitted for convenience. Without loss of generality we assume that

h is a zero mean stochastic process. This is the result after a deterministic model has been optimized. Thus the second term in eq.(II.4) is equal to zero and eq.(2.5) becomes

$$E\{v(t_1)v(t_2)\} = J_{t_1+t_2}v_0 + \int_0^{t_1}\int_0^{t_2} J_{t_1+t_2-s-\xi}E\{h(s)h(\xi)\}dsd\xi. \qquad \text{(II.6)}$$

Note that the calculation of eq.(II.6) requires knowledge of the correlation of h and that towards this end should the field measurements be oriented. Higher order moments may be easily calculated in a similar way.

If the operator A in eq.(II.2) is stochastic because one or more of the parameters is defined as a stochastic process, then is a non-linear stochastic partial differential equation which in general has no exact solution. We follow in this case a procedure similar to the one used in [1] to decompose an ordinary stochastic differential operator into an infinite series in order to approximate the corresponding stochastic Green's function. We shall present a semigroup formulation for a general stochastic partial differential operator, such as the one introduced by Serrano and Unny (1987(1)) for the groundwater flow equation subject to stochastic transmissivity.

Let us write the operator A as

$$A(x, t, \omega) = A(x) + R(t, \omega), \qquad \text{(II.7)}$$

where $A(x)$ is the deterministic, time independent, component and $R(t, \omega)$ the random part or the portion of the partial differential operator containing the random in time parameters. It is clear that this time stochastic representation is equally valid for spatial stochasticity and that we prefer for now to solve the advective-dispersive equation with time stochastic parameters. Substituting eq.(II.7) into eq.(II.2), placing R in the write hand side and assuming for simplicity that g and k are equal to zero, we have a randomly forced equation again whose solution is

$$v = J_t v_0 + \int_0^t J_{t-s}h(s)ds - \int_0^t J_{t-s}Rv(s)ds \qquad \text{(II.8)}$$

It is not possible to solve eq.(II.8) explicitly because v is in the right hand side. Now we decompose v in the right hand side as an infinite series $v = \sum_{i=1}^{\infty} v_i$. Eq.(II.8) becomes

$$v = J_t v_0 + \int_0^t J_{t-s} h(s) ds - \int_0^t J_{t-s} R(v_1 + v_2 + v_3 + ...) ds \tag{II.9}$$

where the semigroup J is now deterministic. Identifying v_1 as the preceding term $\int_0^t J_{t-s} v(s) ds$, we can determine each v_i in terms of the preceding v_{i-1}. Thus

$$v = J_t v_0 + \int_0^t J_{t-s} h(s) ds + \int_0^t \int_0^s J_{t-s} R J_{s-\tau} h(\tau) d\tau ds \tag{II.10}$$

$$- \int_0^t \int_0^s \int_0^\tau J_{t-s} R J_{s-\tau} R J_{\tau-\xi} h(\xi) d\xi d\tau ds - \ldots,$$

where the last term in the series contains v. The basic idea here is that a random semigroup operator, which may be difficult to derive in particular cases, can be determined in an easily computable series by decomposition of the differential operator $A(x, t, \omega)$ into a deterministic operator $A(x)$ whose semigroup is known or found with little effort, and a random operator $R(t, \omega)$ whose contribution to the total semigroup $J_{t,\omega}$ modification can be found in series form. The convergence question will not be treated here, since it has been discused elsewhere (Adomian, 1983).

The mean value of v is obtained by truncating eq.(II.13) and taking expectations:

$$E\{v\} = J_t v_0 + \int_0^t J_{t-s} E\{h(s)\} ds - \int_0^t \int_0^s J_{t-s} E\{R J_{s-\tau}\} E\{h(\tau)\} d\tau ds, \tag{II.11}$$

where statistical separability occurs between the semigroup and the forcing term. Physically this stems from the independent behaviour of the input function and the system parameters (i.e., there is not a functional relationship between the dispersion coefficient and the source terms).

Similarly, the correlation function is given by

$$E\{v(t_1)v(t_2)\} = E\{\ [J_{t_1}v_0 + \int_0^{t_1} J_{t_1-s}h(s)ds - \int_0^{t_1}\int_0^{s} J_{t_1-s}RJ_{s-\tau}h(\tau)d\tau ds] \qquad \text{(II.12)}$$

$$\cdot[J_{t_2}u_0 + \int_0^{t_2} J_{t_2-\rho}h(\rho)d\rho - \int_0^{t_2}\int_0^{\beta} J_{t_2-\beta}RJ_{\beta-\gamma}h(\gamma)d\gamma d\beta]\ \}$$

Assuming h a zero-mean temporal stochastic process and solving,

$$E\{v(t_1)v(t_2)\} = J_{t_1+t_2}v_0^2 + \int_0^{t_1}\int_0^{t_2} J_{t_1+t_2-s-\rho}E\{h(s)h(\rho)\}dsd\rho \qquad \text{(II.13)}$$

$$-2\int_0^{t_1}\int_0^{t_2}\int_0^{\beta} J_{t_1+t_2-s-\beta}E\{RJ_{\beta-\gamma}\}E\{h(s)h(\gamma)\}d\gamma d\beta ds$$

$$+\int_0^{t_1}\int_0^{t_2}\int_0^{s}\int_0^{\beta} J_{t_1+t_2-s-\beta}E\{RJ_{s-\tau}RJ_{\beta-\gamma}\}.E\{h(\tau)h(\gamma)\}d\tau ds d\gamma d\beta,$$

These are the results obtained by considering one term v_1 in the series of eq.(II.9). Obviously calculations can be extended up to a desired degree of accuracy by considering more terms. However, it is known that the series converges rapidly and that in some circumstances considering one term is sufficiently accurate, as demonstrated by the sensitivity analysis on the semigroup for the stochastic boussinesq equation in groundwater flow presented by Serrano, and Unny (1987(1)).

In the chapter III, I shall illustrate the application of the above theory to the modeling of groundwater flow and pollution in engineering problems. The example problems show the solution of special cases of eq.(II.1) which appear in applications. The emphasis is on the illustration of the methodology rather than on the routine modeling steps. I use a well-known stochastic process in the applications, namely the White Gaussian Noise. This is done for simplicity and because the properties of this process closely resemble many physically-realizable processes after the deterministic

trend has been removed. It is clear, however, that any process in $L_2(\Omega)$ could be used, the properties of which should be derived from sample field measurements followed by an estimation algorithm (i.e., Godambe and Thompson, 1984). Other more "realistic" random process I use in the applications, particularly in spatially random problems, is the colored-Gaussian noise, which offers a generalization of correlated processes often found in the field.

CHAPTER III - APPLICATION PROBLEMS:

III.1. Modeling Contamination at a Well Subject to Measurement Errors

In chapter II we described a contamination problem in a shallow phreatic aquifer due to a pond receiving industrial waste. Suppose the facility is new and that due to budgetary restrictions, only one monitoring well was drilled. After studying the average amplitude of the chloride concentration in the pond it was decided to locate this well at a distance from the pond X such that the random variations in the boundary condition could be neglected and replaced by their average value C_0. Assume also that the uncertainty in the dispersion coefficient is minimum, and that the reaction term is negligible. However, the instrumentation used in measurement concentration is rudimentary and the individuals performing the measurement are not experienced, in which case there are important errors in the concentration. The modeling problem reduces to predicting the concentration at the well over time. The modeling equation will be eq.(II.1) with a constant source boundary condition $k = C_0$, an initial condition $C(x, 0) = 0$ and a forcing term at the well $g(X, t, \omega) = w(t)$.

We now assume that we may express C as the superposition of two problems:

$$C(x, t, \omega) = C_1(x, t, \omega) + C_2(x, t), \tag{III.1}$$

where C_1 is the solution to the differential equation satisfying the random forcing term and $C_2(x, t)$ is the solution to the differential equation satisfying the deterministic boundary condition. In this case, the operator A in eq.(II.1) such that

$$AC = (-D\frac{\partial^2}{\partial x^2} + u\frac{\partial}{\partial x})C$$

generates a strongly continuous semigroup J_t given by

$$J_t f(x) = \frac{1}{(4\pi Dt)^{1/2}} \int_0^\infty \{ \exp[-\frac{(x - ut - s)^2}{4Dt}] - \exp[-\frac{(x - ut + s)^2}{4Dt}] \} f(s)ds. \tag{III.2}$$

This is easy to see by analogy of eq.(II.1) with the classical heat flow (diffusion) equation (Cannon, 1984; Zauderer, 1983; Li, 1972; Carslaw and Jaeger, 1971;Crank, 1979). It is easy to show that J_t in this case is a strongly continuous semigroup with the properties of semigroups described in section 2 ([6]). These properties permit the calculation of the concentration at time $t+\tau$, knowing some intermediate concentration at time t. Most importantly, knowing the form of the semigroup we may obtain the solution of our differential equation. For the random component of the solution we have, according to eq.(II.3),

$$C_1(x,\, t,\, \omega) = J_t f(x) + \int_0^t J_{t-\tau} w(\tau) ds \tag{III.3}$$

or

$$C_1(x,\, t,\, \omega) = \int_0^t \frac{w(\tau,\, \omega)}{(4\pi D(t-\tau)^2} \int_0^\infty \{ \exp[-\frac{(x-u(t-\tau)-s)^2}{4D(t-\tau)}] \tag{III.4}$$

$$- \exp[-\frac{(x-u(t-\tau)+s)^2}{4D(t-\tau)}] \} ds d\tau.$$

From this expression we can generate sample functions of the process C_1 if sample functions of the process w are available. Sample functions are useful for testing models and for observing the qualitative behaviour of the system due to different types of excitations. Statistical properties of the process C_1 may be calculated by applying eqs.(II.4) and (II.6), as we shall show.

Now the solution of the deterministic component in eq.(III.1) may be approached in two ways: As stated in section 2, We may transform our functional space $H^1(0,\, \infty)$ into a Sobolev space with compact support $H_0^1(0,\, \infty)$ by defining C_2 in terms of a smooth function satisfying the boundary conditions and replacing it into the differential equation. This procedure will generate a forcing term and the problem can be solved as above by using the concepts of semigroups. The second approach results

after applying the Fourier transformation to a reduced differential equation and produces the same solution. Since this classical solution already exists in the literature, we will use it (Mariño, 1974; Ogata and Banks, 1961):

$$C_2(x,\,t) = \frac{x}{(4\pi D)^{1/2}} \int_0^t \exp[-\frac{(x-u(t-\tau))^2}{4D(t-\tau)}] \frac{C_0}{(t-\tau)^{3/2}} d\tau. \tag{III.5}$$

Since C_0 = is a constant, eq.(III.5) becomes (Ogata and Banks, 1961)

$$C_2(x,\,t) = \Phi(x,\,t) = \frac{C_0}{2} \{erfc[\frac{x-ut}{(4Dt)^{1/2}}] + \exp(\frac{ux}{D}) erfc[\frac{x+ut}{(4Dt)^{1/2}}]\}, \tag{III.6}$$

where $erfc(\ )$ denotes the "error function complement" given by

$$erfc(z) = \frac{2}{\pi^{1/2}} \int_z^\infty e^{-\xi^2} d\xi.$$

Simplifying the inner integral in eq.(III.4), and replacing eqs.(III.4) and (III.6) into eq.(III.1) we find the general solution of our model differential equation:

$$C(x,\,t,\,\omega) = \Phi(x,\,t) + \int_0^t erf[\frac{x-u(t-\tau)}{4\pi D(t-\tau)}] w(\tau,\,\omega) d\tau. \tag{III.7}$$

As an illustration of the behaviour of the solution, assume that the process $w = \frac{d\beta(t)}{dx}$ has been identified as a White Gaussian Noise process in time with the properties

$$E\{w(t)\} = 0, \qquad E\{w(t_1)w(t_2)\} = q\delta(t_2 - t_1), \tag{III.8}$$

where q is the variance parameter ($\frac{mgr}{lit.day}$) and $\delta(\ )$ is the Dirac's delta function. This would indicate that the randomness in the system comes from non-systematic measurement errors due to the limitations of the instrumentation and the data processing.

Now taking expectations on both sides of eq.(III.7) and using eq.(III.8) we find the mean concentration to be

$$E\{C(x,\,t)\} = \Phi(x,\,t). \tag{III.9}$$

Now following eqs.(II.6), (III.7) and (III.8), the second moment of C is

$$E\{C(x,t_1)C(x,t_2)\} = \Phi(x,t_1)\Phi(x,t_2) \tag{III.10}$$

$$+ q\int_0^{t_1}\int_0^{t_2} erf[\frac{x-u(t_1-\tau)}{(4D(t_1-\tau))^{1/2}}]erf[\frac{x-u(t_2-\xi)}{(4D(t_2-\xi))^{1/2}}]\delta(t_1-t_2)d\xi d\tau.$$

If we let $t_1 = t_2 = t$ and subtract the square of the mean, eq.(III.10) becomes the variance of C:

$$\sigma_c^2 = q\int_0^t erf^2[\frac{x-u(t-\tau)}{(4D(t-\tau))^{1/2}}]d\tau. \tag{III.11}$$

In order to have a quantitative observation of the above solution, eqs.(III.7), (III.9) and (III.11) were programmed in the micro-computer and numerical values of the mean concentration, a sample function and the standard deviation of the concentration with time where computed. An average pore velocity $u = 0.2\ m/day$, a dispersion coefficient $D = 0.1\ m^2/day$, a concentration at the origin $C_0 = 10.0\ mgr/lit$, and a variance parameter $q = 0.01$ were assumed. The value of q is entirely arbitrary here. It is clear that the actual value should be determined from field measurements and an estimation algorithm (see for example Godambe and Thompson, 1984). The integrals were numerically. Fig. III.1 is a digital plotter output of the program for a well located $X = 6.0\ m$ from the pond. The solid line represents the evolution with time of the mean concentration, the continuous sinuous line represents the sample concentration, and the dotted lines represent the mean concentration plus and minus one standard deviation respectively. For high values of t, the calculations are more efficient if the differential equation is solved step wise with the output from one step becoming the initial condition to the next one. This procedure could be easily adapted to eq.(III.7).

The implications of the above results are crucial. The mean concentration coincides with the deterministic solution, whereas the sample concentration oscillates above and below the mean concentration with and increasing departure from the mean as

time increases. The exact measurement of the dispersion around the mean is given by the standard deviation function, which clearly shows a direct monotonic increasing magnitude with time. Thus the results indicate a Brownian type of behaviour of the concentration with a continuously increasing variance value, as one might have expected. This increasing departure between model values and measured values has been acknowledged in the hydrologic literature (Smith and Schwartz, 1980; Sudiky and Cherry, 1979) as one of the difficulties in using the existing models. Thus we may conclude that a model such as the one presented replicates concentration distribution values with the same characteristics of the ones measured in the field.

Validation of the above model can be performed by comparing the statistical measures of the predicted concentration process at the well with the sample statistical measures of the concentration values measured at the well. When the set of predicted measures approach the corresponding observed measures the model is validated. This is a "weak" validation procedure though, and we know that a complete model validation may never be accomplished, since the ergodic assumption in the input stochastic quantities does not necessarily imply ergodicity in the output processes.

With a validated model as above, we may predict the concentration stochastic properties at the well or at any other drinking water well downstream. The model can be used to assess the risk of contamination in a more realistic statistical sense.

III.2. Modeling of Non-Conservative Contaminant Migration

Consider the groundwater modeling problem depicted in chapter II and assume that the most important source of uncertainty comes from the difficulty in identifying a fixed deterministic function representing the spatial erratic variation in the main contaminant concentration due to the reaction between the main contaminant and the chemical constituents of the aquifer porous media. For the purpose of the present

illustration, assume that other sources of uncertainty can be neglected, or are very small in magnitude with respect to the reaction term uncertainty. The modeling equation is eq.(II.1) with the uncertain term appearing as a spatially random forcing function $g(x, \omega) = w(x)$, a constant source at the origin $k = C_0$, and with initial condition $C(x, 0) = 0$. We assume that the deterministic trend in the reactive term has already been removed and that we may represent the purely random component of this term as a White Gaussian Noise process in space and smooth in time $w(x) = \frac{d\beta(x)}{dx}$ with the properties given by eq.(III.8) with the dependent variable x instead of t. It is clear that the actual properties of the uncertain term will have to be obtained after an analysis of field concentration measurements along x and an appropriate ergodic assumption.

The solution to the differential equation in this case is given by eq.(III.1), where C_2 is given by eq.(III.6) and C_1 is obtained from eqs.(II.3) and (III.2) as

$$C_1(x,t,\omega) = \int_0^t \frac{1}{(4\pi D(t-\tau)^{1/2}} \int_0^\infty \{ \exp[-\frac{(x-u(t-\tau)-s)^2}{4D(t-\tau)}] \qquad \text{(III.12)}$$

$$- \exp[-\frac{(x-u(t-\tau)+s)^2}{4D(t-\tau)}]\} w(s,\omega) ds d\tau.$$

Eq.(III.12) may be simplified for the calculation of sample functions by defining the sample functions of the w process as a limiting form of the random walk process (Papoulis, 1984). Thus we may define the sample functions of the w process as staircase functions with constant values within each interval. The interval length is a modeling decision problem which depends on the availability of the sample data for w and the scale of the problem. For the purposes of this example, we will assume the interval length to be equal to one. Thus, w may be approximated as a step function $w_i(x)$, such that w_i is constant for $i - 1 < x < i + 1$. Thus eq.(III.12) may be written as

$$c_1(x, t, \omega) = \sum_{k=0}^{k=t} \sum_{i=1}^{N} w_i M_i(t - k), \qquad \text{(III.13)}$$

where N is a suitable truncation index, The function M_i is given by

$$M_i(t-k) = \frac{1}{(\pi b)^{1/2}} \int_{i-1}^{i} \{\exp[-\frac{(a-s)^2}{b}] - \exp[-\frac{(a+s)^2}{b}]\} ds, \qquad \text{(III.14)}$$

where $a = x - u(t-k)$, and $b = 4D(t-k)$. This equation can be written as

$$M_i(t-k) = \frac{1}{2}\{erfc(\frac{i-1-a}{b^{1/2}}) - erfc(\frac{i-a}{b^{1/2}}) - erfc(\frac{i-1+a}{b^{1/2}}) + erfc(\frac{i+a}{b^{1/2}})\}. \qquad \text{(III.15)}$$

Now the mean concentration is given by eq.(III.9), and the concentration variance for the case when $x_1 = x_2 = x$ can be deduced from eqs.(II.6), (III.1), (III.8) and (III.12) to be

$$\sigma_c^2 = q \int_0^t \int_0^t \frac{1}{4\pi D[(t-\tau)(t-\rho)]^{1/2}} \qquad \text{(III.16)}$$

$$\int_0^\infty \int_0^\infty \{\exp[-\frac{(x-u(t-\tau)-s)^2}{4D(t-\tau)} - \exp[-\frac{(x-u(t-\tau)+s)^2}{4D(t-\tau)}]\}$$

$$\cdot \{\exp[-\frac{(x-u(t-\rho)-\xi)^2}{4D(t-\rho)}] - \exp[-\frac{(x-u(t-\rho)+\xi)^2}{4D(t-\rho)}]\}\, \delta(s-\xi) ds d\xi d\tau d\rho.$$

Integrating with respect to ξ and solving the product of exponentials, we obtain two spatial integrals which may be manipulated into integrals of exponentials of second degree polynomials whose solutions are exact (Spiegel, 1968). Thus eq.(III.16) becomes

$$\sigma_c^2 = q \int_0^t \int_0^t \frac{1}{(4\pi b d m_1)^{1/2}} \qquad \text{(III.17)}$$

$$\{\exp(\frac{m_2^2 - 4m_1m_3}{4m_1}) erfc[\frac{m_2}{(4m_1)^{1/2}}] - \exp(\frac{g_2^2 - 4m_1m_3}{4m_1}) erfc[\frac{g_2}{(4m_1)^{1/2}}]$$

$$- \exp(\frac{h_2^2 - 4m_1m_3}{4m_1}) erfc[\frac{h_2}{(4m_1)^{1/2}}] + \exp(\frac{p_2^2 - 4m_1m_3}{4m_1}) erfc[\frac{p_2}{(4m_1)^{1/2}}]\} d\rho d\tau,$$

where $a = x - u(t-\tau)$, $b = 4D(t-\tau)$, $c = x - u(t-\rho)$, $d = 4D(t-\rho)$,

$$m_1 = \frac{b+d}{bd},\ m_2 = \frac{-2cb-2da}{bd},\qquad m_3 = \frac{da^2+bc^2}{bd},\qquad g_2 = \frac{2bc-2da}{bd},$$

$$h_2 = \frac{2da-2bc}{bd},\ \text{and}\ p_2 = \frac{2ad+2bc}{bd}.$$

Eqs.(III.1), (III.9), (III.13) and (III.17) where programmed in the computer in order to calculate the mean concentration, a sample function and the standard deviation of the concentration at particular times. In the computation of eq.(III.13) for the sample function a special flags system was created in order to detect the proper raising and falling limbs of the M_i's functions. Otherwise eq.(III.13) converges in 3 to 4 iterations to desired levels of accuracy. Generally the longer the time t at which the simulation was desired, the longer the CPU time required for the computation. Again this problem could be solved by solving the differential equation iteratively in short time intervals as explained before. Fig. III.2 shows an example of the simulations carried out at $t = 15$ *days*. The variation of either the mean, a sample function and the standard deviation of the concentration around the mean with respect to distance is represented. The same parameter values used in the previous application were inserted in the equations, except that the variance parameter was chosen as $q = 0.1$. The mean values coincide with the deterministic solution.

The results demonstrate the expected direct increase in the dispersion of the concentration around the mean with distance. This phenomenon has been noted in the hydrologic literature and it is interesting to observe that a model like this one may explain the stochastic nature of a set of field data whose erratic nature accounts for the reactive features of the main contaminant. However the most important result here indicates a direct increase in the statistical dispersion of the concentration around the mean with time. Although intuitively we should not expect time stochasticity because we are dealing with a disturbing space stochastic process, the results suggest that by disturbing the advective-dispersive equation with a spatial stochastic process, the output concentration function will be a space-time stochastic process. This may be easily

observed by studying the form of eq.(III.12). We may add that this phenomenon has not been mentioned in previous work related to the spatial stochasticity of the dispersion process and that assumptions ignoring the time stochasticity of the system are probably not appropriate. We may conclude that the problem of space-time stochasticity is a most interesting one and that much future research should be devoted to the analysis and implications of space-time stochasticity on the predictability of the concentration function. In particular, measurement efforts should be devoted to the identification of the random processes involved.

III.3. Investigating Pollution Variability Near a Source

Let us now consider the groundwater pollution problem of chaptyer II when the highest degree of uncertainty comes from the time variability of the concentration of the source at the origin and other uncertain terms are comparatively small. Assume that in this extremely practical case there is a high degree of uncertainty associated with the history of deposition of solid or liquid wastes in the pond, and that the objective of the modeling tasks is to predict the variability of the concentration near the pond. That is, some monitoring wells have been constructed a short distance from the pond and we wish to develop a model which would predict the random nature of the concentration at the wells. This will allow authorities to forecast the concentration values and to design and test remedial measures if appropriate. Assume that the average concentration in the pond tends to be a constant C_0 but there is a totally unpredictable component $w(t, \omega)$ derived from the illegal nature of waste dump site.

For the purpose of the illustration, assume that field measurements have demonstrated that the function w is described by a White Gaussian Noise process in time with the properties described by eq.(III.8). The governing differential equation is eq.(II.1) subject to a boundary source $k(t) = C_0 + w(t)$ and with the forcing function,

the parameters and initial condition equal to zero. From eqs.(III.1), (III.5) and (III.6), the general solution of the differential equation is given by

$$C(x,\,t) = \Phi(x,\,t) + \frac{x}{(4\pi D)^{1/2}} \int_0^t \exp[-\frac{(x - u(t-\tau))^2}{4D(t-\tau)}] \frac{w(\tau,\,\omega)}{(t-\tau)^{3/2}}\, d\tau. \qquad \text{(III.18)}$$

The mean concentration is $E\{C(x,\,t)\} = \Phi(x,\,t)$. By following a procedure similar to the above section one finds the variance of the concentration at time t to be given by

$$E\{C^2(x,\,t)\} = \sigma_c^2 = \frac{qx^2}{4\pi D} \int_0^t \frac{1}{(t-\tau)^3} \exp[-\frac{(x - u(t-\tau))^2}{2D(t-\tau)}]\, d\tau. \qquad \text{(III.19)}$$

As in the previous sections, eqs.(III.18) and (III.19) were used in the generation of sample functions, the calculation of the mean and the standard deviation of the concentration with respect to time. The sample function was calculated by generating a sample of w as a limiting random walk function for an interval of one day and solving eq.(III.18). The integrals were solved numerically and the singularities were treated by using the Gauss-Legendre quadrature method (Hornbeck, 1975).

Fig. III.3 shows the stochastic evolution of the concentration with respect to time for $x = 0.5\ m$. The mean concentration at the pond was assumed $C_0 = 1.0\ mgr/lit$. The variance parameter was chosen as $q = 0.01$ and the rest of the parameters as before. The results indicate that the effect of time stochasticity at the boundary decreases as the distance from the boundary increases for a zero-mean stationary process. This of course depends on the type and variance of the disturbing process, but in general the concentration variance approaches to zero beyond several meters of distance from the boundary and the process is then governed by the mean source concentration. This may indicate qualitatively that the effect of stochasticity of the boundaries is relatively less important than the effect of distributed-source stochasticity on the overall stochasticity of the concentration function.

III.4. Modeling Large-Scale Groundwater Pollution Under Uncertainty

A practical situation of uncertainty analysis in groundwater pollution arises when we wish to predict the evolution of the contaminant deep in a geologic formation. Consider the case of a deep well discharging a highly toxic liquid waste in a homogeneous consolidated sandstone. Secondary permeability with low values of hydraulic conductivity allows seepage through the rock and this poses the question of the long term effect of the contaminating source on the regional groundwater quality. Using a larger representative scale, the governing differential equation is the randomly-forced advective-dispersive equation in a three-dimensional domain subject to a point source at the origin. After eq.(II.1),

$$\frac{\partial C}{\partial t} - D_1\frac{\partial^2 C}{\partial x^2} - D_2\frac{\partial^2 C}{\partial y^2} - D_2\frac{\partial^2 C}{\partial z^2} + u\frac{\partial C}{\partial x} = \frac{d\beta(t)}{dt} \tag{III.20}$$

$$C(\pm\infty,\, y,\, z,\, t) = C(x,\, \pm\infty,\, z,\, t) = C(x,\, y,\, \pm\infty,\, t) = 0;$$

$$C(x,\, y,\, z,\, 0) = 0;\; C(0,\, 0,\, 0,\, t) = C_0,$$

where $C(x,\, y,\, z,\, t,\, \omega) \in H^1(R^3)$ is the stochastic process representing the concentration of a principal contaminant in the fluid (mgr/lit); D_1 is the longitudinal dispersion coefficient in the x direction (m^2/day); D_2 is the lateral dispersion coefficient in the y and z direction (m^2/day); u is the average pore velocity in the x direction; x, y, z are the the three-dimensional cartesian coordinates; C_0 is a constant point source at the origin; and $d\beta(t)/dt = w$ represents a White Gaussian Noise process in time disturbing the system and with the properties given by eq.(III.8).

We assume that the solution to this equation may be written as eq.(III.1), with x representing the three-dimensional coordinate system. The operator A, such that

$$AC_1 = (-D_1\frac{\partial^2}{\partial x^2} - D_2\frac{\partial^2}{\partial y^2} - D_2\frac{\partial^2}{\partial z^2} + u\frac{\partial}{\partial x})C_1$$

generates a strongly continuous semigroup given by

$$J_t f(x, y, z) = \frac{1}{8(\pi^3 D_1 D_2^2 t^3)^{1/2}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp[-\frac{1}{4t}\{\frac{(x-ut-x')^2}{D_1} + \frac{(y-y')^2}{D_2} + \frac{(z-z')^2}{D_2}\}] f(x', y', z')dx'dy'dz'. \tag{III.21}$$

This is easy to see by analogy with eq.(III.2). Thus according to eq.(II.3), the solution for the random component C_1 is

$$C_1 = \int_0^t \frac{w(\tau)}{8[\pi^3 D_1 D_2^2 (t-\tau)^3]^{1/2}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp[-\frac{1}{4(t-\tau)}\{\frac{(x-u(t-\tau)-x')^2}{D_1} + \frac{(y-y')^2}{D_2} + \frac{(z-z')^2}{D_2}\}] dx'dy'dz'd\tau. \tag{III.22}$$

The space integrals have exact solutions. Thus

$$C_1 = \int_0^t \{1 + erf[\frac{x-u(t-\tau)}{(4D_1(t-\tau))^{1/2}}]\}.\{1 + erf[\frac{y}{(4D_2(t-\tau))^{1/2}}]\}. \{1 + erf[\frac{z}{(4D_2(t-\tau))^{1/2}}]\}w(\tau)d\tau, \tag{III.23}$$

where $erf(\ )$ denotes the "error function" such that $erf(z) = 1 - erfc(z)$. Similarly the solution for the deterministic component C_2 in eq.(III.1) is deduced from eqs.(II.3) and (III.21) as

$$C_2 = \int_0^t \frac{C_0}{8[\pi^3 D_1 D_2^2 (t-\tau)^3]^{1/2}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp[-\frac{1}{4(t-\tau)}\{\frac{(x-u(t-\tau)-x')^2}{D_1} + \frac{(y-y')^2}{D_2} + \frac{(z-z')^2}{D_2}\}\delta(x')\delta(y')\delta(z')dx'dy'dz'd\tau. \tag{III.24}$$

or

$$C_2 = C_0 \int_0^t \frac{1}{8[\pi^3 D_1 D_2^2 (t-\tau)^3]^{1/2}} \tag{III.25}$$

$$\exp[-\frac{1}{4D(t-\tau)}\{\frac{(x-u(t-\tau))^2}{D_1}+\frac{y^2}{D_2}+\frac{z^2}{D_2}\}]d\tau.$$

This integral has an exact solution. Thus

$$C_2=\Phi=\frac{C_0}{8\pi D_2 R}\exp(\frac{ux}{2D_1})\{\exp(\frac{uR}{2D_1})[1-erf(\frac{ut+R}{(4D_1t)^{1/2}})] \tag{III.26}$$

$$+\exp(-\frac{uR}{2D_1})[1+erf(\frac{ut-R}{(4D_1t)^{1/2}})]\},$$

where

$$R^2=x^2+\frac{D_1}{D_2}(y^2+z^2).$$

After eq.(II.4), the mean concentration function is given by eq.(III.9). Let us set

$$E_{rx}(\tau)=\{1+erf[\frac{x-u(t-\tau)}{(4D_1t)^{1/2}}]\}, \tag{III.27}$$

$$E_{ry}(\tau)=\{1+erf[\frac{y}{(4D_2(t-\tau))^{1/2}}]\}, \tag{III.28}$$

and

$$E_{rz}(\tau)=\{1+erf[\frac{z}{(4D_2(t-\tau))^{1/2}}]\}. \tag{III.29}$$

After eqs.(II.6) and (III.8), we calculate the variance function by using eqs.(III.1), (III.9) and (III.27) through (III.29).

$$E\{(C-\Phi)^2\}=\sigma_c^2=q\int_0^t\int_0^t\delta(\tau-\xi)E_{rx}(\tau)E_{rx}(\xi)E_{ry}(\tau)E_{ry}(\xi)E_{rz}(\tau)E_{rz}(\xi)d\xi d\tau, \tag{III.30}$$

or

$$\sigma_c^2=q\int_0^t E_{rx}^2(\tau)E_{ry}^2(\tau)E_{rz}^2(\tau)d\tau. \tag{III.31}$$

This singular integral could easily and accurately be calculated by a numerical procedure (i.e., Gaussian-Legendre quadrature). Contour lines representing sample functions, the mean and the variance of the concentration can be obtained to produce a three-dimensional representation of the evolution of the principal contaminant.

III.5. Modeling Groundwater Pollution Subject to Evolving Heterogeneities

In this section we consider the groundwater pollution problem of chapter II when the modeler has identified the parameters as the most important source of uncertainty and other sources of uncertainty are negligible. To illustrate the theory presented in chapter II concerning the case of stochastic parameters, I consider here the contaminant transport equation subject to time-stochastic dispersion coefficient. As stated in chapter 1, much of the emphasis on parameter stochasticity in the hydrologic literature has been confined to the problem of small spatial stochasticity in the hydraulic conductivity and the dispersion coefficient. The results of the present research demonstrate that it may not be appropriate to ignore the inherent temporal dynamic behaviour of the system. Therefore I introduce in this section a new solution to the mass transport equation in aquifers which acknowledges the dispersion coefficient as a fluctuating environmental parameter. This time-random fluctuations are due to the uncertainty generated by the complex dispersion process and the natural evolution of the system. The following development may also be applied to a spatially-random dispersion coefficient and velocity field, but we choose to analyze an untried temporal stochasticity for cases when the spatial stochasticity could be neglected. The following solution also has the same advantages exhibited by all semigroup solutions, that is, it is not restricted to small variance in the parameter and that any stochastic process in $L_2(\Omega)$ could be used.

In this case the modeling equation is

$$\frac{\partial C}{\partial t} - (\overline{D}(t) + D'(t, \omega))\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} = 0, \quad 0 \leq x \leq \infty, \; t > 0, \tag{III.32}$$

$$C(x, 0) = 0; \qquad C(0, t) = C_0; \qquad C(\infty, t) = 0,$$

where $\overline{D}(t)$ is a deterministic trend in the dispersion coefficient D; $D'(t, \omega)$ is a stochastic process disturbing D. For this example, let us assume that $\overline{D}(t) = D$ is a constant and that $D'(t, \omega) = w(t, \omega)$ is a White Gaussian Noise process in time with the properties given by eq.(III.8). Following the procedure described in section 2, we write eq.(III.57) as

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} = D'\frac{\partial^2 C}{\partial x^2}. \tag{III.33}$$

The solution of this equation is given by eq.(II.10) and (III.1) as

$$C = \Phi(x, t) + \int_0^t \frac{1}{(4\pi D(t-\tau)^{1/2}} \tag{III.34}$$

$$\int_0^\infty \{\exp[-\frac{(x-u(t-\tau)-s)^2}{4D(t-\tau)}] - \exp[-\frac{(x-u(t-\tau)+s)^2}{4D(t-\tau)}]\} D'\frac{\partial^2 C}{\partial x^2} ds d\tau,$$

where the semigroup in eq.(II.10) is given by eq.(III.2); D' is spatially independent of C; and $\Phi(x, t)$ is given by eq.(III.6)

Next we define $C = C_1 + C_2 + C_3 + \cdots$, and

$$W(\tau, s) = \exp[-\frac{(x-u(t-\tau)-s)^2}{4D(t-\tau)}] - \exp[-\frac{(x-u(t-\tau)+s)^2}{4D(t-\tau)}] \tag{III.35}$$

Eq.(III.34) becomes

$$C = \Phi(x, t) + \int_0^t \frac{D'(\tau)}{(4\pi D(t-\tau))^{1/2}} \int_0^\infty W(\tau, s)\frac{\partial^2}{\partial s^2}[C_1 + C_2 + C_3 + \ldots] ds d\tau \tag{III.36}$$

The calculation of the series can be carried on to a desired accuracy. This is a computational problem in which the number of terms will vary according to the variance of

the stochastic processes involved and the desired accuracy. Let us truncate, for now, at the first term in the series and assume it to be equal to the first solution, that is, $C_1 = \Phi$. Thus we re-write eq.(III.36) as

$$C = \Phi + \int_0^t \frac{D'(\tau)}{(4\pi D(t-\tau))^{1/2}} \int_0^\infty W(\tau, s) \frac{\partial^2 \Phi(\tau, s)}{\partial s^2} ds d\tau. \tag{III.37}$$

Integrating by parts twice with respect to s and calculating the second derivative of W, it is easy to show that eq.(III.37) becomes

$$C(x, t, \omega) = \Phi(x, t) + \int_0^t \frac{D'(\tau)}{(4\pi D(t-\tau))^{1/2}} \gamma(\tau) d\tau + \int_0^t \frac{D'(\tau) d\tau}{(4\pi D(t-\tau))^{1/2}} \int_0^\infty \psi(s, \tau) \Phi(s, \tau) ds, \tag{III.38}$$

where

$$\gamma(\tau) = (x - u(t-\tau) \exp[-\frac{(x-u(t-\tau))^2}{4D(t-\tau)}]; \tag{III.39}$$

$$\psi(\tau, s) = \frac{1}{2D(t-\tau)} \{\exp[-\frac{(x-u(t-\tau)-s)^2}{4D(t-\tau)}][1 + \frac{(x-u(t-\tau)-s)^2}{2D(t-\tau)}] \tag{III.40}$$

$$+ \exp[-\frac{(x-u(t-\tau)+s)^2}{4D(t-\tau)}][1 - \frac{(x-u(t-\tau)+s)^2}{2D(t-\tau)}]\}.$$

From this expression we can generate sample functions. The mean value of the concentration is obtained by taking expectations on both sides of eq.(III.38) and using eq.(III.8):

$$E\{C(x, t)\} = \Phi(x, t) \tag{III.41}$$

In order to calculate the concentration variance we use eqs.(II.13), (III.8) and (III.38). After some algebraic manipulation we obtain

$$E\{(C - \Phi)^2\} = \sigma_c^2 = q \int_0^t \frac{\gamma^2(\tau) d\tau}{4\pi D(t-\tau)^2} + 2q \int_0^t \int_0^\infty \frac{\psi(s, \tau) \Phi(s, \tau) ds d\tau}{4\pi D(t-\tau)^2} \tag{III.42}$$

$$+ q \int_0^t \int_0^\infty \int_0^\infty \frac{\psi(s, \tau) \psi(\rho, \tau) \Phi(s, \tau) \Phi(\rho, \tau)}{4\pi D(t-\tau)^2} d\rho ds d\tau.$$

Higher order moments can be obtained in a similar manner.

Eqs.(III.6) and (III.38) through (III.42) were programmed in the micro-computer in order to obtain several numerical examples of the stochastic properties of the concentration. An average pore velocity $u = 0.2\ m/day$, a mean dispersion coefficient $D = 0.1\ m^2/day$, a concentration at the origin $C_0 = 1.0\ mgr/lit$, and a variance parameter $q = 0.1$ were assumed. The integrals were numerically evaluated using 24 points Gauss-Legendre quadrature, which gives very accurate values for singular integrals. It was found that the space integrals converge very rapidly. Fig. III.4 is a digital plotter output of the program for a point in space $x = 6.0\ m$ from the origin. It is interesting to note that as the observation distance increases the sample functions become smoother. The mean concentration coincides with the deterministic solution, whereas the sample concentration oscillates above and below the mean concentration with and increasing departure from the mean as time increases. The exact measurement of the dispersion around the mean is given by the standard deviation function, which shows a direct monotonic increasing magnitude with time. Thus the results indicate a Brownian type of behaviour of the concentration with a continuously increasing variance value, as one might have expected. Thus we may conclude that a model such as the one presented in this section may explain the stochastic nature of the concentration in an aquifer.

CHAPTER IV - APPLICATIONS TO UNSATURATED FLOW MODELING:

This chapter of the report deals with new applications of the methodology to the modeling of groundwater flow in the unsaturated zone. It is intended to illustrate the wide range of applications of the methodology and the treatment and importance of different sources of uncertainty. For a more detailed description of the model development and verification, the reader is referred to Serrano (1990(1) and 1990(2)). I also chose section IV.1 for the illustration of the case of spatially random coefficients. The iteration algorithm is shown along with verification of the model with experimental data. For the micro-computer implementation of this fascinating technique to approximate non-linear stochastic systems please see Serrano (1990(3)).

Laboratory and field infiltration data exhibit a degree of erratic variability usually associated with measurement errors and uncertainties in the phenomenon of unsaturated porous media flow. Traditionally, these uncertainties are ignored and averaged soil characteristic curves are used in the inverse and direct modeling problems. However it is highly desirable to develop models capable of reproducing the inherent variability of soil moisture in order to study the true physics of flow at the laboratory level and to reproduce more realistic infiltration data in natural watersheds. In section IV.1 two models are tested as to their ability to replicate the erratic variability of experimental horizontal infiltration data. The first model is based on the exact differential equation of infiltration, and the second model is based on the Boltzman-transformed differential equation. Both models are subject to a space or a time and space random soil-water diffusivity defined as uncertainty term. In section IV.2 a model is introduced as a new approach to predict vertical infiltration in hysteretic soils in real watersheds. For this purpose, the effect of time variability of point rainfall is represented as a shot noise process, the hysteretic loops resulting from the natural wetting and drying cycles generate a correlated random soil-water diffusivity process, and a solution of the verti-

cal infiltration equation is presented along with statistical properties.

IV.1. Modeling Space and Time Variability of Infiltration

We begin our analysis by writing the equation representing the horizontal water content evolution in a horizontal homogeneous media.

$$\frac{\partial \theta}{\partial t} - \frac{\partial}{\partial x}[D(\theta)\frac{\partial \theta}{\partial x}] = 0, \tag{IV.1}$$

$$\theta(0, t) = \theta_0, \quad \theta(\infty, t) = \theta_n, \quad \theta(x, 0) = \theta_{in},$$

where θ is the volumetric water content; t is the time coordinate (hr); x is the horizontal spatial coordinate (mm); and D is the soil-water diffusivity (mm^2/hr).

Assuming that the most important element of variability, due to the combined effect of uncertainties in the unsaturated transport phenomenon and measurement errors, is the uncertainty in the spatial variability of D, we define this parameter as a random process of the form

$$D(x, \omega) = \overline{D} + D'(x, \omega), \tag{IV.2}$$

where $\overline{D}$ represents the expected value in the soil-water diffusivity, assumed to be constant, $D'(x, \omega)$ represents the random spatial variability of this parameter; and ω is the probability variable. We further assume that this random variability is one which increases erratically with distance, and thus we choose a suitable random process such as a Brownian motion process given by (Jazwinski, 1970)

$$E\{D'(x)\} = 0, \qquad E\{D'(x_1)D'(x_2)\} = q\min(x_1, x_2), \tag{IV.3}$$

where $E\{\ \}$ denotes the expectation operator; q is the variance parameter; and $\min(x_1, x_2)$ denotes the minimum between the distances x_1 and x_2.

Substituting eq.(IV.2) into eq.(IV.1), placing the terms containing random coefficients in the right hand side of the equation and rearranging, we obtain

$$\frac{\partial\theta}{\partial t} - \bar{D}\frac{\partial^2\theta}{\partial x^2} = D'\frac{\partial^2\theta}{\partial x^2} + w\frac{\partial\theta}{\partial x}, \tag{IV.4}$$

where $w = \frac{\partial D'}{\partial x}$ is the formal derivative of the Brownian motion process, that is a White Gaussian noise process given by

$$E\{w(x)\} = 0, \qquad E\{w(x_1)w(x_2)\} = q\delta(x_1 - x_2), \tag{IV.5}$$

where $\delta(\ )$ is the Dirac's delta function. In the above equations ω has been dropped for convenience, but it is clear that because the differential equation contains random functions, the dependent variable, θ, is also a random process. Eq.(IV.4) can be treated as a stochastic evolution equation whose solution is given by (see eq.(II.8))

$$\theta(x,\ t) = J_t\theta_{in} + \Phi(x,\ t) + \int_0^t J_{t-\tau}R\theta(\tau)d\tau, \tag{IV.6}$$

where J_t is the strongly continuous semigroup associated with the diffusion operator $\bar{D}\frac{\partial^2}{\partial x^2}$ and it is given by (see eq.(III.2))

$$J_t\theta(x,\ t) = \frac{1}{(4\pi\bar{D}t)^{1/2}}\int_0^\infty \{exp[-\frac{(x-s)^2}{4\bar{D}t}] - exp[-\frac{(x+s)^2}{4\bar{D}t}]\}\theta(s,\ t)ds. \tag{IV.7}$$

$\Phi(x,\ t)$ in eq.(IV.6) is the particular solution due to the source boundary condition given by

$$\Phi(x,\ t) = \frac{x}{(4\pi\bar{D})^{1/2}}\int_0^t exp[-\frac{x^2}{4\bar{D}(t-\tau)}]\frac{\theta_0 - \theta_n}{(t-\tau)^{3/2}}d\tau. \tag{IV.8}$$

Since the source boundary condition is constant over time, this equation becomes

$$\Phi(x,\ t) = (\theta_0 - \theta_n)erfc[\frac{x}{(4\bar{D}t)^{1/2}}], \tag{IV.9}$$

where $erfc[\ ]$ denotes the "error function complement". Finally the operator R in

eq.(IV.6) represents

$$R\theta(x,\,t) = [D'(x,\,\omega)\frac{\partial^2}{\partial x^2} + w(x,\,\omega)\frac{\partial}{\partial x}]\theta(x,\,t). \tag{IV.10}$$

The third term in the right hand side of eq.(IV.6) contains θ. Thus we will approximate this integral by expanding θ as an infinite series of partial solutions $\theta = \theta_1 + \theta_2 + \cdots$ (see eq.(II.9)). Since the initial condition is a constant equal to the right boundary condition, $\theta_{in} = \theta_n$, eq.(IV.6) reduces to

$$\theta(x,\,t) = \theta_n + \Phi(x,\,t) + \sum_{i=1}^{\infty}\int_0^t J_{t-\tau}R\theta_i(\tau)d\tau. \tag{IV.11}$$

For dissipative systems such as the one in question, the convergence speed of this approximation series is extremely fast and ordinarily only a few terms in the series are needed, as I intend to show. Furthermore, since this is not a perturbation approximation, arbitrarily large variances in the stochastic terms can be included. We initiate the approximation by setting $\theta_1 = \Phi$, which is the previous approximation and compute recursively subsequent terms in the series by setting $\theta_i = \int_0^t J_{t-\tau}R\theta_{i-1}d\tau$.

Eq.(IV.11) can be used to generate sample functions of the water content and, thus replicate experimental infiltration data, by generating sample functions of D' and w and solve for θ numerically. We are also interested in computing the mean and the variance of the water content as a function of x and t. After taking expectations on both sides of eq.(IV.11) one obtains

$$E\{\theta(x,\,t)\} = \theta_n + \Phi(x,\,t) \tag{IV.12}$$

Similarly from eq.(IV.11) it is possible to derive an expression for the second moment of θ and after some algebraic manipulation one obtains

$$\sigma_\theta^2 = q\int_0^t\int_0^t\int_0^\infty\int_0^\infty f(x,\,s,\,t-\tau)\,f(x,\,u,\,t-\xi)E\{R(s)R(u)\}\Phi(s,\,\tau)\Phi(u,\,\xi)du\;ds\;d\xi\;d\tau. \tag{IV.13}$$

$$f(x,\ s,\ t-\tau) = = \frac{1}{(4\pi\bar{D}(t-\tau))^{1/2}}\{exp[-\frac{(x-s)^2}{4\bar{D}(t-\tau)}] - exp[-\frac{(x+s)^2}{4\bar{D}(t-\tau)}]\}; \qquad \text{(IV.14)}$$

$$E\{R(s)R(u)\}=[\min(s,u)\nabla_s^2\nabla_u^2+U(s-u)\nabla_s^2\nabla_u+U(u-s)\nabla_s\nabla_u^2+\delta(s-u)\nabla_s\nabla_u; \qquad \text{(IV.15)}$$

$\nabla_s^2 = \frac{\partial^2}{\partial s}$; $U(\ )$ denotes the unit step function, and the rest of the terms as before.

It was found that eq.(IV.4) and its solution only offered a partially satisfactory model for the variability of soil moisture data. Thus it was decided to study an alternative model and the choice was the Boltzman-transformed equation of eq.(IV.1) because of its importance as a classical solution of the corresponding deterministic problem. By defining a new independent variable $\lambda = x/t^{1/2}$, eq.(IV.1) reduces to the non-linear ordinary differential equation given by

$$\frac{d}{d\lambda}(D\frac{d\theta}{d\lambda}) + \frac{\lambda}{2}\frac{d\theta}{d\lambda} = 0, \qquad \text{(IV.16)}$$

subject to

$$\theta(0) = \theta_0,\ \theta(\infty) = \theta_n,\ \frac{d\theta}{d\lambda}(\infty) = 0.$$

For consistency we define the uncertainty term D as a stochastic process of $(\lambda,\ \omega)$ following the same rules of eqs.(IV.2), (IV.3) and (IV.5). Thus eq.(IV.16) becomes

$$\frac{d^2\theta}{d\lambda^2} + \alpha\lambda\frac{d\theta}{d\lambda} = 2\alpha R(\lambda,\ \omega)\theta, \qquad \text{(IV.17)}$$

where the operator

$$R(\lambda,\ \omega)\theta = [-D'(\lambda,\ \omega)\frac{d^2}{d\lambda^2} - w(\lambda,\ \omega)\frac{d}{d\lambda}]\theta; \qquad \text{(IV.18)}$$

and $\alpha = \frac{1}{2\bar{D}}$.

The general solution of eq.(IV.17) is given by

$$\theta(\lambda) = \Psi(\lambda) + \int_0^\infty G(\lambda, \xi)R(\xi)\theta(\xi)d\xi, \qquad \text{(IV.19)}$$

where the function Ψ is the solution satisfying the boundary conditions, and the kernel G is the impulse response function. With the aim of deriving a practical solution to model the water content variability in the soil domain, it was decided to simplify the right boundary condition of eq.(IV.16) and to represent the unsaturated flow problem as a two-point boundary value problem. Thus a simple expression for the Ψ function is

$$\Psi(\lambda) = \theta_0 - A\lambda + B\lambda^3 - C\lambda^5, \qquad 0 \leq \lambda \leq a, \qquad \text{(IV.20)}$$

where a is the the limiting right value of λ as given by the laboratory experiment, and A, B and C are constants. Eq.(IV.20) is actually an approximation of the series solution

$$\Psi(\lambda) = \theta_0 - E(\lambda - \frac{\alpha\lambda^3}{3!} + \frac{3\alpha^2\lambda^5}{5!} - \ldots,$$

where E is a constant.

$$G(\lambda, \xi) = U(\lambda - \xi)\{\frac{Z(\xi)Z(\lambda)}{Z'(\xi)Z(a)} - \frac{Z(\xi)}{Z'(\xi)}\} + U(\xi - \lambda)\{\frac{[Z(\xi) - Z(a)]Z(\lambda)}{Z'(\xi)Z(a)}\}, \qquad \text{(IV.21)}$$

where $Z(\xi) = [\Psi(\xi) - \theta_0]/E$, and $Z'(\xi)$ is the first derivative of Z evaluated at ξ.

The integral term in eq.(IV.19) contains θ. Thus we approximate this integral successively in the same way as that of eq.(IV.6). That is we define $\theta = \sum_{i=1}^{\infty}\theta_i$ and eq.(IV.19) reduces to

$$\theta(\lambda) = \Psi(\lambda) + \sum_{i=1}^{\infty}\int_0^a G(\lambda, \xi)R(\xi)\theta_i(\xi)d\xi, \qquad \text{(IV.22)}$$

where the first approximation $\theta_1 = \Psi$, and subsequent approximations are recursively evaluated as

$$\theta_i(\lambda, \xi) = \int_0^a G(\lambda, \xi)R(\xi)\theta_{i-1}(\xi)d\xi.$$

From eq.(IV.22) the mean of the water content is

$$E\{\theta(\lambda)\} = \Psi(\lambda), \tag{IV.23}$$

and the variance of the water content can be deduced after some algebraic manipulation to be

$$\sigma_\theta^2 = \int_0^a \int_0^a G(\lambda, \xi)G(\lambda, \rho)E\{R(\xi)R(\rho)\}\Phi(\xi)\Phi(\rho)d\rho d\xi, \tag{IV.24}$$

where $E\{R(\xi)R(\rho)\}$ is given by eq.(IV.15).

We now proceed to verify the models with the aid of the laboratory experiments. A somewhat qualitative verification of model eq.(IV.11) is provided through a visual comparison between observed water content versus distance profiles with respect to simulated sample functions of the water content versus distance at the same times of breakthrough. This was easily accomplished by adopting an average diffusivity $\bar{D} = 100\ cm^2/hr$ observed in the experiment, generating a Brownian motion sequence and a White Gaussian noise sequence for an interval $\Delta x = 1\ cm$ (Jazwinski, 1970) and solving eq.(IV.11) numerically for the same experimental times $t = 1, 3$ and $6\ hr$ respectively.

Unfortunately, the comparison of observed and simulated values of water content at corresponding times was not satisfactory. The reason for this discrepancy is the fact that at the heart of eq.(IV.11) is the function Φ given by eq.(IV.9), which is a solution of the linearized deterministic unsaturated flow equation. Therefore, a substantial improvement would be obtained if the function Φ is taken as the solution of the non-linear deterministic equation. However, this task was not attempted since it was also observed that the computation of sample functions using eq.(IV.11) already took too long time in a micro-computer.

A more objective verification of model eq.(IV.11) is provided after a comparison of the mean and variance of observed water content profiles with respect to the

corresponding simulated mean and variance values of the water content (Serrano and Unny, 1987(2)). The mean observed values were deduced from the experiments and the mean simulated values were computed after eq.(IV.12) for the same experimental times above. The comparison of the observed means with the simulated means confirmed the observations on the qualitative verification: Contrary to the observed means, the simulated means exhibited an exponential type of decay with respect to distance.

Now the observed variance was computed from the experimental values at the different breakthrough times, after assuming that the observed variances were generated by a stationary random process. This would produce a constant value of the variance with respect to distance for every breakthrough time. We realize it is not possible to assess this assumption, but this is the best one can do with the available information, and at least the experimental variance values will help establish some bounds for the simulated variances. The observed variance at $t = 1\ hr$ was equal to 1.003×10^{-4}. The first experiment at $t = 3\ hr$ produced a variance in the water content equal to 2.549×10^{-4}, and the second experiment at $t = 3\ hr$ produced a variance equal to 6.809×10^{-4}. The observed variance at $t = 6\ hr$ produced a variance equal to 6.429×10^{-4}. The simulated variances were computed using a numerical approximation of eq.(IV.13), which exhibited constant magnitudes with respect to distance for every specific time. For an average value of $q = 0.0035$ in eq.(IV.13), the simulated values of the variance at times $t = 1, 3$ and $6\ hr$ were respectively 6.119×10^{-4}, 5.073×10^{-4} and 3.461×10^{-4}. Thus the simulated variances fall within the same range of corresponding experimental variances. It was then concluded that eqs.(IV.11), (IV.12), and (IV.13) are an unsatisfactory model for the sample functions and the mean of the water content evolution, but they constitute a good model for the replication of the variability of soil moisture around the mean. A substantial improvement of this model could be accomplished by incorporating a solution to the non-linear deterministic equation in the function Φ. This, however was not attempted since the

computation of these equations required considerable micro-computer time.

Following a similar procedure, the qualitative verification of the second model we presented in chapter III is accomplished by comparing observed experimental profiles of θ versus λ with corresponding sample functions generated from eq.(III.22). The following parameter values based on the experiments were used: $D = 2.77\ mm^2/s$, $\alpha = 0.1801\ s/mm^2$, $a = 2.7\ mm/s^{1/2}$, $\theta_0 = 0.458$, $\theta_n = 0.086$, $q = 0.0002$, $A = E = 3.217 \times 10^{-3}$, $B = 9.651 \times 10^4$, $C = 2.6057 \times 10^{12}$, and the computation interval $\Delta\lambda = 0.1\ mm/s^{1/2}$. It was noted that only two or three terms in the summation series in eq.(IV.22) was necessary since the convergence speed was very fast and the computer time required was substantially less than the required for the previous model. Fig. IV.3 illustrates the first three approximations of θ versus λ. The fourth iteration is negligible in magnitude (or insignificant at the usual scale of measurement of water content). Please see Serrano (1990(3)) for the computational features and an algorithm in the C computer language. Fig. IV.1 illustrates the qualitative verification of this second model by depicting the evolution of θ with respect to λ for all of the experiments and a plot of one simulated sample function. Other simulated sample functions not illustrated were found to be similar and to evolve in a similar manner with respect to experimental values.

This exercise demonstrates the the speed of convergence of the approximation technique for non-linear stochastic systems. The algorithm implementation in a micro-computer is extremely simple. The three iterations required about 3 seconds for the execution in a HARRIS HCX-7 mini-computer and about 15 seconds in an AT&T 7300 micro-computer.

A more objective verification of this second model was accomplished after comparing the experimental mean values and variances of the water content with respect to the corresponding simulated mean values and variances. The simulated mean of the water content as a function of λ was easily computed from eq.(IV.23) and the simulated

variance as a function of λ was computed after an approximation of eq.(IV.24). Fig. IV.2 shows a plot of the observed mean, the simulated mean, the observed mean plus and minus one observed standard deviation, and the simulated mean plus and minus one simulated standard deviation, al with respect to λ. Generally the observed and simulated means are close one another, and the only discrepancy worth noting is the somewhat lower slope of the simulated mean at the wetting front. Also the simulated mean does not level to zero slope at $\lambda = a$, following the simplification of the right boundary condition described previously, a small price to pay in the name of simplicity. Now the observed standard deviation is a constant equal to 0.0214, whereas the simulated standard deviation starts with zero at $\lambda = 0$ and monotonically increases with λ up to a value of about 0.09 at $\lambda = a$. Both simulated and observed are within the same order of magnitude. Thus it was concluded that the second model based on Boltzman-transformed equation represents a good tool for the prediction of the variability of soil moisture evolution.

IV.2. Applications to Modeling Infiltration in Hysteretic Soils

Modeling vertical infiltration in soils has been approached in the past in two main ways. In the first approach, hydrologists have recognized the difficulties associated with the solution of physically-based unsaturated flow equations and have opted for a large variety of empirical expressions with parameters to calibrate in optimization procedures (i.e., Viessman et al., 1977). This approach, which has produced acceptable results for surface hydrologic computations, has not generated much understanding on the phenomenon of infiltration and distribution of water in unsaturated soils. In the second approach, soil physicists have attempted to produce solutions to physically-based equations describing horizontal or vertical infiltration in soils. Several quasi-analytical solutions of the non-linear unsaturated flow equation have been reported in the literature (i.e., Philip, 1955, 1972; Philip and Knight, 1974; Parlange, 1971, among others). Recently exact non-linear solutions for constant flux infiltration using Lie-Backlund transformations was reported (Sander et al., 1988; Broadbridge and White, 1988). This approach has given much understanding of the phenomenon of infiltration in soils and in general the solutions have been in good agreement with experimental data. Other solutions in this category use a numerical algorithm to implement in a computer (i.e., Freeze, 1971; Neuman, 1973; Mohsenisaravi, 1981; and Nieber, 1979, 1982 among others). These models have given valuable computational information to use in watershed simulation models.

Most analytical solutions restrict their validity to specific laboratory conditions in which the infiltration rate at the source boundary is constant in time, and the soil is continuously wetted. In this situation the natural effects of hysteresis in the soil-water functional relationships are minimized. Therefore the application of these solutions to field conditions in watersheds where the rainfall regime is a highly erratic process composed of periods of rainfall followed by periods of drought is limited. Rainfall periods

will produce a partial wetting cycle in the soil profile and drought periods will produce a partial drying cycle in the soil profile. This situation will produce a set of soil-water functional relationships in which hysteresis is very important. The solution of the unsaturated groundwater flow equation subject to hysteretic functional relationships is very difficult to obtain.

Most numerical solutions can handle time variability in the source boundary for specific rainfall patterns known *a priori*. Nevertheless, hysteresis in the soil-water functional relationships is seldom incorporated and a unique, usually empirical, set of relationships is used. The use of empirical, single-valued, functional relationships obviates the difficulties associated with the unpredictability of hysteresis, although the predicted water content values do not represent the natural variability associated with the hysteretic soil.

Other approaches have attempted to use stochastic concepts in an effort to describe the uncertainty of the infiltration phenomenon in a statistical manner. One of these studies (Dagan, 1983) defined the saturated hydraulic conductivity as a log-normally distributed random variable and by assuming analytical, single-valued, expressions for the soil-water functional relationships a solution of a simplified "piston flow" model of the infiltration equation was obtained. A constant flux infiltration during rainfall was assumed and spatial variability of infiltration was studied. Another interesting study (Mtundu and Koch, 1987) derived two ordinary differential equations describing the surplus and the deficit conditions in the unsaturated zone. These equations are forced by the random infiltration process, modeled as a Poisson process, and the evapotranspiration, modeled as a Brownian motion process. In an innovative approach the study in mention solved the resulting random differential equations and derived expressions for the first two moments. The above study motivates two questions. The first question, one may ask, is what would be the random form of the soil-water diffusivity, D, which results from a Poissonian type of infiltration? This is a

question which can not be answered without considering hysteresis in the soil-water functional relationships. The next question is: Is it possible to obtain a solution of the physically-based non-linear unsaturated flow equation when the top boundary is a Poisson process and D is a stochastic process? This is a question which involves the solution of a random partial differential equation, which would describe the time and space variability of the water content. The present setion of the report attempts to respond these questions.

This section presents a new methodology for the analysis and solution of the unsaturated groundwater flow equation subject to the uncertainty inherent to hysteresis. It is a theoretical analysis on the general form of the point precipitation process forcing infiltration in natural watersheds and the subsequent hysteretic loops in the soil-water functional relationships. The solution of the infiltration equation subject to the resultant random processes is the main objective of the study with the hope to develop a more realistic statistical representation of the infiltration phenomenon. First a simplified Poisson process is assumed to represent the time variability of point rainfall in a hypothetical watershed. The water content variation over time at the top layer due to the Poissonian rainfall pattern is found to follow a shot noise process, in agreement with existing literature on the topic. Second, a simulation experiment to synthesize realizations of the D process in a hypothetical soil is performed. In this experiment sample values of the shot noise process describing water content in the root zone are used to reproduce the hysteretic loops in the water content versus pressure head relationship and in the hydraulic conductivity versus pressure head relationship, by emulating experimental scanning curves published in the literature. Using these simulated functional relationships, a sample function of D is obtained. While this approach only gave qualitative information on the form of D, it was observed that the hysteretic wetting and drying cycles produced a highly erratic D process, which would be better described as a random process of an exponential type of correlation. It was then

assumed that D can be represented by a colored noise. Third a new semigroup solution of the infiltration equation subject to a shot noise boundary condition and a colored noise D was obtained. Finally a computational procedure of each of the components of the stochastic solution, and of the first two moments is presented, along with observations about the role of each of the components and the procedure for reduction of the model variance in practical field situations.

It is hoped that the results will encourage hydrologists and water resources scientists to use physically based equations subject to the natural environmental fluctuations encountered in the field, rather than empirical expressions. Since the theory and solutions of stochastic partial differential equations are now available, the modeler can now use a predictive tool which may give a better insight on the physical processes.

IV.2.1. The Water Content at the Root Zone: Definition of the Top Boundary Condition

We begin our analysis by considering a typical homogeneous soil profile in a natural watershed having a gentle slope and a deep mean water table elevation for now. The regional hydrology is such that in the area considered the vertical infiltration is the main source of aquifer recharge. This would be the situation in an agricultural watershed whose regional groundwater flow occurs through an alluvial aquifer. The problem we consider is the statement and the solution of the boundary value problem modeling the vertical infiltration at a point in the recharge zone, and in particular the prediction of the evolution of the volumetric soil-water content.

The first difficulty the hydrologist faces is the fact that the upper boundary is the ground surface which is subject to the complex time variation of the rainfall occurrence in the area, alternated by dry periods which allow the redistribution of moisture in the

soil. This erratic nature of the rainfall time distribution would pose serious difficulties in the exact solution of the differential equation governing infiltration, except in limited cases when assumptions of constant infiltration rate at the top boundary are made. The problem is further aggravated by recent hydrologic evidence of the existence of a macropore flow zone in the top layer of most natural soils (see Sloan et al., 1983), usually in the first 10 to 20 *cm* of the soil profile corresponding to the agricultural *A* horizon. This macropore zone is created by the penetration of roots from plants, animal burrows and natural soil weathering.

The exact hydraulic interaction between the rainfall intensity and the soil-water content in the root zone is still unknown, although some mathematical models have been proposed in the literature. One of these models (Tsakiris et al, 1988) approximates point rainfall depth as a Poisson process in time. This is indeed a simplification since it is well known that point rainfall follows a much more complex stochastic process (see Kavvas et al., 1987). Behind this assumption is the recognition of the root zone as a filtering entity of the rainfall intensity signal. For example, the complex hourly rainfall intensity curves would generate a daily infiltrated rainfall depth time series which can be easily observed as a Poisson process such that (Papoulis, 1984)

$$p(N(t)=n) = \frac{(\lambda t)^n}{n!} e^{-\lambda t}, \qquad \text{(IV.25)}$$

where $p(N(t) = n)$ is the probability of n storms in the interval (0, t]; t is time (*days*); $n = 0, 1, 2,...$; and λ is the mean storm arrival rate in (0, t]. This process has the properties

$$E\{N(t)\} = \lambda t, \qquad E\{N^2(t)\} = \lambda^2 t^2 + \lambda t, \qquad \text{(IV.26)}$$

where $E\{\ \}$ represents the expectation operator. The time $T = t_a$ in *days* between storms can be modeled as an exponential distribution of the form

$$p_T(t_a) = \lambda e^{-\lambda t}, \qquad \text{(IV.27)}$$

with the properties

$$E\{T\} = \frac{1}{\lambda}, \qquad E\{T^2\} = \frac{2}{\lambda^2}. \tag{IV.28}$$

Tsakiris et al (1988) assumed that the moisture depletion during rainless periods in the root zone is a function of the potential evapotranspiration and the field capacity and adopted the Thornthwaite and Mather equation for this purpose:

$$\theta_0(t) = \theta' e^{-\frac{PET}{FC}t}, \tag{IV.29}$$

where $\theta_0(t)$ is the water content in the root zone (mm); θ' is the initial water content (mm); PET is the potential evapotranspiration (mm); and FC is the soil field capacity.

Because of its simplicity, in the present study we will adopt the Tsakiris et al (1988) model to represent the water content in the root zone in order to to obtain a description of the conditions at the top boundary, which we will call "boundary layer", in our boundary value problem. This transition layer will resemble a similar conception in fluid dynamics except that in this case the representative scale (the depth) of the boundary layer is significantly greater than that used in fluid dynamics problems because of the presence of the porous media. Therefore acceptable typical dimensions for the soil boundary layer will have to be of the order of the scale of existing measurement devices for soil moicture (see Cushman, 1987). For the present study we assumed a boundary layer depth of 10 cm, a dimension appropriate for core sampling which also corresponds to the depth of the A horizon in many natural soils.

Recognizing that this is only an approximative abstraction of the complex conditions in the top boundary, this model will serve our objective to develop a methodology to solve the infiltration equation when the top boundary is a time stochastic process. It is clear that the hydrologist will have to identify the particular time stochastic process representing soil moisture in the root zone by measuring the water content at the root zone over time. Then s/he can use a methodology such as the one presented in this

article to predict the statistical nature of the evolution of the water content at different depths.

Summarizing, we assume that the input infiltration to the boundary layer is a Poisson sequence of pulses of the form (Papoulis, 1984)

$$Z(t) = \sum_{i=0}^{N(t)} X_i \delta(t - t_i), \tag{IV.30}$$

where $Z(t)$ is the moisture depth input (mm) in (0, t]; $N(t)$ is the number of pulses in (0, t], which is Poisson distributed as in eq.(IV.25); X_i is the infiltration pulse magnitude at t_i, which is modeled in this case as an exponential distribution of the form of eq.(IV.26) with parameter γ; t_i are the random points in time with the intervals $(t_i - t_{i-1})$ modeled as an exponential distribution; and $\delta(\ )$ is the Dirac's delta function.

Following eq.(IV.29) we regard the unit impulse response, $h(t)$, of the boundary layer as

$$h(t) = e^{-\alpha t}, \tag{IV.31}$$

where α is a parameter to determine. Then the output water content of the boundary layer system is found as

$$\theta_0(t) = \int_0^t Z(\tau) h(t - \tau) d\tau = \int_0^t \sum_{i=0}^{N(t)} X_i \delta(\tau - t_i) e^{-\alpha(t-\tau)} d\tau. \tag{IV.32}$$

Thus the water content at the boundary layer will be

$$\theta_0(t) = \sum_{i=0}^{N(t)} X_i e^{-\alpha(t - t_i)}, \tag{IV.33}$$

where the random variables $N(t)$, X_i and t_i are assumed to be independent. The mean of $Z(t)$ is

$$E\{Z(t)\} = \lambda E\{X\}, \tag{IV.34}$$

and the mean of $\theta_0(t)$ is given by

$$E\{\theta_0(t)\} = \int_0^t E\{\sum_{i=0}^{N(t)} X_i \delta(t - t_i)\} e^{-\alpha\tau} d\tau. \qquad \text{(IV.35)}$$

Solving,

$$E\{\theta_0(t)\} = \frac{\lambda}{\alpha\gamma}(1 - e^{-\alpha t}). \qquad \text{(IV.36)}$$

Now the correlation of $Z(t)$ is found as

$$E\{Z(t_1)Z(t_2)\} = [\lambda^2 + \lambda\delta(t_1 - t_2)]\ E\{X^2\}. \qquad \text{(IV.37)}$$

Thus the correlation function of $\theta_0(t)$ is given by

$$E\{\theta_0(t_1)\theta_0(t_2)\} = \int_0^{t_1}\int_0^{t_2} [\lambda^2 + \lambda\delta(\tau-\rho)E\{X^2\}e^{-\alpha(t_1-\tau)}e^{-\alpha(t_2-\rho)}d\rho d\tau. \qquad \text{(IV.38)}$$

Solving we obtain,

$$E\{\theta_0(t_1)\theta_0(t_2)\}=\frac{2\lambda}{\alpha\gamma^2}\ [\frac{\lambda}{\alpha}-\frac{\lambda}{\alpha}e^{-\alpha t_2}-\frac{\lambda}{\alpha}e^{-\alpha t_1}+(\frac{\lambda}{\alpha}-\frac{1}{2})e^{-\alpha(t_1+t_2)}+\frac{1}{2}e^{-\alpha(t_1-t_2)}. \qquad \text{(IV.39)}$$

The process $\theta_0(t)$ now defines the time distribution of the water content in the boundary layer. As a simulation experiment, two months of daily water content data in the root zone were generated using arbitrary values for the parameters which reflected typical conditions of a homogeneous sandy soil in the torrid zone. It was decided for simplicity to model the number of storms $N(t)$ as an exponential distribution with parameter $\varsigma = 0.2\ day^{-1}$; the interarrival times t_i as an exponential distribution with parameter $\lambda = 0.2\ day^{-1}$; the infiltration depths X_i as an exponential distribution with parameter $\gamma = 0.3\ mm^{-1}$; the removal rate of moisture from the root zone was assumed to be $\alpha = 0.1\ day^{-1}$; the the depth of the root zone $d = 100.0\ mm$; a residual minimum water content was assumed as $r_m = 10\%$; and a maximum saturated water content (or porosity) of $\theta_{\max} = 30\%$. These values do not intend to specify actual field conditions in a particular soil, but rather some hypothetical conditions in a soil in order to investigate the effect of time and space distribution of soil moisture due to general Poissonian

conditions of the water content at the top boundary. These Poissonian conditions at the top boundary will reflect the effect of the complex time variability of point rainfall in real situations.

Using appropriate algorithms for the generation of exponential realizations ([8]Haan, 1977) and eq.(IV.33), Fig. IV.4 was obtained. It describes the time variability of the water content with respect to time at the root zone. Note that wetting takes place almost instantaneously, whereas drying is a slow decay process. Such a wide variability in the water content should be expected in the root zone of natural soils.

IV.2.2. The Random Nature of the Soil-Water Diffussivity: A Simulation Experiment

In the vertical infiltration equation the soil-water diffusivity, $D(\theta)$, is defined as

$$D(\theta) = K(\theta)\frac{d\psi}{d\theta}, \tag{IV.40}$$

where θ is the soil-water content; $K(\theta)$ is the soil-water hydraulic conductivity $(m.day^{-1})$; and ψ is the soil-water pressure head (m).

Several laboratory techniques have been proposed to determine the functional relationships of θ versus ψ and of K versus ψ in soil samples (i.e., Klute, 1965; Tanner and Elrick, 1958; Miller and Elrick, 1958; Rijtema, 1959; Kunze and Kirkham, 1962; Moore, 1939; Youngs, 1964, Watson, 1966; Rose et al., 1965). These functional relationships are used to numerically solve eq.(IV.40) to obtain the relationship of D versus θ, which will subsequently be used to solve the vertical infiltration equation. Most of the existing solutions of the vertical infiltration equation assume a fixed set of soil functional relationships and a unique relationship of D versus θ. However, it is well known that the soil functional relationships are not unique and are subject to hysteretic effects (see Hillel, 1980 for discussion). Thus the shape of the soil functional relationships will be

dependent on the way the soil was wetted or dryed in the experiment. For example a continuous and gradual wetting of the soil will generate the "main wetting curves" in the soil functional relationships, and a continuous and gradual drying of the soil will generate the "main drying curves" in the soil functional relationships. When neither continuous wetting or continuous drying occurs, that is when the soil is subjected to cycles of partial wetting followed by partial drying, secondary or "scanning curves" between the main wetting curve and the main drying curve are generated. The location of the scanning curves will depend on the value of the relationships at the instant of time when a cycle changes from wetting to drying or from drying to wetting, and from soil physical properties not yet well understood.

The unpredictability of the soil functional relationships subject to the cyclic conditions will produce an uncertain relationship between D and θ, which will in turn generate an uncertain solution of the vertical infiltration equation. The degree of uncertainty will depend on the degree of hysteresis in the soil in question. The hysteretic phenomenon, which has puzzled scientists for a long time, has been the reason why solutions of the vertical infiltration equation have only been obtained under idealistic conditions of constant infiltration. These conditions are only realizable in laboratory settings which are rarely attained in natural soils of hydrologic watersheds, where rainfall periods are followed by dry periods. Hysteresis is also the reason why hydrologists mainly rely on empirical equations, rather than physically-based equations, for the calculation of infiltration and for the watershed simulation models requiring infiltration estimates.

In order to investigate the effect of hysteresis in the soil functional relationships on the form of the soil-water diffusivity a simulation experiment was performed. The simulation was based on the results of Liakopoulus (1965), where detailed experimental information on the soil functional relationships of a fine sand was presented. We used the Liakopoulus data to represent the physical bounds of the main wetting curve, the

main drying curve and the general direction of the scanning curves of a hypothetical sandy soil. The hypothetical soil was assumed to represent a typical soil profile in a watershed whose point rainfall regime follows the Poisson process described in the previous section.

We showed in the previous section that the water content in the root zone of a soil forced by a Poissonian rainfall follows a shot noise process. A sample function of the shot noise process was used to generate (Fig. IV.4) realizations of daily water content at the root zone. Using this information on the time variability of the water content, realizations of the daily pressure head in the root zone were generated. The pressure head was computed by emulating the main wetting curve, the main drying curve and the secondary scanning curves according to the Liakopoulus data. Fig. IV.5 shows a digital plotter output of 57 days of simulation. Note the main wetting and drying curves and the cyclic loops (scanning curves) as a result of partial wetting and drying of the rainfall inputs. We remark that the objective of the experiment is not to calculate exact absolute values of the pressure head, but rather to reproduce the phenomenon of hysteresis in the soil functional relationships and to observe the sort of stochastic process representing pressure head in a soil subject to the complex rainfall characteristics affecting real watersheds.

A similar procedure was used to generate 57 realizations of the hydraulic conductivity. Fig. IV.6 shows the results of one of such simulations. Subsequently the two sets of synthetic data (Figs. IV.5 and IV.6) were used in conjunction with eq.(IV.40) to approximate realizations of the daily soil-water diffusivity. It is known that the numerical approximation of the derivative in eq.(IV.40) is not very accurate, but again the objective is to observe the nature of the time stochastic process representing daily soil-water diffusivity.

Fig. IV.7 shows the 57 realizations of such process. Note the high variability in D and that, at least in the root zone, D "jumps" to high values in relatively short periods

of time, whereas D recedes slowly in low values. The reason behind this resides in the fact that wetting takes place in shorter periods of time than drying. This differences in the timing of wetting and drying may be significantly attenuated as depth increases. There is also an indication that the extreme high values in D are probable unattainable in real field conditions. In the simulation, these extreme high values are obtained as the soil-water content approaches saturation. However, it is known that except under prolonged ponding in the ground surface and because of capillary fringe effects in fine soils with shallow water table (Gillam, 1982) a condition not considered here, saturation rarely occurs. Under conditions of intense rainfall, the value of the water content would be somewhat below saturation because of the presence of entrapped air. This would suggest that the variance in the D process is probably lower than the one exhibited by our simulation.

It is also noted that during dry periods some persistence exist in the daily time series of D. To obtain a quantitative evaluation of this aspect, the serial correlation coefficient of the generated D series was computed. It was found that the correlation coefficient follows an exponential decay of the form

$$r_l = e^{-\rho l}, \tag{IV.41}$$

where r_l is the lag l serial correlation coefficient; and ρ a recession parameter found to be equal to 0.5 on this example. No further analysis of the D series was done since it was considered that the data only represents a hypothetical condition rather than an actual field situation. Further research is needed to determine the correlation structure of the time variability in the soil-water diffusivity, its marginal probability density function, and its degree of stationarity. The research should involve some repetitive type of test in a soil profile in which the soil is excited by a rainfall process of known stochastic properties, the soil functional relationships and the soil-water diffusivity are determined on a continuous basis.

The preliminary results of this simulation indicate that the random time variability in the rainfall occurrence generates hysteretic loops and an important degree of uncertainty in the time variability of the soil-water diffusivity which should be accounted for in the solution of the vertical infiltration equation. This uncertainty in D will generate an important uncertainty in the water content evolution in the soil profile. Since the main aim of the present study was the development of a methodology to solve the vertical infiltration equation which accounted for the time variability in the rainfall input and the variability in the soil-water diffusivity resulting from the inherent hysteretic process, several assumptions were made on the stochastic properties of the D process. Knowing that this is only an illustration of the methodology in the next section, future research will have to be done to determine the exact stochastic properties of D in actual soil profiles.

It was assumed that the D process can be represented as

$$D = \overline{D} + D'(t, \omega), \tag{IV.42}$$

where $\overline{D}$ represents a deterministic component; and $D'(t, \omega)$ represents a random component in the probabilistic variable ω. Following the previous observation on the boundedness of D we adopted a significantly lower value for the mean D, that is $\overline{D} = 0.0162\ m^2.day^{-1}$. The effect of seasonality was neglected in this example, knowing that its inclusion will not significantly complicate the procedure. The random component was assumed to follow a colored Gaussian noise. The latter follows in view of the evidence of persistence in our previous simulation of D:

$$E\{D'(t)\} = 0, \qquad E\{D'(t_1)D'(t_2)\} = qe^{-\rho(t_1-t_2)}, \tag{IV.43}$$

where q is the variance parameter equal to $1.56\ m^2.day^{-1}$.

IV.2.3. Solution of the Vertical Infiltration Equation

Following the definition of the top boundary condition and the form of the soil-water diffusivity in the last two sections, we attempt in this section the solution of the vertical infiltration equation. The partial differential equation governing the one-dimensional vertical infiltration in a homogeneous soil is given by (Bear, 1979)

$$\frac{\partial\theta}{\partial t} - \frac{\partial}{\partial z}[D\frac{\partial\theta}{\partial z}] + \frac{dK}{d\theta}\frac{\partial\theta}{\partial z} = 0, \qquad \text{(IV.44)}$$

$$\theta(0,\, t,\, \omega) = \theta_0(t,\, \omega), \qquad \theta(\infty,\, t) = 0, \qquad \theta(z,\, 0) = \theta_i(z),$$

where θ is the volumetric water content; t is the time coordinate ($days$); z is the vertical spatial coordinate, positive downward (m); D is the soil-water diffusivity ($m^2.day^{-1}$), which we propose to be a stochastic process of the form of eq.(IV.42) when the top boundary is subject to the rainfall regime in a watershed; $K(\theta)$ is the unsaturated hydraulic conductivity of the soil ($m^2.days^{-1}$); $\theta_0(t,\, \omega)$ is the stochastic process representing the time variability in the water content at the top boundary, the "boundary layer", which we assume to follow a shot noise process of the form of eq.(IV.33) when this layer is subject to the time variability typical of natural point rainfall patterns; and $\theta_i(z)$ is the known initial water content along the soil profile.

The assumption on the form of D implies that we are neglecting its spatial variability. This means that in this study the time random variations in D occur in the entire soil profile, a condition feasible in small reaches of soil where a bulk D value can be measured. The effect of the spatial variability in D on the evolution of θ was discussed in section IV.1.

The term $\frac{dK}{d\theta} = u$ is assumed constant in the present study and equal to 0.0216 $m.day^{-1}$, which is an average value taken from the Liakopoulus data. Clearly this term is not constant and varies directly with θ. Thus strictly speaking u would be

another time stochastic process presumably correlated with the D process. In the absence of experimental data on the correlation structure of of this term, we leave the investigation of this aspect to a future study.

Another simplification of the formulation is the assumption of independence between the boundary process, θ_0 and the D process. Intuitively one may think that high rainfall intensity is associated with high values in D and low rainfall intensity is associated with low values in D. Therefore, some correlation could be expected between the above two processes. However, because of the attenuation effect of hydrodynamic dispersion in unsaturated soils, this possible degree of correlation may be significantly reduced as depth increases. The issue is further complicated because the nature and the behaviour of D is not well understood yet. Once again we are in unknown territory and the absence of experimental information refrains us from speculating further. Thus in the following treatment we assume that D is a system parameter which is physically independent of the input functions. This statistical independence between system parameters and environmental inputs has been reported in many other physical systems (see Adomian, 1983).

The objective in this section is then the solution to the partial differential eq. (IV.44) subject to a colored noise soil-water diffusivity and a shot noise boundary condition. The following solution of the stochastic partial differential equation (IV.44) is based on the results presented in chapters II and III of this report (also see Serrano et al., 1985(1), 1985(2), 1985(3); Serrano and Unny, 1986; Serrano and Unny, 1987(1), 1987(2); and Serrano, 1988(1), 1988(2)), where functional analytic concepts were applied to obtain new solutions to similar stochastic partial differential equations in subsurface hydrology.

Let us replace eq.(IV.42) into eq.(IV.44) and put the random component on the right hand side to obtain

$$\frac{\partial\theta}{\partial t} - \bar{D}\frac{\partial^2\theta}{\partial z^2} + u\frac{\partial\theta}{\partial z} = D'\frac{\partial^2\theta}{\partial z^2}, \tag{IV.45}$$

subject to the same boundary and initial conditions of eq.(IV.44). The solution to this transport evolution equation is (Serrano, 1988(1); Serrano, 1985(2))

$$\theta(z,\, t) = \Phi(z,\, t) + J_t\theta_i(z) + \int_0^t J_{t-\tau}D'(\tau)\frac{\partial^2\theta}{\partial z^2}d\tau, \tag{IV.46}$$

where $\Phi(z,\, t)$ is the solution due to the stochastic boundary condition given by (Serrano, 1988(1))

$$\Phi(z,\, t) = \frac{z}{(4\pi\bar{D})^{1/2}}\int_0^t \exp[-\frac{(z-u(t-\tau))^2}{4\bar{D}(T-\tau)}]\frac{\theta_0(\tau)}{(t-\tau)^{3/2}}d\tau. \tag{IV.47}$$

$J_t\theta_i(z)$ in eq.(IV.44) is the solution due to the deterministic initial condition, where J_t is the strongly continuous semigroup (Serrano et al., 1985(2)) associated with the evolutional operator in eq.(IV.44). The semigroup operator in this case is given by (Serrano, 1988(1))

$$J_t\theta_i(z) = \frac{1}{(4\pi\bar{D}t)^{1/2}}\int_0^\infty \{\exp[-\frac{(z-ut-s)^2}{4\bar{D}t}] - \exp[-\frac{(z-ut+s)^2}{4\bar{D}t}]\}\theta_i(s)ds. \tag{IV.48}$$

We now define θ in the right hand side of eq.(IV.46) as the series $\theta = \theta_1 + \theta_2 + \theta_3 + \cdots$. Eq.(IV.46) becomes

$$\theta(z,\, t) = J_t\theta_i(z) + \Phi(z,\, t) + \int_0^t J_{t-\tau}D'(\tau)\frac{\partial^2}{\partial z^2}(\theta_1 + \theta_2 + \ldots)d\tau. \tag{IV.49}$$

Now set θ_1 equal to the previous part of the solution, $\Phi(z,\, t)$, and truncate at the first term to obtain

$$\theta(z,\, t) = J_t\theta_i(z) + \Phi(z,\, t) + \int_0^t J_{t-\tau}D'(\tau)\frac{\partial^2}{\partial z^2}\Phi(z,\tau)d\tau. \tag{IV.50}$$

For a justification of the above approximation procedure and a discussion on the convergence see Serrano (1988(2)). We are truncating at the first term in the expansion

for simplicity and because we assume we are dealing with relatively small variances in D. Obviously more terms will have to be included in the case of arbitrary large variances. Note that the solution we are presenting is not a perturbation solution, and therefore it is not limited to small variances in the stochastic functions, which is the most important limitation in the existing perturbation solutions.

From eq.(IV.50) we may obtain sample functions of the water content at different depths and at different times. These sample functions help us observe the evolution of the water content distribution under different conditions. We are also very interested in obtaining statistical measures of the water content, which characterize the stochastic properties of the water content process. In particular it is very desirable to derive expressions to calculate the mean and the variance of the water content as a function of the same measures of D and θ_0. In most engineering applications the modeler only has available the first two moments of the input processes and rarely information on their join probability density function. Therefore the first two moments of the solution are the only feasible statistical measures. In order two obtain such measures, we examine first each of the terms in eq.(IV.50).

The mean of the boundary solution is given by

$$E\{\Phi(z,\,t)\} = \frac{z}{(4\pi\bar{D})^{1/2}}\int_0^t \exp[-\frac{(z-u(t-\tau))^2}{4\bar{D}(t-\tau)}]\frac{E\{\theta_0(\tau)\}}{(t-\tau)^{3/2}}d\tau. \qquad \text{(IV.51)}$$

Using eq.(IV.36) this becomes

$$E\{\Phi(z,\,t)\} = \frac{\lambda z}{\alpha\gamma(4\pi\bar{D})^{1/2}}\int_0^t \exp[-\frac{(z-u(t-\tau))^2}{4\bar{D}(t-\tau)}]\frac{(1-e^{-\alpha\tau})}{(t-\tau)^{3/2}}d\tau. \qquad \text{(IV.52)}$$

The correlation function of the boundary solution is, from eq.(IV.47),

$$E\{\Phi(t_1)\Phi(t_2)\} = \frac{z^2}{4\pi\bar{D}}\int_0^{t_1}\int_0^{t_2} \exp[-\frac{(z-u(t_1-\tau))^2}{4\bar{D}(t_1-\tau)}]\exp[-\frac{(z-u(t_2-\xi))^2}{4\bar{D}(t_2-\xi)}] \qquad \text{(IV.53)}$$

$$\frac{E\{\theta_0(\tau)\theta_0(\xi)\}}{(t-\tau)^{3/2}(t-\xi)^{3/2}}d\xi d\tau.$$

Using eq.(IV.39) this becomes

$$E\{\Phi(t_1)\Phi(t_2)\} = \frac{2\lambda z^2}{4\alpha\gamma^2\pi\overline{D}}\int_0^{t_1}\int_0^{t_2}\exp[-\frac{(z-u(t_1-\tau))^2}{4\overline{D}(t_1-\tau)}]\exp[-\frac{(z-u(t_2-\xi))^2}{4\overline{D}(t_2-\xi)}] \qquad \text{(IV.54)}$$

$$\cdot[\frac{\lambda}{\alpha}-\frac{\lambda}{\alpha}e^{-\alpha\xi}-\frac{\lambda}{\alpha}e^{-\alpha\tau}+(\frac{\lambda}{\alpha}-\frac{1}{2})e^{-\alpha(\tau+\xi)}+\frac{1}{2}e^{-\alpha(\tau-\xi)}]\frac{d\xi d\tau}{(t-\tau)^{3/2}(t-\xi)^{3/2}}.$$

Using eqs.(IV.52) and (IV.54) the variance of Φ will then be

$$Var\{\Phi(z,\,t)\} = E\{\Phi^2(z,\,t)\} - E^2\{\Phi(z,\,t)\}. \qquad \text{(IV.55)}$$

Now the mean of the third term, which we shall call $I(t)$, in the solution eq.(IV.50) is simply

$$E\{I(t)\} = 0, \qquad \text{(IV.56)}$$

in which eq.(IV.43) has been used. Using again eq.(IV.43) we find an expression for the correlation function of $I(t)$:

$$E\{I(t_1)I(t_2)\} = \int_0^{t_1}\int_0^{t_2} J_{t_1-\tau}J_{t_2-\xi}E\{D'(\tau)D'(\xi)\frac{\partial^2}{\partial z^2}[\Phi(\tau)]\frac{\partial^2}{\partial z^2}[\Phi(\xi)]\}d\xi d\tau. \qquad \text{(IV.57)}$$

Using Eqs.(IV.56), (IV.57) and (IV.43), setting $t_1 = t_2 = t$, and the previously mentioned assumption of independence between Φ and D', we obtain the variance of $I(t)$:

$$Var\{I(t)\} = q\int_0^t\int_0^t J_{t-\tau}J_{t-\xi}e^{-\rho(\tau-\xi)}\frac{\partial^2}{\partial z^2}[E\{\Phi(\tau)\Phi(\xi)\}]d\xi d\tau, \qquad \text{(IV.58)}$$

where the correlation of Φ is given by eq.(IV.54). We are now in a position to calculate the first two moments of the water content. In eq.(IV.50) the mean water content is given by

$$E\{\theta(z,\,t)\} = E\{\Phi(z,\,t)\} + J_t\theta_i(z), \qquad \text{(IV.59)}$$

where eq.(IV.56) has been used, and the mean of Φ is given by eq.(IV.52).

Finally, using eqs.(IV.55) and (IV.58), it is easy to show that the variance of the water content is given by

$$Var\{\theta(z,\ t)\} = E\{\theta^2(z,\ t)\} - E^2\{\theta(z,\ t)\} = Var\{\Phi(z,\ t)\} + Var\{I(z,\ t)\}. \quad \text{(IV.60)}$$

The above derived expressions for sample functions, the mean and the variance were used in the numerical computations of the next section. Computation of each of the partial terms involved in the expressions was done in order to observe the contribution of each of the stochastic components to the combined random behaviour of the water content. The objective of the exercise was to evaluate the relative importance of each of the terms in order to identify the individual components crucial in the reduction of the variance of the water content forecast.

IV.2.4. Computational Results and Analysis

In this section we explore the computational features of each of the terms in the stochastic solution of the vertical infiltration equation, its mean and its variance as developed in the previous section. We begin by considering the deterministic component in the solution eq.(IV.50), $J_t\theta_i(z)$, which is defined by eq.(IV.48). Assuming that the typical scale of the instrument measuring field water content is 0.1 m, then the bulk water content will be constant at 0.1 m intervals. Thus the deterministic component will reduce to

$$J_t\theta_i(Z) = \sum_{j=1}^{N} \theta_j M_j, \quad \text{(IV.61)}$$

where the depth Z takes the discrete values 0.1, 0.2, 0.3, $\cdots$; θ_j is the measured initial water content at the above discrete intervals; $j = 1, ,2, \ldots, N$; and the function M_j is the spatial integral of eq.(IV.48) solved at 0.1 m intervals in which θ_j is constant. For example, when $j = 1$,

$$M_1 = \frac{1}{(\pi b)^{1/2}} \int_0^{0.1} \{\exp[-\frac{a-s)^2}{b}] - \exp[-\frac{(a+s)^2}{b}]\} ds, \qquad \text{(IV.62)}$$

where $a = Z - ut$; and $b = 4\bar{D}t$. This equation can be written as

$$M_1 = \frac{1}{\pi^{1/2}} \{ \int_{\frac{-a}{b^{1/2}}}^{\frac{0.1-a}{b^{1/2}}} e^{-\xi^2} d\xi - \int_{\frac{a}{b^{1/2}}}^{\frac{0.1+a}{b^{1/2}}} e^{-\xi^2} d\xi \}, \qquad \text{(IV.63)}$$

which in turn can be written as

$$M_1 = \frac{1}{2} \{ erfc(-\frac{a}{b^{1/2}}) - erfc(\frac{0.1-a}{b^{1/2}}) - erfc(\frac{a}{b^{1/2}}) + erfc(\frac{0.1+a}{b^{1/2}}) \}, \qquad \text{(IV.64)}$$

where $erfc(\ )$ denotes the "error function complement". In general, for any j

$$M_j = \frac{1}{2} \{ erfc(\frac{j-0.1-a}{b^{1/2}}) - erfc(\frac{j-a}{b^{1/2}}) - erfc(\frac{j-0.1+a}{b^{1/2}}) + erfc(\frac{j+a}{b^{1/2}}) \}. \qquad \text{(IV.65)}$$

Interestingly, convergence of eq.(IV.61) to a desired accuracy was achieved after two or three steps. The accuracy of the above scheme was tested by setting $\theta_j = 1.0$,for all j, and noting that $J_t \theta_i$ was equal to one. It was also found that a stepwise computation, at 1 *day* intervals, was the most accurate.

The deterministic solution results from a linearization of the infiltration equation. It is known that this solution by itself is a poor model for vertical infiltration. In the present study the deterministic solution was compared with the observed data presented by Liakopoulus (1965), by computing eq.(IV.61) with the same initial condition presented in the above study. It was found that the deterministic solution substantially underestimates the values of the water content. This may indicate that the simulated values of D and u are probably lower in magnitude than the ones adopted. However this modification of the parameters would not produce a good fit with the observed data because the deterministic solution does not include the physical dependence between the parameters and θ. This suggests that a better deterministic solution should account for the high values in D and u in zones of high θ and the low values in

the parameters in zones of low θ. However, a deterministic solution which includes this parameter dependence with the water content is very difficult to derive. No further analysis or "calibration" of this component was attempted, since the motivation of the present work is the understanding that the deterministic, linearized, solution is not an appropriate tool to represent real field conditions. In the present study this component is only a part of the total stochastic solution.

For the rest of this study an arbitrary initial condition was assumed and its evolution over time was computed after eq.(IV.60). Fig. IV.8 illustrates the behaviour of the deterministic component.

Now the second term in eq.(IV.50) is the partial solution due to the stochastic boundary condition, $\Phi(z, t)$, which is given by eq.(IV.47). Here the sample boundary water content values were discretized at 1 *day* intervals. Thus

$$\Phi(z, t, \omega) = \frac{Z}{(4\pi D)^{1/2}} \sum_{j=1}^{j=t} \int_{j-1}^{j} \exp[-\frac{(Z - u(t-\tau))^2}{4D(t-\tau)}] \frac{\theta_j' e^{-\alpha\tau}}{(t-\tau)^{3/2}} d\tau, \qquad \text{(IV.66)}$$

where θ_j' is the initial value of the boundary water content, θ_0, at the left boundary of the time interval (that is at the time $\tau = j-1$); and $\tau \in (j-1, j]$. Each step-wise integral was solved by a 24 point Gauss-Legendre quadrature with good results. Again accuracy was tested first by setting θ_j' and $e^{-\alpha\tau}$ equal to one and assuring that Φ was equal to one.

Fig. IV.9 shows the boundary component of the stochastic solution with respect to time at three different depths. It was found that the closer the observation point is to the upper boundary, the higher the variability in the water content due to the random nature of rainfall. This would explain the difficulty in forecasting the water content near the ground surface. As depth increases, the boundary component of the water content will take longer time to react and its variation over time is smoother. Thus for depths beyond 0.8 m the water content will slowly increase to a steady mean value and its variability over time with respect to this mean value will be small. This feature is

in agreement with field observations of the water content which seem to indicate that the water content in deep soils tend to maintain a steady constant value even though the rainfall on the surface is highly variable.

It is interesting to observe the spatial variability of the water content at different times. Fig. IV.10 illustrates the water content versus depth at different times. Note that as time increases, the water content profile tends to a smooth steady curve.

The calculation of the third term in eq.(IV.50) involves the generation of sample functions of the colored noise process representing the time variations in the soil-water diffusivity, D'. Generation of sample functions of a colored noise process with correlation function given by eq.(IV.43) can be easily achieved by making the transformation $q = \frac{\sigma^2\rho}{2}$ and noting that a zero-mean stationary Gaussian process with exponential correlation

$$E\{D'(t_1)D'(t_2)\} = \frac{\sigma^2\rho}{2}e^{-\rho(t_1-t_2)} \tag{IV.67}$$

can be generated by an ordinary differential equation forced by white Gaussian noise (Jazwinski, 1970):

$$\frac{dD'(t)}{dt} + \rho D\,(t) = \sigma\rho\frac{d\beta(t)}{dt}, \tag{IV.68}$$

subject to $D'(t=0) = D_0'$, where D_0' follows a normal distribution $N(0, \frac{\sigma^2\rho}{2})$; and $\frac{d\beta(t)}{dt} = w(t)$ is white Gaussian noise with

$$E\{w(t)\} = 0, \qquad E\{w(t_1)w(t_2)\} = \delta(t_1 - t_2). \tag{IV.69}$$

The solution of eq.(IV.68) is

$$D'(t) = D_0'e^{-\rho t} + \sigma\rho\int_0^t e^{-\rho(t-s)}w(s)ds, \tag{IV.70}$$

which can be used to generate sample functions of D'.

This equation can be further reduced after recalling that the typical time scale in our simulations is one day and assuming that any time variation in an interval of less than a day is not recognized. This is equivalent to assume that the w process is constant in intervals of one day. Thus eq.(IV.70) becomes

$$D'(t) = D_0' e^{-\rho t} + \sigma\rho \sum_{j=1}^{j=t} w(j) \int_{j-1}^{j} e^{-\rho(t-s)} ds, \tag{IV.71}$$

where $w(j)$ is the value of the white Gaussian noise process at discrete times $j = 1, 2, \ldots, t$. Solving the integral this equation reduces to

$$D'(t) = D_0' e^{-\rho t} + \sigma e^{-\rho t}(1 - e^{-\rho}) \sum_{j=1}^{j=t} w(j) e^{-\rho j}. \tag{IV.72}$$

This equation was used to generate realizations of the D' process which was needed in the calculation of the third term in eq.(IV.50). Since the colored noise variance parameter was previously chosen as $q = 1.56\ m^2.day^{-1}$, and $\rho = 0.5$, then $\sigma = 2.5$.

The third term in eq.(IV.50) is due to the random component in the soil-water diffusivity, D', in the stochastic equation (IV.44). This term was first approximated as

$$I(t) = \sum_{j=1}^{j=t} D_j' \int_{j-1}^{j} J_{t-\tau} \Delta^2 (J_\tau \Phi_{j-1}) d\tau, \tag{IV.73}$$

where $\Delta^2(\ )$ is a suitable forward finite difference approximation of the spatial second derivative; D_j' is the value of D' at time j; and Φ_{j-1} is the value of the boundary solution along depth at time $j-1$. Since the differentiation operation may be an unstable procedure, some smoothing of the function $J_\tau \Phi_{j-1}$ may be useful. Each of the t integrals was solved using a Gaussian quadrature. It was found that this procedure took too long in a micro-computer and a further simplification was formulated as follows:

$$I(t) = \sum_{j=t-1}^{j=t} J_{t-j} D_j' \Delta^2 (J_j \Phi_{j-1}). \tag{IV.74}$$

In this case $I(t)$ was approximated stepwise and computational time was drastically reduced.

Fig. IV.11 shows a sample function of the I component of the water table generated from eq.(IV.74). Note that sometimes this component will lead the total value of the water content beyond the interval 0-30%. As with any statistical analysis, the physical bounds will limit the numerical value of the sample function.

Adding the three components of eq.(IV.50) (Figs. IV.8, IV.9, and IV.11, corresponding to eqs.IV.69, IV.74 and IV.82 respectively), we obtain the total sample water content, an illustration of which is shown in Fig. IV.12. In this example the first 0.6 m of the soil profile is maintained at saturation. This only reflects the particular choice of parameters and the nature of the forcing rainfall used in the present example. It was earlier noted that saturation may rarely occur in the boundary layer and therefore the boundary water content values used in this example are probably too high. In any case, the soil moisture profiles will be spatially smooth curves, varying erratically in time, which describe the random nature of the water content due to the random nature of the forcing rainfall and the random nature of the hysteresis process.

The next step is the calculation of the mean water content as given by eq.(IV.59). First we compute the mean boundary component, $E\{\Phi(z, t)\}$, by using eq.(IV.52). This equation was approximated using a similar procedure to the one used to calculate the sample $\Phi(z, t)$ values, except that in this case the integral was much easier to solve. Fig. IV.13 shows the mean boundary component with respect to time at three different depths in the soil. It is illustrative to compare these means with the sample boundary components at corresponding depths (Fig. IV.9). Using this information and eq.(IV.59), the mean water content was computed and plotted with respect to time for the same typical depths (Fig. IV.14). Again the shape of these curves reflect the particular choice in the parameters, the properties of the forcing rainfall, and the particular choice in the initial condition for the simulation.

The next step is the calculation of the variance of the water content as described by eq.(IV.60). First we compute the variance of the boundary component $Var\{\Phi\}$, which was done in a similar way to the calculation of the mean, $E\{\Phi\}$. Fig. IV.15 describes the mean and one standard deviation of the boundary component with respect to time at $z = 1.0\ m$. The large values in the variance reflect the high variability of the rainfall used in the simulation. It was also found that low values in the parameter α, that is an upper layer of soil which quickly looses water through evapotranspiration, results in significantly lower values in the variance of the boundary component at depth.

The second term in eq.(IV.60) is the variance of I, $Var\{I(t)\}$, which was approximated from eq.(IV.58) as follows:

$$Var\{I(t)\} = q \sum_{k=t-1}^{k=t} \sum_{j=t-1}^{j=t} J_{t-k} J_{t-j} e^{-\rho(k-j)} \Delta^2 [E\{\Phi(k)\Phi(j)\}], \qquad \text{(IV.75)}$$

where the correlation of Φ is given by similar approximation of eq.(IV.54). It was found that the mean of I was about 7.2 and the standard deviation was 9.6. In Fig. IV.11 the mean plus and minus one standard deviation of I was plotted. Finally eq.(IV.60) will give the variance of the water content.

The results indicate that the variance of the predicted water content is largely dominated by the variance of the boundary component. The particular selection in the parameters of the boundary component produced large variance values which in some cases force the theoretical water content beyond the physically realizable values. This indicates that the variability of rainfall selected for the example calculations is probably too high. The results also suggest that the modeler should perform a series of measures of the upper-soil water content in order to determine the stochastic properties of the boundary component. this exercise will in turn tend to reduce the variance in the predicted water content at depth.

CHAPTER V - PRACTICAL MODELS FOR THE DIRECT AND INVERSE PROBLEMS

In this section we attempt to present a balanced methodology to investigate the effect of random variability, or uncertainty, in the values of physical parameters involved in groundwater differential equations on the behaviour of the dependent variables. A "balanced" methodology, in our opinion, implies a procedure the modeler may use to either forecast the statistical properties of the dependent variable knowing the corresponding statistical properties of the uncertain parameter, or estimate the parameters of the random process assumed to describe the random nature of the parameter knowing the statistical properties of the groundwater dependent variable. Since parameter uncertainty seems to pose a challenging problem in subsurface hydrology today, a methodology which draws from the same consistent theoretical background for either the direct of the inverse problem may be found useful.

The procedure is based on the concepts introduced in chapter II, which may be found to be related to linear systems theory of deterministic ordinary differential equations, and its extension to some non-linear cases, and therefore a fundamental element is the derivation of a system impulse response function, which we previously called the semigroup operator. In this section new extensions to the important case of spatial parameter variability and to cases where popular numerical methods can be used. It is emphasized throughout the necessary steps to transform the governing differential equation subject to parameter uncertainty into a stochastically-forced evolution equation whose solution is straight forward. Thus the solution will employ a deterministic impulse response function which will be contained within every term of the approximation. The method is specifically suited for the investigation of the effect of high variability or high uncertainty in the parameters; the solution of the equations is systematic; the method is accurate and the computational effort is small; it does not require

artificial logarithmic transformations of the parameter; it does not require parameter variability to be small (small perturbation methods); and it does not require spectral decomposition or any other domain transformation for the solution.

Section V.1 concentrates on models applicable to cases where the input random processes are general space and time random functions. First a deterministic example is presented with the purpose of illustrating the general methodology, the stability of the approximations and the convergence rate. Then an application to the investigation of groundwater pollution subject to spatial variability in the velocity field is studied. Section V.2 introduces models based on semi-analytical solutions of the stochastic differential equation, which can be employed when the input uncertainty occurs with respect to only one of the independent variables and therefore use the convenient features of numerical methods. The handling of the resulting stochastic matrices is with a groundwater flow case subject to time variability in the transmissivity. The case when spatial erratic variability in the transmissivity is present is discussed, and a groundwater pollution case when spatial erratic variability in the velocity field is the most important uncertainty term is also discussed. Finally in section V.3 we introduce a method for the parameter estimation of random processes involved in groundwater differential equations and for the estimation of the mean value of the equation physical parameters. This method utilizes the solution of the stochastic differential equation, and therefore the system impulse response function, rather than the differential equation itself along with field measurements of the dependent variable.

V.1.1. Models to Investigate the Effect of Parameter Variability

Before studying the effect of random variability of a system parameter on the dependent variable of a groundwater differential equation, let us visualize the accuracy

of the decomposition method with a simple deterministic example. Consider the problem of groundwater pollution by a conservative contaminant in an infinite homogeneous aquifer, as governed by the advective-dispersive equation:

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} = 0, \tag{V.1}$$

$$C(-\infty, t) = C(\infty, t) = 0, \quad C(x, 0) = C_0(x),$$

where C is the contaminant concentration (mgr/lit); D is the average aquifer dispersion coefficient (m^2/day); u is the average aquifer pore velocity (m/day); x is horizontal distance from an origin (m); t is time (day); and the initial condition, C_0 is a smooth known function of x.

The solution to this differential equation is (Serrano, 1988(2))

$$C(x, t) = J(x, t)C_0 = \frac{1}{(4\pi Dt)^{1/2}} \int_{-\infty}^{\infty} \exp[-\frac{(x - ut - s)^2}{4Dt}] C_0(s)ds, \tag{V.2}$$

where J is the impulse response function (in this case the strongly continuous semigroup) associated with the spatial differential operator in eq.(V.1). Now assume that the initial condition may be represented as an impulse function of magnitude equal to 10 mgr/lit for $30 \leq x \leq 50$, and equal to zero everywhere else, that is

$$C_0(x) = 10H(x - 30).H(x - 50), \tag{V.3}$$

where $H(\ )$ denotes the unit step function. This initial condition would represent an accidental spill penetrating the saturated zone at an average concentration of 10 mgr/lit over an area 20 m in length. Substituting eq.(V.3) into eq.(V.2) yields

$$C(x, t) = \Phi(x, t) = 5\{erf[\frac{30 - x + ut}{(4Dt)^{1/2}}] - erf[\frac{50 - x + ut}{(4Dt)^{1/2}}]\}, \tag{V.4}$$

where $erf(\ )$ denotes the "error function".

Let us now assume that we wish to investigate the effect of an increase of 100% in the magnitude of the velocity field u. In that case, eq.(V.1) becomes

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} = -u\frac{\partial C}{\partial x}. \tag{V.5}$$

The solution to this equation is

$$C(x,\, t) = J(x,\, t)C_0 - u\int_0^t J(x,\, t-\tau)\frac{\partial C}{\partial x}d\tau, \tag{V.6}$$

which can be expanded as

$$C(x,\, t) = \Phi(x,\, t) - u\int_0^t \frac{1}{(4\pi Dt)^{1/2}}\int_{-\infty}^{\infty} \exp[-\frac{(x-ut-s)^2}{4Dt}]\frac{\partial C(s,\, \tau)}{\partial s}dsd\tau, \tag{V.7}$$

after using eqs.(V.2) and (V.4).

We now expand C in the right side of eq.(V.7) as the series (Serrano, 1988(2)) $C = C_1 + C_2 + \cdots$, and set $C_1 = \Phi$, which is the first and most important partial solution. In general

$$C_i = -u\int_0^t J(x,\, t-\tau)\frac{\partial C_{i-1}}{\partial x}d\tau, \quad i \geq 2. \tag{V.8}$$

Thus the equation describing concentration in the aquifer subject to a 100% increase in the velocity field will read

$$C(x,\, t) = \Phi(x,\, t) - u\sum_{i=1}^{N}\int_0^t J(x,\, t-\tau)\frac{\partial C_{i-1}}{\partial x}d\tau, \tag{V.9}$$

subject to eq.(V.8). N is a suitable number of iterations such that C reaches a degree of accuracy on the order of the representative scale of resolution of the concentration measurement device used in the field. In cases when the impulse response function has well-behaved first and second derivatives, and when the domain has homogeneous boundary conditions, integration by parts of the integral term in eq.(V.9) may significantly simplify the solution and increase the convergence speed. In that case numerical evaluation of the derivatives of previous iterations is not necessary and stability improves substantially.

As an illustrative example, assume an initial velocity $u = 0.2\ m/day$, $D = 0.1\ m^2/day$ and and compute the breakthrough curves at $t = 30\ days$ after the spill. Fig. V.1 illustrates the exact concentration magnitude versus distance, the concentration as obtained by the one approximation, and the concentration as obtained by two approximations. The exact concentration versus distance, was calculated from eq.(V.4) for $u = 0.4\ m/day$, after the 100% increase in the original velocity. The concentration by one approximation was computed from eq.(V.9) with $u = 0.2\ m/day$, and corresponds to the first term in the equation. The concentration by two approximations was obtained by adding the first two terms in eq.(V.9) with $N = 1$. Thus Fig. V.1 illustrates that the concentration profile after an increase in the velocity field of as much as 100% of the original magnitude is accurately estimated after the first two approximations in eq.(V.9). The effect of an increase of 120%, or higher, in the original value of the velocity field can be accurately estimated by three approximations. Fig. V.2 illustrates the first three approximations individually. Note the uniform convergence of the approximation.

The programming effort or computer time required for the implementation of eq.(V.9) is not high. A simple 24-point Gauss-Legendre quadrature was employed for the integral term with a first-order central finite difference approximation for the derivative within the integral. The term $\frac{\partial C_1(s,\tau)}{\partial s}$ was approximated as $\frac{\partial C_1(s,\,t)}{\partial s}$, under the assumption that the change in the basic shape of C_1 is small within the simulation period of 30 *days*, as compared to its spatial variability. As with any other numerical approximation scheme, care should be taken to control unstability between iterations. In the example in question, the infinite integral was accurately estimated by dividing it into three parts: $0 \leq x < 36$, $36 \leq x < 56$, and $56 \leq x < 80$. Observing that every subsequent iteration is based on the previous approximation (see eq.(V.8)), error propagation or magnification should be minimized by smoothing, or curve interpolation, of each iteration. This is specially true after the third iteration and when the

equation contains random terms.

The above example illustrates the important advantages of the decomposition method we already mentioned.

V.1.2. Groundwater Pollution Subject to a Spatially Erratic Velocity Field

Consider again the modeling problem of section V.1.1 and assume that the hydrogeology of the area is such that the measured groundwater velocities at discrete points in the aquifer over a long period of time suggest that the velocity field is a highly variable (uncertain) function which could be described as $u(x, \omega) = \bar{u} + u'(x, \omega)$, where $\bar{u}$ is a long-term mean, $u'(x, \omega)$ represents the zero-mean spatially random component in the velocity field, and ω is the probability variable. In this case eq.(V.1) becomes

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + \bar{u}\frac{\partial C}{\partial x} = -u'\frac{\partial C}{\partial x}, \tag{V.10}$$

subject to the same set of boundary conditions. Proceeding in a similar manner as before, the solution to this equation is

$$C(x,t)=\Phi(x,t)-\sum_{i=2}^{N}\int_0^t \frac{1}{(4\pi D(t-\tau))^{1/2}}\int_{-\infty}^{\infty}\exp\left[-\frac{(x-\bar{u}(t-\tau)-s)^2}{4D(t-\tau)}\right]u'(s,\omega)\frac{\partial C_{i-1}(s,\tau)}{\partial s}\,ds\,d\tau, \tag{V.11}$$

subject to $C_1(x, t) = \Phi(x, t)$, $\Phi(x, t)$ as given by eq.(V.4) if we use the same initial condition eq.(V.3), and

$$C_i=-\int_0^t \frac{1}{(4\pi D(t-\tau))^{1/2}}\int_{-\infty}^{\infty}\exp\left[-\frac{(x-\bar{u}(t-\tau)-s)^2}{4D(t-\tau)}\right]u'(s,\omega)\frac{\partial C_{i-1}}{\partial s}\,ds\,d\tau,\ i\geq 2. \tag{V.12}$$

Note that the impulse response function is the same as that given by eq.(V.2) with $\bar{u}$ instead of u, and $(t - \tau)$ instead of t. Eq.(V.11) can be used to generate sample functions to observe the qualitative nature of the concentration evolution if sample functions of u' are available. In most engineering applications, however, only the first lower

order moments are available after statistical inference on the limited historical measurements of the velocity field. Thus it seems natural to develop expressions which would describe the corresponding lower order moments of the concentration field. According to the earlier results in this section a value of $N = 1$ in eq.(V.11) produced an accurate estimation of the concentration. After taking expectations on both sides of eq.(V.12) we obtain the mean concentration:

$$E\{C(x, t)\} = \Phi(x, t), \tag{V.13}$$

where $E\{\ \}$ denotes the expectation operator. For $N = 1$ the mean concentration coincides with the deterministic component. It is a modeling decision to include additional terms if it is judged that the variances of u' are so high that the first approximation is crude. The computational effort required by additional terms is small. Fig. V.3 shows the mean concentration versus distance 30 *days* after the spill according to eq.(V.13), and one sample realization of the concentration using eq.(V.11) with the same deterministic parameters as before. In this experiment the random component of the velocity field, u', was assumed to follow a Gaussian colored noise process in space with variance parameter $q = 0.1$ and decay parameter $\rho = 0.01$ (see eq.(V.14)). This is a common assumption adopted by researchers, but of course in practical applications the functional form of u' must be supported by long-term field measurements. A sample function of a colored-noise groundwater velocity with the above properties is necessary in eq.(V.11) in order to obtain a sample function of the concentration. For the practical details about the numerical generation of such a sequence the reader is referred to Serrano (1990(1)). Fig. V.3 indicates that the lowest variability in the concentration field appear where the concentration gradients tend to zero.

The variance and the covariance of the concentration can be derived from the two-point (time or space) correlation function, which in turn depends on the correlation structure of the groundwater velocity as derived from field measurements. The correlation function of the colored-noise velocity field assumed before is defined as

$$E\{u'(x_1, t)u'(x_2, t)\} = R_u(x_1, x_2) = qe^{-\rho|x_1-x_2|}, \tag{V.14}$$

where q and ρ are constants. Using eq.(V.11), the variance of the concentration at a particular point in time and space reduces to

$$\sigma^2_{C(x,t)} = q\int_0^t\int_0^t J(x, s, t-\tau)J(x, \xi, t-\gamma)e^{-\rho|s-\xi|}\frac{\partial\Phi(s, \tau)}{\partial s}\frac{\partial\Phi(\xi, \gamma)}{\partial\xi}d\gamma d\tau, \tag{V.15}$$

where the approximation $N = 1$ has been adopted again. An additional approximation which seems to produce reasonable results is $\frac{\partial\Phi(s, \tau)}{\partial s} = \frac{\partial\Phi(s, t)}{\partial s}$ for all τ. Care should be taken to minimize unstability in the computation of the concentration variance. Fig V.4. shows the standard deviation of the concentration versus distance 30 *days* after the spill according to eq.(V.15). Once again, the lowest values of the standard deviation occur at locations where the concentration gradient tends to zero, that is at $x \leq 33$, $x \geq 57$, and particularly at the peak concentration, $43 \leq x \leq 48$. The highest values of the standard deviation (the expected highest variability in concentration values) occur at locations where the concentration gradients are maximum, that is at $36 \leq x \leq 40$ and at $51 \leq x \leq 55$. This phenomenon can be interpreted from eq.(V.15) and an observation of Fig. V.3. All the computations in this section were done by writing corresponding programs in C and running them in UNIX-based micro and mini-computers.

V.2. Special Cases with Semi-Analytical Solutions

The methodology illustrated in the previous sections is systematic and general enough to handle cases when the parameter uncertainty entering the differential equation is modeled as a time and space random process. In such a case the development of numerical solutions of the stochastic differential equation is not straight forward, since

the solution of the equation constitutes a family of functions (a random process) for which the finite difference derivatives have to be defined. Thus the discretization of the differential equation has to be carefully investigated to assure that the solution of the discretized equation satisfies in some specified sense the original differential equation.

Some modeling problems allow a discretization in certain dimension and therefore the advantages of numerical methods can be beneficial. In certain circumstances the modeler observes that the variability associated with one or more of the parameters is more important with respect to one of the independent variables. In these cases where the stochasticity is important with respect to one of the independent variables, and negligible with respect to the other independent variables, certain simplifications which reduce the complexity of the impulse response function and that of the solution are possible.

V.2.1. Regional Groundwater Flow Subject to Time-Variable Transmissivity

Consider the case of a two-point boundary-value problem describing regional groundwater flow in a horizontal phreatic aquifer bounded by rivers. Assume that the fluctuation of the aquifer transmissivity is a highly variable time function while at the same time its bulk magnitude, as estimated by a series of pumping tests, does not change drastically with respect to distance. The governing differential equation reduces to

$$\frac{\partial h}{\partial t} - \frac{T(t,\omega)}{S}\frac{\partial^2 h}{\partial x^2} = \frac{i(t)}{S}, \qquad \text{(V.16)}$$

$$h(0,t) = h_1, \quad h(L,t) = h_2, \quad h(x,0) = h_0(x),$$

where $h(x, t, \omega)$ is the elevation of the water table (Dupuit assumptions) with respect to the bottom of the aquifer (m); x is the horizontal distance from the left boundary

(m); h_1 and h_2 are the constant left and right heads at the rivers respectively (m); h_0 is a smooth initial head across the aquifer, as interpolated from a few field piezometers; L is the length of the aquifer (m); t is the time coordinate $(days)$; S is the aquifer specific yield; $T(t, \omega)$ is the time random process representing the aquifer transmissivity (m^2/day); and $i(t)$ is the aquifer recharge, which in this case is assumed spatially independent (m).

Eq.(V.16) can be further reduced after assuming $h(x, t) = V(x) + u(t, x, \omega)$ where $V(x) = h_1 + \frac{h_2 - h_1}{L}x$ is a smooth steady state function and u is the stochastic transient function satisfying

$$\frac{\partial u}{\partial t} - \frac{T(t, \omega)}{S}\frac{\partial^2 u}{\partial x^2} = \frac{i(t)}{S}, \tag{V.17}$$

$$u(0, t) = u(L, t) = 0, \quad u(x, 0) = h_0(x) - V(x).$$

Now assume that the transmissivity function can be defined as $T(t, \omega) = \bar{T} + T'(t, \omega)$, where $\bar{T}$ represents the average transmissivity and T' represents the zero-mean random component. Thus eq,(V.17) becomes

$$\frac{\partial u}{\partial t} - \frac{\bar{T}}{S}\frac{\partial^2 u}{\partial x^2} = \frac{i(t)}{S} + \frac{T'}{S}\frac{\partial^2 u}{\partial x^2}. \tag{V.18}$$

The similarity of eq.(V.18) to eq.(V.10) may suggest a straight-forward solution at this stage. However due to the fact that eq.(V.18) is an evolution equation forced by a time stochastic process a discretization with respect to distance is plausible.

Let us formally subdivide the spatial domain into $n + 2$ nodes equally spaced by a distance Δx, so that $k = 0$ at $x = 0$ and $k = n + 1$ at $x = L$. Discretizing the spatial derivatives with a simple central finite-difference approximation, eq.(V.18) for the node k at time t will be

$$\frac{\partial u_k}{\partial t} - \frac{T}{S}\left(\frac{u_{k-1} - 2u_k + u_{k+1}}{\Delta x^2}\right) = \frac{i}{S} + \frac{T'}{S}\left(\frac{u_{k-1} - 2u_k + u_{k+1}}{\Delta x^2}\right). \qquad \text{(V.19)}$$

After applying this equation to every node, including the boundary nodes, we can write the resulting system of differential equations in matrix form:

$$\frac{dU(t,\omega)}{dt} - \bar{A}U(t,\omega) = G(t) + A'(t,\omega)U(t,\omega), \quad U(0) = U_0, \qquad \text{(V.20)}$$

where U is a $n \times 1$ unknown column vector containing the values of u_k at the different nodes; $\bar{A}$ is a $n \times n$ conductivity matrix containing values of $\bar{a} = \dfrac{T}{S.\Delta x^2}$; G is the known column vector containing recharge values, $b = \dfrac{i(t)}{S}$; A' is a square random matrix identical in form to A, except that instead of constants, a, it contains the random processes $a' = \dfrac{T'}{S\ \Delta x^2}$; and U_0 is the known column vector containing the initial condition, u_{0_k}. The arrays are respectively

$$U = \begin{bmatrix} u_1 \\ u_2 \\ . \\ . \\ . \\ u_n \end{bmatrix}; \quad \bar{A} = \begin{bmatrix} -2\bar{a} & \bar{a} & 0 & 0 & . & . & . \\ \bar{a} & -2\bar{a} & \bar{a} & 0 & . & . & . \\ 0 & \bar{a} & -2\bar{a} & \bar{a} & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{bmatrix}; \quad G = \begin{bmatrix} b \\ b \\ b \\ . \\ . \\ . \end{bmatrix}; \quad U_0 = \begin{bmatrix} u_{0_1} \\ u_{0_2} \\ . \\ . \\ . \end{bmatrix}$$

Thus we have reduced the stochastic partial differential equation (V.18) into an ordinary vector stochastic differential equation (V.20) whose impulse response function, and therefore its solution, is simpler. However the price to be paid is measured in terms of loss of stability, increased computer space and time requirements.

The solution to eq.(V.20) is

$$U(t,\omega) = J(t)U_0 + \int_0^t J(t-s)A'(s,\omega)U(s)ds, \qquad \text{(V.21)}$$

where

$$J(t) = e^{\bar{A}t} = I - \bar{A}t + \frac{\bar{A}^2t^2}{2!} - \frac{\bar{A}^3t^3}{3!} + \cdots$$

is the impulse response function; and I is the identity matrix. The computation of the impulse response function, or the exponential of a matrix in this case, should not be done by the approximation of its formal Taylor series expansion, since the results may prove inaccurate. Many different methods about how to approach the problem are contained in Moler and Van Loan (1978) and Umari and Gorelick (1986). For the present application we note that if the eigenvectors associated with the matrix $\bar{A}$ are linearly independent, then an $n \times n$ modal matrix M may be formed (that is a square matrix whose columns each contain an eigenvector of $\bar{A}$) from the eigenvectors and the similarity transformation (Kraus, 1987)

$$S = M^{-1}\bar{A}M,$$

with M^{-1} the inverse of M, can be used to diagonalize $\bar{A}$ into the spectral matrix S composed of the eigenvalues, λ, of $\bar{A}$:

$$S = \begin{bmatrix} \lambda_1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ 0 & 0 & \lambda_3 & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdots & 0 \\ 0 & 0 & 0 & \cdots & \lambda_n \end{bmatrix}.$$

The matrix $\bar{A}$ can be reclaimed from its spectral matrix via $\bar{A} = MSM^{-1}$. Any functional of $\bar{A}$ can be expressed as $f(\bar{A}) = f(MSM^{-1}) = Mf(s)M^{-1} = Mf(\lambda)M^{-1}$. This expression may well be the simplest method for the evaluation of of the exponential of a matrix, that is $J(t) = e^{\bar{A}t} = Me^{st}M^{-1}$.

Returning to the solution equation (V.21), and following the same procedure of

and following the same procedure of section 2 for the approximation of the third term in the equation we obtain

$$U(t,\omega) = J(t)U_0 + \int_0^t J(t-s)G(s)ds + \sum_{i=1}^{N}\int_0^t J(t-s)A'(s,\omega)U'_i(s,\omega)ds. \quad \text{(V.22)}$$

For practical applications sample functions of a' in A' and measured values of b in G are approximated as staircase sequences. Setting $t = 1$ *day* (an assumed representative time scale for the recharge), then we can simulate realizations of U recursively at intervals of time one day apart:

$$U(t) = J(1)U_{t-1} + [\int_0^1 J(1-s)ds]G(t) + \sum_{i=1}^{N}\int_0^1 J(1-s)A'(t)U'_i(s)ds, \quad \text{(V.23)}$$

where G and A' are constants within the integration limits. A further simplification is obtained with the trapezoidal rule, valid for small Δt,

$$U(t) = J(1)U_{t-1} + \tfrac{1}{2}(I + J(1))G(t) + \tfrac{1}{2}(I + J(1))A'(t)\sum_{i=1}^{N}U'_i, \quad \text{(V.24)}$$

where the semigroup properties of the impulse response matrix have been used (Serrano, 1988(1)); $U'_1 = J(1)U_{t-1}$, the first term in eq.(V.24), and in general

$$U'_i = \tfrac{1}{2}(I + J(1))A'(t)U'_{i-1}.$$

Eq.(V.24) indicates that realizations of the groundwater table elevation U_t can be forecasted based on the previous realization U_{t-1}. This can be easily done if sample functions of the elements a' of A' are available. In the present experiment we assumed a' to be a white Gaussian noise process, that is $E\{a'(t)\} = 0$ and $E\{a'(t_1)a'(t_2)\} = q\delta(t_1 - t_2)$, where $\delta(\ )$ is the Dirac's delta function and q is the variance parameter. Thus sample functions of the vector U in eq.(V.24) can be computed by using generated white Gaussian noise sequences (Jazwinski, 1970).

From eq.(V.22), assuming $N = 1$ is sufficiently accurate, we may derive the mean of U as

$$E\{U(t)\} = J(t)U_{t-1} + \int_0^t J(t-s)G(s)ds, \tag{V.25}$$

which coincides with the deterministic solution. $E\{U(t)\}$ is a $n \times 1$ vector whose elements are $E\{u_k\}$, $k = 1,..., n$. From eq.(V.22) the two-point correlation function can be derived. Combining the correlation function and the mean, it is easy to show that the variance of U is

$$\sigma^2_{U(t)} = q\int_0^t J(V. - 2s)A^2 J(V.)[U_{t-1}.U_{t-1}]_{n\times n}, \tag{V.26}$$

where the product of the U_{t-1} vectors is the "outer product" making a square matrix; and the matrix A^2 contains as elements the coefficients (either 0, 1 or -2) of A'. We can approximate a variance expression consistent with the sample functions model (eq.(V.24)) by integrating at $\Delta t = 1$ *day* intervals.

$$\sigma^2_{U(t)} = \frac{q}{2}\{[J(V.A^2[U^2_{t-1}]_{n\times n}] + [J(1)A^2 J(V.[U^2_{t-1}]_{n\times n}]\}, \tag{V.27}$$

where $\sigma^2_{U(t)}$ is a $n \times n$ covariance matrix. This equation indicates that the head variance at any point at time t in the aquifer may be calculated based on the aquifer heads at time $t-1$. We note in passing that we are dealing with matrices whose unstability should be minimized, particularly when high recharge values are present.

As an illustration, simulations were conducted by assuming $S = 0.14$, $L = 10.0\ m$, $\Delta x = 1.0\ m$, $h_1 = h_2 = 1.0\ m$,
$K = 0.06\ m/day$, $T = 0.06\ m^2/day$, and $q = 0.25^2$. Since the calculations involve the estimation of an impulse response matrix, and the recursive evaluation of head vectors and variance matrices, the problem is best suited for a spreadsheet software application. We used a Smart Spreadsheet with Graphics application on a AT&T 7300 UNIX microcomputer. The spreadsheet package offers an ideal environment for the automatic computation of the matrix eigenvalues and eigenvectors necessary for the evaluation of the impulse response matrix. Many other functions can be accessed and

controlled by the user such as the generation of a matrix with random values as elements, which is indispensable in the calculation of heads sample functions. The matrix stability and error propagation can be step-by-step observed in the spreadsheet.

Fig. V.5 is a graphical output from the spreadsheet package implementing eq.(V.24),which illustrates an arbitrary initial head versus distance and two sample functions at $t = 5$ *days* and at $t = 10$ *days*, after an assumed recharge sequence. Fig. V.6 is a breakthrough curve of the groundwater head with time at $x = 5$ m. Fig. V.7 shows the head standard deviation with distance at three different days, as computed from eq.(V.27). As expected the maximum standard deviation occurs in the middle of the aquifer, where the heads are maximum, and zero at the boundaries, where the heads are deterministic. Finally Fig. V.8 shows the mean groundwater head and the mean head plus one standard deviation with respect to time at $x = 5.0$ m.

The above procedure is well suited for the investigation of the variability and the forecasting of groundwater flow subject to the time uncertainty associated with the transmissivity. In general a similar methodology could be developed for the investigation of groundwater pollution when there is a time uncertainty associated with one of the parameters. In either case the discretization in the spatial domain reduces the partial differential equation into an ordinary vector differential equation whose solution is mathematically simpler. However the computational procedure involved in the numerical evaluation of the corresponding matrices has an associated degree of unstability which the modeler has to face.

V.2.2. Regional Groundwater Flow Subject to Spatially-Variable Transmissivity

Consider a similar situation to the one depicted in section V.2.1, but in this case

the dominant uncertainty is associated with spatial variability in the transmissivity, rather than time variability. For instance the series of field-scale values of transmissivity, as obtained from long-term pumping tests, exhibit an erratic behaviour with respect to distance, while they tend to be constant with respect to time at a particular location. This situation is realistic when the evolution of groundwater heads at the chosen representative time scale (i.e., one *day*) is very slow compared with its variability with respect to the spatial coordinates (i.e., the head changes considerable along the aquifer length). Thus the transmissivity may be represented as the random function $T(x, \omega) = T + T'(x, \omega)$, where again T represents the mean value and $T'(x, \omega)$ is a zero-mean spatially random process representing the variability with respect to the mean in the values of the transmissivity. Eq.(V.17) reduces to

$$\frac{\partial u}{\partial t} - \frac{T}{S}\frac{\partial^2 u}{\partial x^2} = \frac{i(t)}{S} + R(x\ \omega)u, \tag{V.28}$$

where the random operator R is given by

$$R(x, \omega)u = \frac{1}{S}(T'(x, \omega)\frac{\partial^2}{\partial x^2} + \frac{\partial T'(x, \omega)}{\partial x}\frac{\partial}{\partial x})u. \tag{V.29}$$

Since the transmissivity varies randomly with respect to distance, then we may discretize the time domain in the differential equation at equal intervals separated by Δt. Replacing the time derivative by a simple backward finite difference approximation, then we can write eq.(V.28) as an ordinary stochastic differential equation whose independent variable is x only and whose dependent variable is is the head at a fixed time t:

$$-\frac{d^2 u}{dx^2} + a^2 u = bi + a^2 u_0 + Ru, \tag{V.30}$$

where $u_0(x)$ is the head across the aquifer at the previous time step $(t - \Delta t)$; $a^2 = \frac{S}{T\Delta t}$; $b = \frac{1}{T}$; i again is the recharge at time t (m); and the operator R is given by eq.(V.29) with the partial derivatives replaced by total derivatives.

The solution to eq.(V.30) is given by

$$u(x, \omega) = \int_0^L J(x, \xi)[bi(\xi) + a^2 u_0(\xi)]d\xi + \int_0^L J(x, \xi)R(\xi, \omega)u(\xi)d\xi, \tag{V.31}$$

where $J(x, \xi)$ is the impulse response function associated with the ordinary differential operator in eq.(V.30). It is easy to show that this function is given by (Serrano, 1990(2))

$$J(x, \xi) = H(\xi - x)J_1(x, \xi) + H(x - \xi)J_2(x, \xi), \tag{V.32}$$

where $H(\ )$ is the unit step function;

$$J_1(x, \xi) = C_2(\xi)\sinh(ax); \tag{V.33}$$

$$J_2(x, \xi) = C_3(\xi)\cosh(ax) + C_4(\xi)\sinh(ax); \tag{V.34}$$

$$C_2(\xi) = C_4(\xi)[1 - \frac{\tanh(aL)}{\tanh(a\xi)}]; \tag{V.35}$$

$$C_3(\xi) = -C_4(\xi)\tanh(aL); \tag{V.36}$$

$$C_4(\xi) = \frac{1}{a\tanh(aL)[\sinh(a\xi) - \frac{\cosh(a\xi)}{\tanh(a\xi)}]}; \tag{V.37}$$

and sinh( ) denotes the hyperbolic sine function. We now follow a procedure similar to the applied in the previous problems for the treatment of u in the last right-hand term of eq.(V.31). Thus the general solution of eq.(V.30) reduces to

$$u(x, \omega) = a\int_0^L J(x, \xi)u_0(\xi)d\xi + b\int_0^L J(x, \xi)i(\xi)d\xi + \sum_{i=1}^{N}\int_0^L J(x, \xi)R(\xi, \omega)u_i(\xi)d\xi \tag{V.38}$$

subject to

$$u_1(\xi) = \Phi(\xi) = a\int_0^L J(x, \xi)u_0(\xi)d\xi,$$

which is the first term in the right side of eq(V.38), and in general

$$u_i(\xi) = \int_0^L J(x, \xi) R(\xi, \omega) u_{i-1}(\xi) d\xi.$$

Eq.(V.38) indicates that we can generate sample realizations of the groundwater head recursively, step by step in time. For instance, the heads across the aquifer at time t can be forecasted if the observed or generated values of the head at time $t - \Delta t$ and sample functions of the processes T' and $\frac{dT'}{dx}$ are available. Generally eq.(V.38) is evaluated numerically using an appropriate quadrature.

Difficulty arises with the evaluation of the third term in the right-side of the equation since it contains derivatives of the u_{i-1}, the previous iteration. For values of $N \leq 2$, and with relatively low variances in the random terms, unstability may be kept under control. For greater values of N and for large variances, "smoothing" of each iteration may increase the speed of convergence and minimize unstability of the solution. The physical reasoning behind this smoothing is the fact that the phreatic surface in between piezometric measurements is a smooth curve whose spatial derivatives are bounded. An objective way to smooth each iteration is to fit a polynomial of the form $u_{i-1} = a_0 + a_1 x + a_2 x^2 + ... + a_n x^n$ and to use its algebraic expression to compute the derivatives of u_{i-1}. By choosing n points from the raw values of the previous iteration, u'_i for $i = 0, ..., n$, forming the Vandermonde matrix (Chapra and Canale, 1988) and the vector equation

$$\begin{bmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ 1 & x_2 & x_2^2 & \cdots & x_2^n \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \cdot \\ \cdot \\ \cdot \\ a_n \end{bmatrix} = \begin{bmatrix} u'_0 \\ u'_1 \\ u'_2 \\ \cdot \\ \cdot \\ \cdot \\ u'_n \end{bmatrix},$$

one can calculate the coefficients a_i. This can be easily done by inter-facing a

subroutine to solve the above vector equation with the main program doing the actual iteration for u.

For the present experiment we assumed the random component of the transmissivity to follow a colored noise process with the properties $E\{T'(x)\} = 0$ and $E\{T'(x_1)T'(x_2)\} = qe^{-\rho\ x_1 - x_2}$. The first spatial derivative of this process has the properties (Jazwinski, 1970)

$$E\{\frac{dT'(x)}{dx}\} = 0, \quad E\{\frac{dT'(x_1)}{dx}\frac{dT'(x_2)}{dx}\} = \frac{\partial^2}{\partial x_1 \partial x_2} E\{T'(x_1)T'(x_2)\} = \rho^2 q e^{-\rho\,|x_1 - x_2|}.$$

Sample functions of these processes can be generated by a linear ordinary differential equation forced by white Gaussian noise (see Serrano, 1990(1) for details). The mean groundwater head can be computed from eq.(V.38). Assuming that $N = 1$ gives an acceptable degree of accuracy (although this is not always the case) it reduces to

$$E\{u(x)\} = a\int_0^L J(x,\,\xi)u_0(\xi)d\xi + b\int_0^L J(x,\,\xi)i(\xi)d\xi. \tag{V.39}$$

Under the same assumption, the head variance can be deduced from eq.(V.38) as

$$\sigma^2_{u(x)} = \int_0^L\int_0^L J(x,\,\xi)J(x,\,\gamma)E\{R(\xi)R(\gamma)\}\Phi(\xi)\Phi(\gamma)d\xi d\gamma, \tag{V.40}$$

where the correlation of the operator R, after some manipulation is given by

$$E\{R(\xi)R(\gamma)\} = \frac{q}{S^2}e^{-\rho\ \xi-\gamma}\ [\nabla^2_\xi\nabla^2_\gamma - \rho\nabla^2_\xi\nabla_\gamma - \rho\nabla_\xi\nabla^2_\gamma + \rho^2\nabla_\xi\nabla_\gamma], \tag{V.41}$$

and the operator $\nabla^2_\xi\Phi(\xi)$ denotes $\dfrac{\partial^2\Phi(\xi)}{\partial\xi^2}$. The evaluation of eqs.(V.40) and (V.41) has to be done numerically. Fig. V.9 illustrates the mean and the mean plus or minus one standard deviation as computed from eqs.(V.39) and (V.40) respectively, when $q = 1.0$, $\rho = 0.1$, $\Delta t = 1.0\ day$, an arbitrary smooth initial condition u_0, and the rest of the parameters as before. A program in C was written for the calculations. The results obtained with a computer program proved more efficient and with less memory

requirements than comparatively a similar problem run in spreadsheets. However the main advantage of using spreadsheets lies in the possibility to visualize and control the partial results step by step, and the graphics capabilities. A model such as this could be used to forecast the groundwater heads across the aquifer subject to strong and erratic spatial variability in the transmissivity.

V.2.3. Groundwater Pollution Subject to Spatially-Variable Velocity Field

Let us consider again the case of dispersion in an infinite aquifer subject to a space stochastic velocity field as described by eq.(V.10) in section V.1.1. Since $u'(x, \omega)$ is a random process in space, we may attempt a discretization of the time domain with the hope that the resulting ordinary stochastic differential equation is simpler to solve, while maintaining an accurate, stable, estimation of the concentration field. A physical justification comes from the observation that the time evolution of the concentration at a point may be small at intervals of time of a few weeks, while its spatial variability is important. Proceeding as in section V.2.2, eq.(V.10) reduces to

$$\frac{d^2C}{dx^2} - a\frac{dC}{dx} - bC = -(bC_0 - m\frac{dC}{dx}), \tag{V.42}$$

where $a = \frac{\bar{u}}{D}$; $b = \frac{1}{D\Delta t}$; $m = \frac{u'}{D}$; $C_0(x)$ is the concentration at time $t - \Delta t$; $C(x, \omega)$ is the concentration profile at time t; and the rest of the terms as before. The solution to this equation is given by

$$C(x, \omega) = b\int_{-\infty}^{\infty} J(x - \xi)C_0(\xi)d\xi - \sum_{i=1-\infty}^{N}\int^{\infty} J(x - \xi)m(\xi, \omega)\frac{dC_i(\xi)}{d\xi}d\xi, \tag{V.43}$$

subject to

$$C_1(x) = \Phi(x) = b \int_{-\infty}^{\infty} J(x-\xi) C_0(\xi) d\xi,$$

and in general

$$C_i(x) = \int_{-\infty}^{\infty} J(x-\xi) m(\xi, \omega) \frac{dC_{i-1}(\xi)}{d\xi} d\xi.$$

The impulse response function in eq.(V.43) can be found by solving the homogeneous eq.(V.42) after applying the Fourier transformation with complex integration, or any other suitable technique. This will give

$$J(x-\xi) = \frac{1}{2k} e^{-k|x-\xi| + \frac{a}{2}(x-\xi)},$$

where $k = \frac{a^2}{4} + b$.

Comparing the analytical solution of eq.(V.10), that is eq.(2.11), to the corresponding semi-analytical solution eq.(V.43), it is possible to observe that the semi-analytical solution is simpler to evaluate.

The mean concentration function is obtained after assuming an appropriate value of N (i.e., $N = 1$) and taking expectations on both sides of eq.(V.43):

$$E\{C(x)\} = \Phi(x). \tag{V.44}$$

From eqs.(V.43) and (V.44) the variance of the concentration at a point can be deduced as

$$\sigma^2_{C(x)} = \frac{q}{D^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} J(x-\xi) J(x-\gamma) e^{-\rho|\xi-\gamma|} \nabla_\xi \Phi(\xi) \nabla_\gamma \Phi(\gamma) d\gamma d\xi. \tag{V.45}$$

Comparing eq.(V.15) with eq.(V.45) we note again that the variance of the semi-analytical solution is simpler to evaluate than that of the analytical solution. Thus we conclude that whenever a semi-analytical solution is reasonably accurate in a problem, it should be attempted.

V.3. On the Parameter Estimation Problem

In the previous sections models for the direct problem of forecasting groundwater variables, and their statistical properties, in the presence of parameter uncertainty were introduced. A fundamental requisite for the application of these procedures was the availability of the statistical properties associated with the uncertain parameter, either from direct field measurement or from an estimation algorithm based on field data. Combining the statistics of the parameters with a solution of the stochastic equation governing the hydrology of the output variable, our objective was accomplished. Alternatively, the inverse problem focus on the estimation of the values of the parameters by using the governing differential equation, an optimization algorithm, and a set of field values of the output variable.

Most of the available results on the parameter estimation of groundwater parameters have been approached from the deterministic point of view and relatively little has been done on the topic for the case when uncertainty is present, which is the general case. A popular approach for the latter is the geostatistical approach, which offers convenient results in some cases, but as pointed by Dietrich and Newsam (1989) the use of a finite-difference representation of the differential equation may lead to serious problems of unstability. Efforts to attack the problem from a stochastic point of view are proliferating in the literature (see Ginn and Cushman, 1990 for a review). A very important fundamental result has been recently introduced by Unny (1989), where a maximum likelihood algorithm in combination with the governing differential equation is proposed in order to obtain the values of the parameters. An advantage of this method is the use of direct field measurements in the presence of uncertainty.

In the present section I would like to propose a method for the parameter estimation in the presence of uncertainty which makes specific use of the solution of the stochastic differential equation. An important role in this process is played by the impulse

response function of the system, in the same way that this function plays a critical role in the direct problem. Using the solution of the stochastic differential equation, rather than the differential equation itself, the numerical evaluation of derivatives is no longer needed thereby minimizing the eventual unstability. We will illustrate this approach for the parameter estimation of stochastic processes assumed to be present in the differential equation, hoping to extend the method to the estimation of the mean of the parameters themselves in a future article. This is done for consistency and completeness with the previous sections in this article, were assumptions of random processes governing the erratic nature of the parameters is always made, thereby raising the question on the estimation of the parameters of these disturbing processes.

Consider the regional groundwater flow problem discussed in section V.2.1, and for simplicity assume an infinite domain, a constant transmissivity, no recharge, and the combined measurement and model uncertainty represented in this case as a white Gaussian noise process in time, W', in the forcing function. Assuming that previous investigations have indicated that this is a correct transient model for the area under study, the governing equation, corresponding to eq.(V.18) is

$$\frac{\partial u}{\partial t} - \frac{T}{S}\frac{\partial^2 u}{\partial x^2} = W'(t, \omega), \quad -\infty < x < \infty, \quad 0 \leq t < \infty, \tag{V.46}$$

$$u(-\infty, t) = u(\infty, t) = 0, \quad u(x, 0) = u_0(x).$$

The objective is to estimate the magnitude of the variance parameter, q, of the process W' forcing the differential equation by using the solution of the stochastic differential equation (V.46), which is written as

$$u(x, t, \omega) = J(x, t)u_0(x) + \int_0^t J(x, t-\tau)W'(\tau, \omega)d\tau, \tag{V.47}$$

where the impulse response function is given by

$$J(x,\ t)u_0 = \frac{1}{(4\pi\frac{T}{S}t)^{1/2}} \int_{-\infty}^{\infty} \exp[-\frac{(x-s)^2}{4\frac{T}{S}t}]u_0(s)ds, \tag{V.48}$$

The mean head is

$$E\{u(x,\ t)\} = J(x,\ t)u_0(x). \tag{V.49}$$

The correlation function at to points of coordinates $(x_1,\ t_1)$ and $(x_2,\ t_2)$ respectively is

$$E\{u(x_1,t_1)u(x_2,t_2)\}=J(x_1,t_1)u_0J(x_2,t_2)u_0+q\int_0^{t_1} J(x_1,t_1-\tau)J(x_2,t_2-\tau)d\tau,\ t_1\leq t_2, \tag{V.50}$$

from which the variance at a particular point $(x,\ t)$ reduces to

$$\sigma^2_{u(x,t)} = q\int_0^t J^2(x,\ t-\tau)d\tau. \tag{V.51}$$

In this equation the function $\psi(x,\ t) = \int_0^t J^2(x,\ t-\tau)d\tau$ is well behaved, deterministic and relatively simple to evaluate. Now eq. (V.51) suggests that the estimate of the variance parameter at a particular point, $\hat{q}_{x,t}$ i simply

$$\hat{q}_{x,t} = \frac{\hat{\sigma}^2_{u(x,t)}}{\psi(x,\ t)}, \tag{V.52}$$

where $\hat{\sigma}^2_{u(x,t)}$ is the head variance as computed from field measurements taken at a piezometer located at the point $(x,\ t)$. It is expected that the point estimate of q will be a function of distance. Taking a spatial measure, the best estimate of q is given by

$$\hat{q} = \int_{-\infty}^{\infty} s.\hat{q}_{s,t}(s)ds = \int_{-\infty}^{\infty} \frac{s.\hat{\sigma}^2_{u(s,t)}ds}{\psi(s,\ t)}; \tag{V.53}$$

where the integrals can be approximated based on a collection of piezometers drilled across the aquifer. This intrinsically implies an assumption of stationarity, which may not be realistic in certain cases, but convenient. Quadrature methods of integration

recommend the evaluation of the integrand at a few points only. This suggests that between 6 to 10 piezometers drilled at the specific locations required by the quadrature would be sufficient. The selection of the value of t should be in agreement with the representative time scale of the measurement strategy. Eq.(V.53) provides a systematic way to estimate the parameter q using field measurements of the head and the impulse response function of the differential equation. Since integration is a more stable procedure than differentiation, the value of q must be bounded.

Since the above result is based on the assumed differential equation (eq.(V.46) in this case), a procedure to define the form of the random process entering the equation is needed. Usually a long-term observation of the behaviour of transient components of groundwater heads would suggest the form of the random process perturbing the differential equation. For instance, a groundwater head following an erratic form characterized by a Brownian motion type of function in time would indicate a model differential equation forced by white Gaussian noise. However we suspect that in many practical applications it would be difficult to deduce such a process.

Let us consider the more general case when the above process is unknown. From eq.(V.47) the solution of the differential equation is

$$u(x, t, \omega) = J(x, t)u_0 + g(x, t, \omega), \tag{V.54}$$

where the random function g results from the convolution integral of the known impulse response function, J, with an unknown perturbing random process. Presumably this function is a zero-mean process since u represents the stochastic transient component, which will result in the mean given by eq.(V.49). This equation provides a criterion for the estimation of the mean of the parameter $\frac{T}{S}$. The estimation problem is simply to find the numerical value of $\frac{T}{S}$ such that the expected value of u, as obtained from measurements across the aquifer, follows eq.(V.49). In fact this is the criterion inherent in many estimation algorithms, including "trial and error", only here

we are providing a mathematical justification.

Let us return to the problem of estimation of the parameters of the random function g. From eq.(V.54) it is possible to obtain sample functions of g, that is $\hat{g}(x, t, \omega) = \hat{u}(x, t, \omega) - J(x, t)u_0$, where $\hat{u}$ comes from field measurements. Studying the correlation structure of many sample functions one can make assumptions on the form of g. Suppose for example that it was found that a correlation function of the form $E\{g(x, t_1)g(x, t_2)\} = qe^{-\rho\ t_1 - t_2}$ could be fitted. This means that the variance of u is equal to q, and therefore an estimate of q is given by

$$\hat{q} = \int_{-\infty}^{\infty} s.\hat{\sigma}^2_{u(s,t)}ds, \tag{V.55}$$

where $\hat{\sigma}^2_u$ is obtained from field measurements. Finally, for the estimation of the parameter ρ we use the two-point correlation function of u,

$$E\{u(x, t_1)u(x, t_2)\} = R_u(x, t_1, t_2) = J(x, t_1)u_0J(x, t_2)u_0 + qe^{-\rho|t_1-t_2|}, \tag{V.56}$$

from which we can obtain a measure of the parameter ρ:

$$\hat{\rho} = -\frac{1}{t_1 - t_2} \int_{-\infty}^{\infty} s.\ln[\frac{C\hat{o}v\{s, t_1, t_2\}}{q}]ds, \quad t_1 \neq t_2, \tag{V.57}$$

where $C\hat{o}v\{\ \}$ denotes the two point covariance obtained from field measurements; and ln[ ] denotes the natural logarithm function.

The above results indicate that a similar methodology could be used to estimate the parameters involved in groundwater pollution models, which would use the solution of the stochastic differential equation along with field measurements of the concentration field. to higher dimensions is straight forward.

CONCLUSIONS

A new methodology to model the time and space evolution of groundwater variables (groundwater potential, contaminant concentration, water content, etc., either in the saturated or the unsaturated zone) in a system of aquifers was presented. The method is specifically suited to handle non-point sources and is capable of handling the case when certain components of the model, such as the geohydrologic information, the boundary conditions, the magnitude and variability of the sources or physical parameters or a combination of the above are uncertain and defined in stochastic terms. Some of the advantages with respect to conventional methodologies are the possibility to include high variances in the stochastic terms; the approach is systematic and easy to implement in a numerical algorithm; it does not require excessive computer time; and it is supported by a well-posed, rigorous mathematical theory.

The method is based on applications of modern mathematics to the solution of the resulting stochastic transport equations. It was found that this new methodology presents considerable advantages over the existing modeling methods. Thus the theory satisfies a more general modeling need by providing, if desired, a systematic global concentration information on the sample functions, the mean, the variance, correlation functions or higher-order moments based on similar information of any "size", anywhere, of the input functions. This more realistic statistical representation of the concentration distribution is a valuable tool in designing and testing preventive or remedial alternatives by engineers and planners.

Several individual applications were shown in order to illustrate the methodology when the different cases of uncertainty appear in groundwater flow and pollution problems. The method could be used to solve more difficult cases of groundwater pollution modeling subject to complex reactive transport problems.

REFERENCES

Adomian, G., 1983. Stochastic Systems. Academic Press, New York.

Aly I., El-Kadi., 1987. Effects of Variability of Infiltration Under Uncertainty on Unsaturated Soil Parameters. J. of Hydrol., 90:61-80.

Arnold, L., Kotelenez, P., and Curtain, R.F., 1981. Linear Stochastic Evolution Equations Models for Chemical Reactions. In Stochastic Nonlinear Systems in Physics, Chemistry and Biology, L. Arnold and R. Lefever (editors). Springer-Verlag.

Anderson, M.P., 1979. Using Models to Simulate The Movement of Contaminants Through Groundwater Flow Systems. CRC Crit. Rev. Environ. Control 9:97-156.

Bear, J., 1979. Hydraulics of Groundwater. McGraw-Hill Book Company, New York, New York.

Belleni-Morante, A., 1979. Applied Semigroups and Evolution Equations. Clarendon Press-Oxford.

Bensoussan , A., 1977. Control of Stochastic Partial Differential Equations, in Distributed Parameter Systems, edited by W.H. Ray and D.G. Lainiotis. Marcel Dekker Inc.

Broadbridge, P., and White, I., 1988. Constant Rate Rainfall Infiltration: A Versatile Non-Linear Model. 1. Analytical Solution. Water Res. Res. 24(1):145-154.

Butzer, P.L., and Berens, H., 1967. Semigroups of Operators and Approximations. Springer.

Cannon, J.R., 1984. The One-Dimensional Heat Equation. Encyclopedia of Mathematics and its Applications edited by G-C Rota. Addison-Wesley Publishing Company.

Carslaw H.S., and Jaeger, J.C., 1971. Conduction of Heat in Solids. Oxford University Press.

Chapra, S.C., and Canale, R.P., 1988. Numerical Methods for Engineers. McGraw-Hill Book Co., Second Ed., New York, N.Y.

Chow, P.L., 1979. Approximate Solution of Random Evolution Equations, in Approximate Solutions of Random Equations, edited by A.T. Bharucha-Reid. North Holland.

Crank, J., 1970. The Mathematics of Diffusion. Oxford University Press.

Curtain, R.F., and Pritchard, A.J., 1978. Infinite Dimensional Linear Systems Theory. Lecture Notes in Control and Information Sciences, Vol. 8, edited by A.V. Balakrishnan and M. Thoma. Springer-Verlag.

Curtain, R.F., and Falb, P.L., 1971. Stochastic Differential Equations in Hilbert Space. J. of Diff. Eqs. 10:412-430.

Cushman, J.H., 1987. Developments of Stochastic Partial Differential Equations in Subsurface Hydrology. J. Stoch. Hydrol. Hydraul., 1(4):241-262.

Dagan, G., 1984. Solute Transport in Heterogeneous Porous Formations. J. Fluid Mech., 145:151-177.

Dagan, G., 1983. Unsaturated Flow in Spatially Variable Fields, 1. derivation of Models of Infiltration and Redistribution. Water Res. Res., 19:413-420.

Dagan, G., 1982. Stochastic Modeling of Groundwater Flow by Unconditional and Conditional Probabilities. 2. Solute Transport. Water Res. Res. 18(4): 835-848.

Dagan, G., and Bresler, E., 1979. Solute Dispersion in Unsaturated Heterogeneous Soil at Field Scale. 1. Theory. Soil Sci. Soc. Am. J. 43:461-467.

Dietrich, C.R., and Newsam, G.N., 1989. A Stability Analysis of the Geostatistical Approach to Aquifer Transmissivity Identification. Stochastic Hydrol. Hydraul. 3(4):293-316.

Freeze, R.A., 1971. Three-Dimensional, Transient, Saturated-Unsaturated Flow in a Groundwater Basin. Water Res. Res. 7(2):347-366.

Fried, J.J., 1975. Groundwater Pollution. Elsevier, New York.

Gelhar, L.W., and Axness, C.L., 1983. Three-dimensional Stochastic Analysis of Macrodispersion in Aquifers. Water Res. Res. 19(1):161-180.

Gelhar, L.W., Gutjahr, A.L., and Naff, R.J., 1979. Stochastic Analysis of Macrodispersion in a Stratified Aquifer. Water Res. Res. 15:1387-1397.

Gillam, R.W., 1982. Influence of the Tension-Saturated Zone on Contaminant Migration in Shallow Water-Table Regimes. Proc. Symp. Unsat. Flow Transp. Mod., March 23-24, 1982, Battelle-Seattle, Seattle, Washington.

Ginn, T.R., and Cushman, J.H., 1990. Inverse Methods for Subsurface Flow: A Critical Review of Stochastic Techniques. Stochastic Hydrol. Hydraul., 4(1):1-26.

Godambe, V.P., and Thompson, M.E., 1984. Robust Estimation Through Estimating Equations. Biometrica, 71(1):115-125.

Goldstain, J.A., 1985. Semigroups of Linear Operators and Applications. Oxford University Press, New York.

Griffel, D.H., 1981. Applied Functional Analysis. Ellis Horwood Ltd.

Gupta, V.K., and Bhattacharya, R.N., 1986. Solute Dispersion in Multidimensional Periodic Saturated Porous Media. Water Res. Res. 22(2):156-164.

Haan, C.T., 1987. Statistical Methods in Hydrology. The Iowa State University Press, Ames Iowa.

Hillel, D., 1980. Fundamentals of Soil Physics. Academic Press, New York, New York.

Hornbeck, R.W., 1975. Numerical Methods. Quantum Publishers Inc., New York, N.Y.

Hunt, B., 1983. Mathematical analysis of Groundwater Resources. Butterworths, London, England.

Hutson and Pym., 1980. Functional Analysis in Applied Mathematics. Academic Press.

Ichikawa, A., 1985. A Semigroup Model for Parabolic Equations with Boundary and Pointwise Noise. In L. Arnold and P. Kotelenez (editors), Stochastic Space-Time Models and Limit Theorems. D. Reidel Publishing Co., Dordrecht, Holland.

Jazwinski, A.H., 1970. Stochastic Processes and Filtering Theory. Academic Press, New York.

Kavvas, M.L., Saquib, M.N., and Puri, P.S., 1987. On a Stochastic Description of the Time-Space Behaviour of Extratropical Cyclonic Precipitation Fields. Stochastic Hydrol. Hydraul., 1(1):37-52.

Klute, A., 1965. Laboratory Measurement of Hydraulic Conductivity of Unsaturated

Soil. In Methods of Soil Analysis, pp. 253-261. Monograph 9. Am. Soc. Agron. Madison, Wisconsin.

Kotelenez, P., 1985. On The semigroup Approach to Stochastic Evolution Equations. In L. Arnold and P. Kotelenez (editors), Stochastic Space-Time Models and Limit Theorems. D. Reidel Publishing Co., Dordrecht, Holland.

Kraus, A.D., 1987. Matrices for Engineers. Hemisphere Publishing Corporation, Washington, D.C.

Kunze, R.J., and Kirkham, D., 1962. Simplified Accounting for Membrane Impedance in Capillary Conductivity Determinations. Soil. Sci. Soc. Am. Proc., 26:421-426.

Ladas, G., and Lakshmikantham, V., 1972. Differential Equations in Abstract Spaces. Academic Press.

Li, W-H., 1972. Differential Equations of Hydraulic Transients, Dispersion and Groundwater Flow. Mathematical Methods in Water Resources. Prentice- Hall, Inc.

Liakopoulus, A.C., 1965. Theoretical Solution of Unsteady Unsaturated Flow Problems in Soils. Bull. Int. Assoc. Sci. Hydrol., 10:5-39.

Mariño, M.A., 1974. Longitudinal Dispersion in Saturated Porous Media. ASCE, J. of Hyd. Div., 100(HY1):151-157.

Matheron, G., and De Marsily, G., 1980. Is Transport in Porous Media Always Diffusive? Water Res. Res. 16:901-917.

Miller, E.E., amd Elrick, D.E., 1958. Dynamic Determination of Capillary Conductivity Extended for Non-negligible Membrane Impedance. Soil Sci. Soc. Am. Proc. 22:483-486.

Mohsenisaravi, M., 1981. Forecasting Subsurface Water Flow and Storage on Forested Slopes Using a Finite Element Model. Ph.D. Thesis, Univ. of Idaho, Univ. Microfilms International, Ann Arbor, MI.

Moler, C., and Van Loan, C., 1978. Nineteen Dubious Ways to Compute the Exponential of a Matrix. SIAM Rev., 20(4):801-836.

Moore, R.E., 1939. Water Conduction from Shallow Water Tables. Hilgardia, 12:383-426.

Mtundu, N.D., and Koch, R.W., 1987. A Stochastic Differential Equation Approach to Soil Moisture. Stochastic Hydrol. Hydraul., 1(2):101-116.

Neuman, S.P., 1973. Saturated-Unsaturated Seepage by Finite Elements. J. Hydraulics Div., A.S.C.E. 99(HY12):2233-2250.

Nieber, J.L., 1982. Hillslope Soil Moisture Flow, Approximation by a One-Dimensional Formulation. A.S.A.E. 82-2026, St. Joseph, MI.

Nieber, J.L., 1979. Hillslope Runoff Characteristics. Ph.D. Thesis, Cornell Univ., Ithaca, NY., Univ. Microfilms International, Ann Arbor Michgan.

Oden, J.T., 1977. Applied Functional Analysis. Prentice-Hall.

Sawaragi, Y., Soeda, T., and Omatu, S., 1978. Modeling, Ogata, A., and Banks, R.B., 1961. A Solution of the Differential Equation of Longitudinal Dispersion in Porous Media. U.S. Geol. Surv. Prof. Paper 411-A, U.S. Government Printing Office, Washington, D.C.

Papoulis, A., 1984. Probability, Random Variables and Stochastic Processes. McGraw-Hill Book Co., New York.

Parlange, J.Y., 1971. Theory of Water Movement in Soils: I. One-Dimensional Absorption. Soil Sci. 111(2):134-137.

Philip, J.R., 1972. On Solving the Unsaturated Flow Equation: 1. The Flux-Concentration Relation. Soil Sci. 16(5):328-335.

Philip, J.R., 1955. Numerical Solution of Equations of The Diffusion Type With Diffusivity Concentration-Dependent. Commonwealth Scientific and Industrial Research Organization. Commonwealth of Australia. Reprinted from the Transactions of the Faraday Society 51(391) Part 7.

Philip, J.R., and Knight, J.H., 1974. On Solving the Unsaturated Flow Equation: 3. New Quasi-Analytical Technique. Soil Sci. 117(1):1-13.

Rijtema, P.E., 1959. Calculation of Capillary Conductivity From Pressure Plate Outflow Data With Non-negligible Membrane Impedance. Neth J. Agr. Sci., 7:209-215.

Rose, C.W., Stern, W.R., and Drummond, J.E., 1965. Determination of Hydraulic Conductivity as a Function of Depth and Water Content for Soil In Situ. Aust. J. Soil Res., 3:1-9.

Sander, G.C., Parlange, J.Y., Kuhnel, V., Hogarth, W.L., Lockington, D., and O'Kane, J.P.J., 1988. Exact Non-Linear Solution for Constant Flux Infiltration. Short Note, J of Hydrol., 97:341-346.

Sawaragi, Y., Soeda, T., and Omatu, S., 1978. Modeling, Estimation, and Their Applications for Distributed Parameter Systems. Lecture Notes in Control and Information Sciences, Vol. 2, edited by A.V. Balakrishnan and M. Thoma. Springer- Verlag.

Schwartz, F.W.,1977. Macroscopic dispersion in Porous Media: The Controlling Factors. Water Res. Res. 13(4):743-752.

Serrano, S.E., 1990(3). Using the C Language to Approximate Non-Linear Stochastic Systems. J. Adv. in Eng. Software, 12(2):59-68.

Serrano, S.E., 1990(2). Stochastic Differential Equation Models of Erratic Infiltration. Water Res. Res. 26(4):703-712.

Serrano, S.E., 1990(1). Modeling Infiltration in Hysteretic Soils. Adv. in Water Res., 13(1):12-23.

Serrano, S.E., 1988(1). General Solution to Random Advective- Dispersive Equation in Porous Media. Part I: Stochasticity in The Sources and in the Boundaries. Stoch. Hydrol. Hydraul. 2(2):79-98.

Serrano, S.E., 1988(2). General Solution to Random Advective- Dispersive Equation in Porous Media. Part II: Stochasticity in the Parameters. Stoch. Hydrol. Hydraul., 2(2):99-112.

Serrano, S.E., and Unny, T.E., 1987(1). Semigroup Solutions of the Unsteady Groundwater Flow Equation with Stochastic Parameters. J. Stoch. Hydrol. Hydraul., 1(4):281-296.

Serrano, S.E., and Unny, T.E., 1987(2): Predicting Groundwater Flow in a Phreatic Aquifer. J. of Hydrol., 95:241-268.

Serrano, S.E., and Unny, T.E., 1986. Boundary Element Solution of the Two-Dimensional Groundwater Flow Equation With Stochastic Free-Surface Boundary Condition. J. Num. Meth. Partial Diff. Eqs. 2:237-258.

Serrano, S.E., Unny, T.E., and Lennox, W.C., 1985(1). Analysis of Stochastic

Groundwater Flow Problems. Part I: Deterministic Partial Differential Equations in Groundwater Flow. A Functional Analytic Approach. J. Hydrol. 82(3-4): 247-263.

Serrano, S.E., Unny, T.E., and Lennox, W.C., 1985(2). Analysis of Stochastic Groundwater Flow Problems. Part II: Stochastic Partial Differential Equations in Groundwater Flow. A Functional-Analytic Approach. J. Hydrol. 82(3-4): 265-284.

Serrano, S.E., Unny, T.E. and Lennox, W.C., 1985(3). Analysis of Stochastic Groundwater Flow Problems. Part III: Approximate Solution of Stochastic Partial Differential Equations. J. Hydrol. 82(3-4): 285-306.

Showalter, R.E., 1977. Hilbert Space Methods for Partial Differential Equations. Pitman.

Simmons, C.S., 1982. A Stochastic-Convective Transport Representation in Dispersion in One-Dimensional Porous Media Systems. Water Res. Res. 18(4):1193-1214.

Sloan, G.S., Moore, I.D., Coltharp, G.B., and Eigel, J.D., 1983. Modeling Surface and Subsurface Stormflow on Steeply-Sloping Forested Watersheds. Research Report No. 142., Water Res. Res. Inst., Univ. of Kentucky, Lexington, Kentucky.

Smith, L., and Schwartz, F.W., 1980. Mass Transport. 1. A Stochastic Analysis of Macroscopic Dispersion. Water Res. Res. 16:303-313.

Spiegel, M.R., 1968. Mathematical Handbook of Formulas and Tables. Schaum's outline series. McGraw-Hill.

Sposito, G., and Jury, W.A., 1986. Fundamental Problems in The Stochastic Convection-Dispersion Model of Solute Transport in Aquifers and Field Soils. Water Res. Res. 22(1):77-88.

Sudiky, E.A., 1986. A Natural Gradient Experiment on Solute Transport in a Sand Aquifer: Spatial Variability of the Hydraulic Conductivity and Its Role in the Dispersion Process. Water Res. Res., 22(13):2069-2082.

Sudiky, E.A., and Cherry, J.A., 1979. Field Observations of Tracer Dispersion Under Natural Flow Conditions in an Unconfined Sandy Aquifer. Water pollut. Res. Can. 14:1-17.

Tang, D.H., Schwartz, F.W., and Smith, L., 1982. Stochastic Modeling of Mass Transport in a Random Velocity Field. Water Res. Res. 18(2):231-244.

Tanner, C.B., and Elrick, D.E., 1958. Volumetric Porous (Pressure) Plate Apparatus for Moisture Hysteresis Measurements. Soil Sci. Soc Am. Proc. 22:575-576.

Tsakiris, G., Agrafiotis, G., and Kiountouzis, E., 1988. A Shot Noise Model for the Generation of Soil Moisture Data. Stochastic Hydrol. Hydraul., 2(1):51-59.

Umari, A.M.J., and Gorelick, S.M., 1986. The Problem of Complex Eigensystems in the Semianalytical Solution for Advancement of Time in Solute Transport Simulations: A New Method Using Real Arithmetic. Water Res. Res. 22(7):1149-1154.

Unny, T.E., 1989. Stochastic Partial Differential Equations in Groundwater Hydrology. Part I: Theory. Stochastic Hydrol. Hydraul., 3(2):135-153.

Viessman, W., Knapp, J.W., Lewis, G.L., and Harbaugh, T.E., 1977. Introduction to Hydrology. Harper and Row Publishers Inc., New York, New York.

Warren, J.E., and Skiba, F.F., 1964. Macroscopic Dispersion. Trans. Am. Inst. Min. Metall. Pet. Eng. 231:215-230.

Watson, K.K., 1966. An Instantaneous Profile Method for Determining the Hydraulic Conductivity of Unsaturated Porous Materials. Water Res. Res. 2:709-715.

Winter, C.L., Newman, C.M., and Neumann, S.P., 1984. A Perturbation Expansion for Diffusion in a Random Velocity field, SIAM J. Appl. Math., 44(2):411-424.

Youngs, E.G., 1964. An Infiltration Method of Measuring the Hydraulic Conductivity of Unsaturated Porous Materials. Soil Sci., 109:307-311.

Zauderer, E., 1983. Partial Differential Equations of Applied Mathematics. John Wiley & Sons.

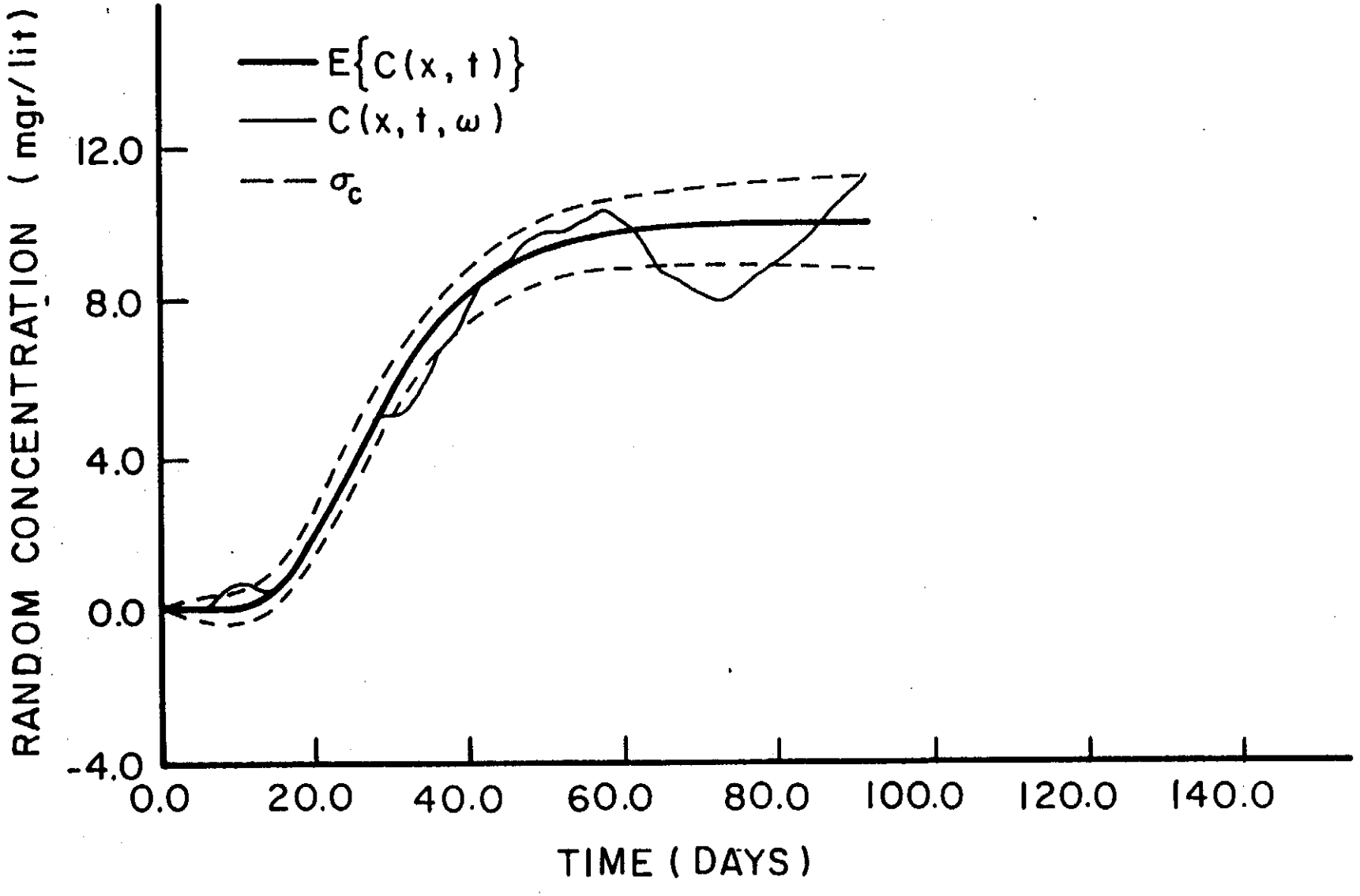

Fig. III.1: Stochastic Concentration witht Time at X=6.0 m

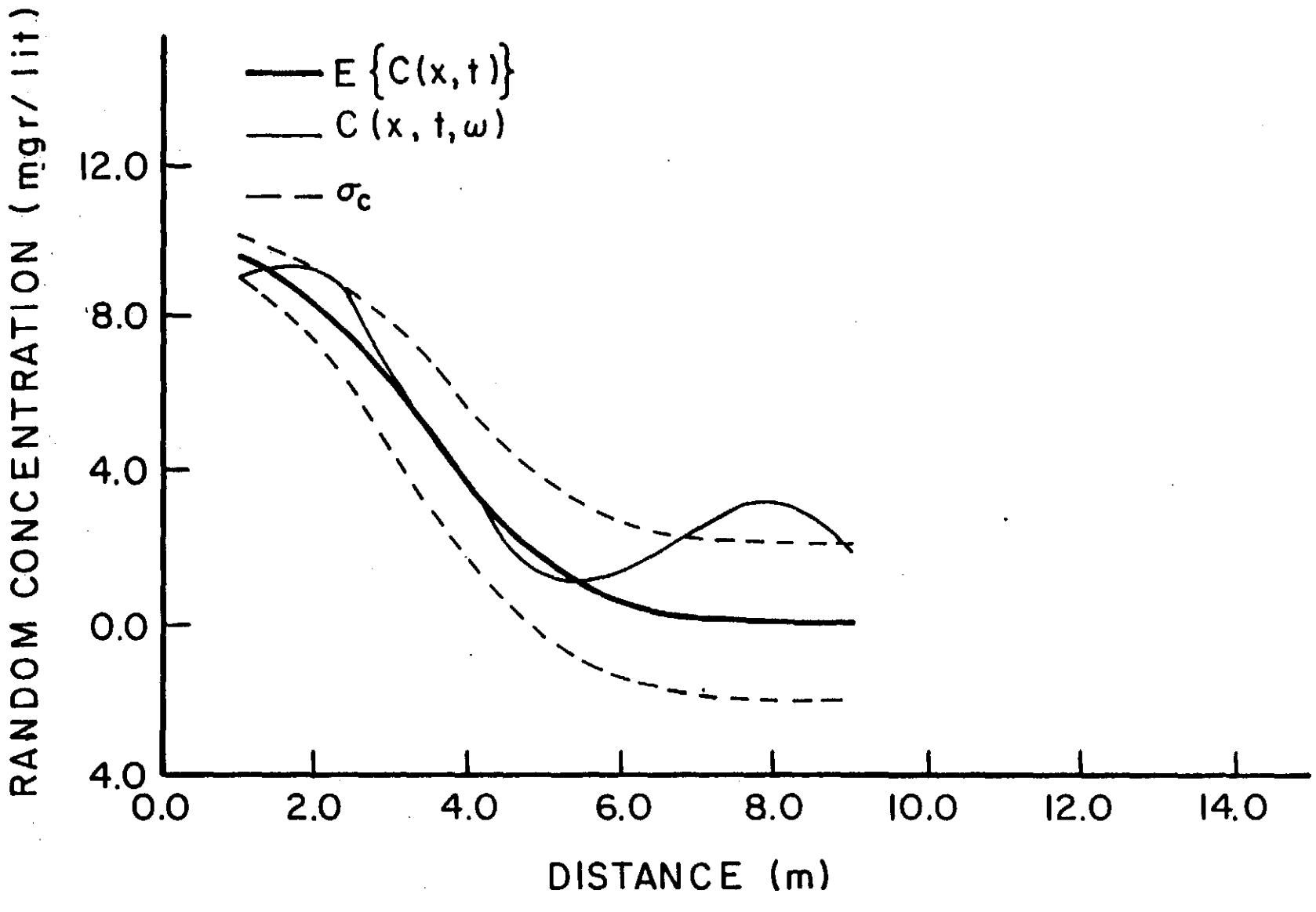

Fig. III.2: Stochastic Concentration in Space at t=15 days

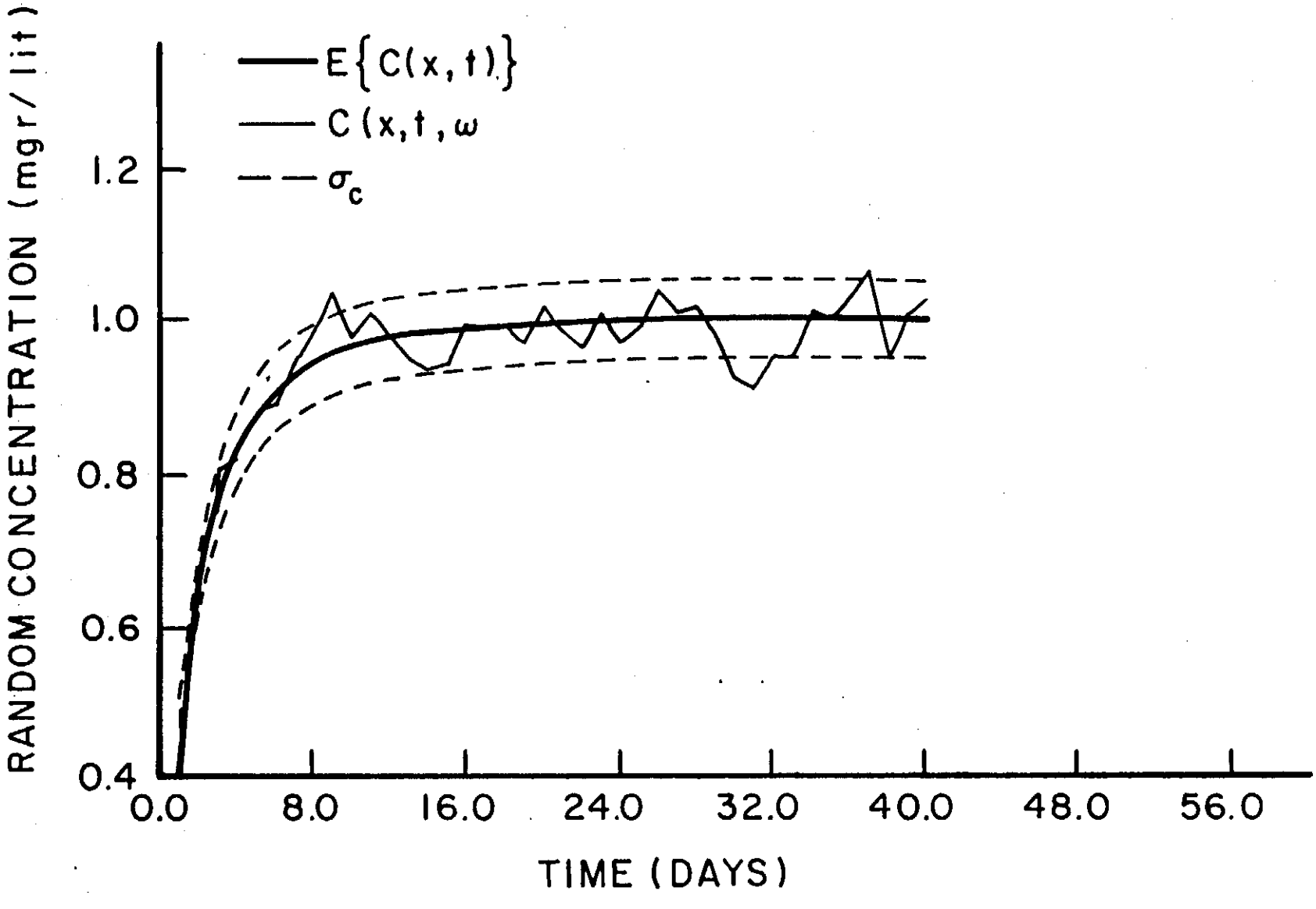

Fig. III.3: Stochastic Concentration with Time at X=0.5m

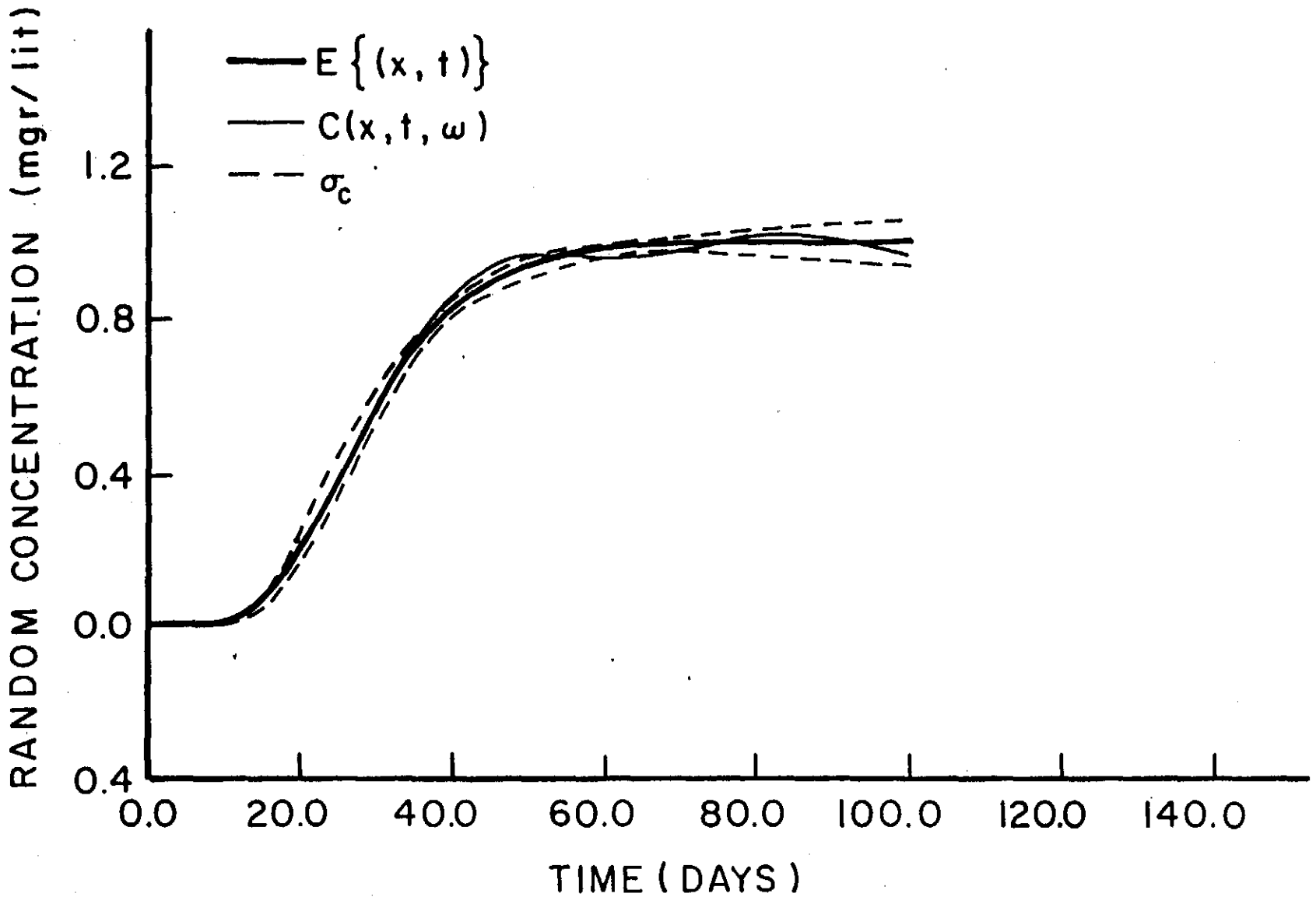

Fig. III.4: Stochastic Concentration with Time at X=6.0 m

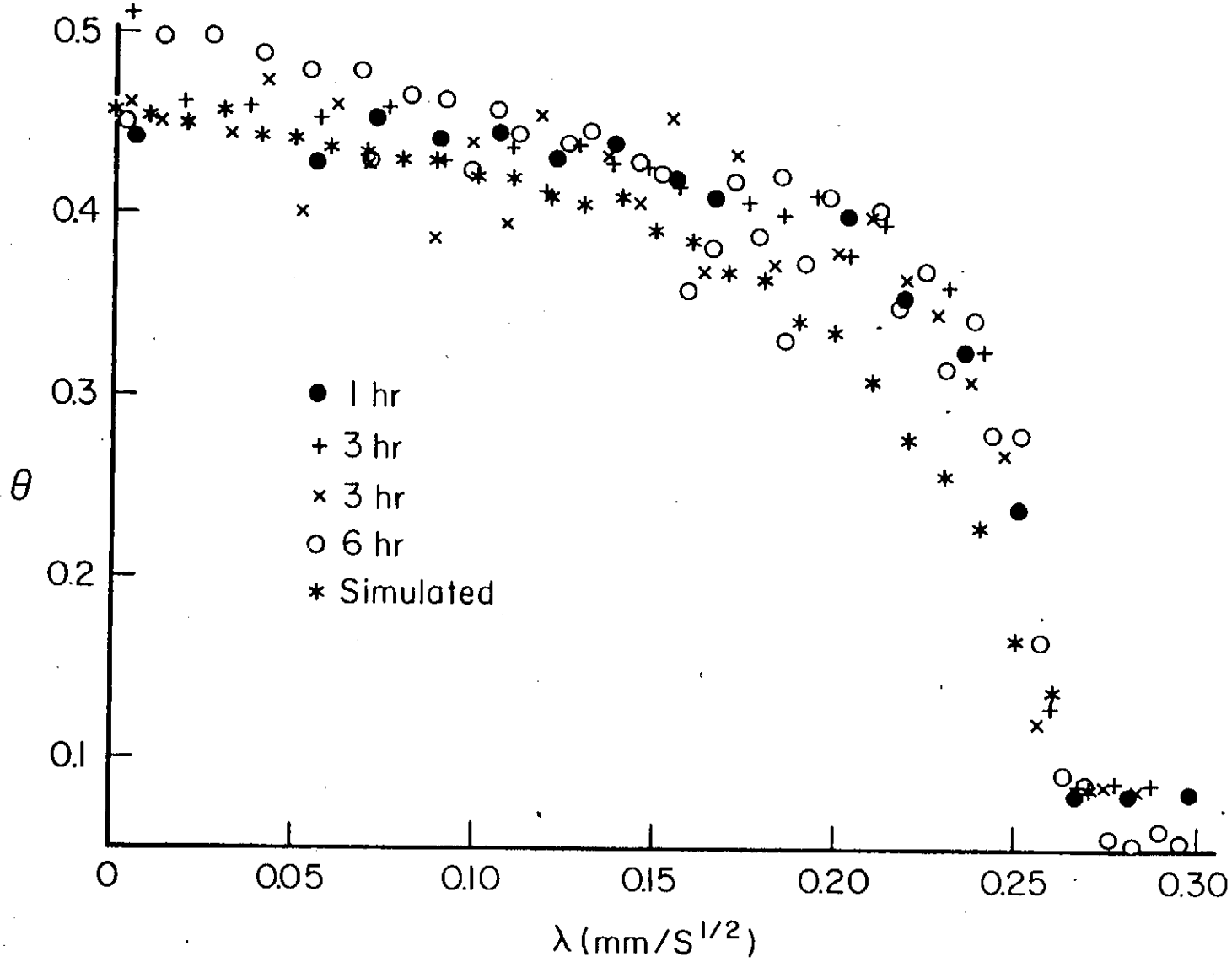

Fig. IV.1: Measured and Sample Simulated Water Content versus λ

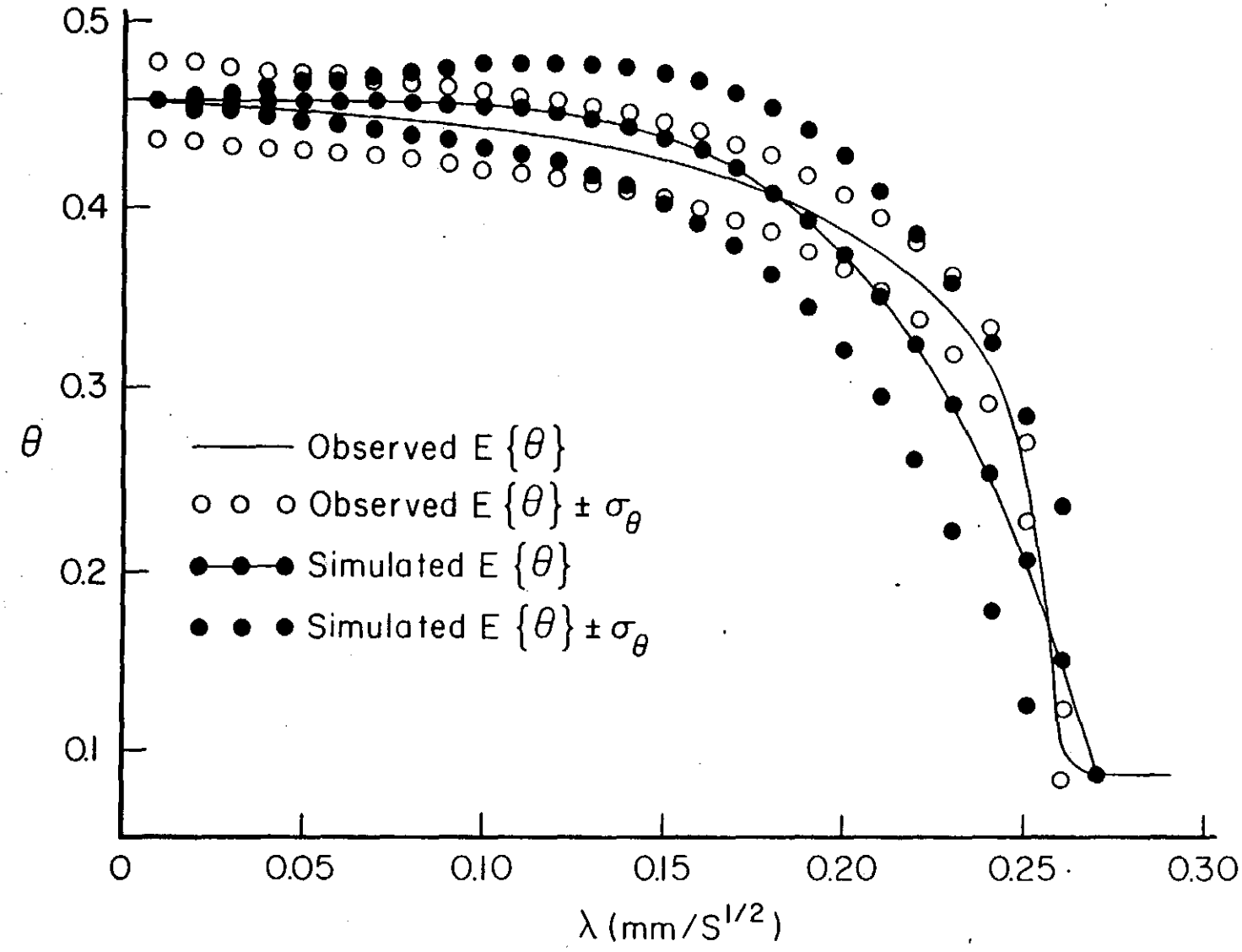

Fig. IV.2: Measured and Simulated Moments of Water Content versus λ

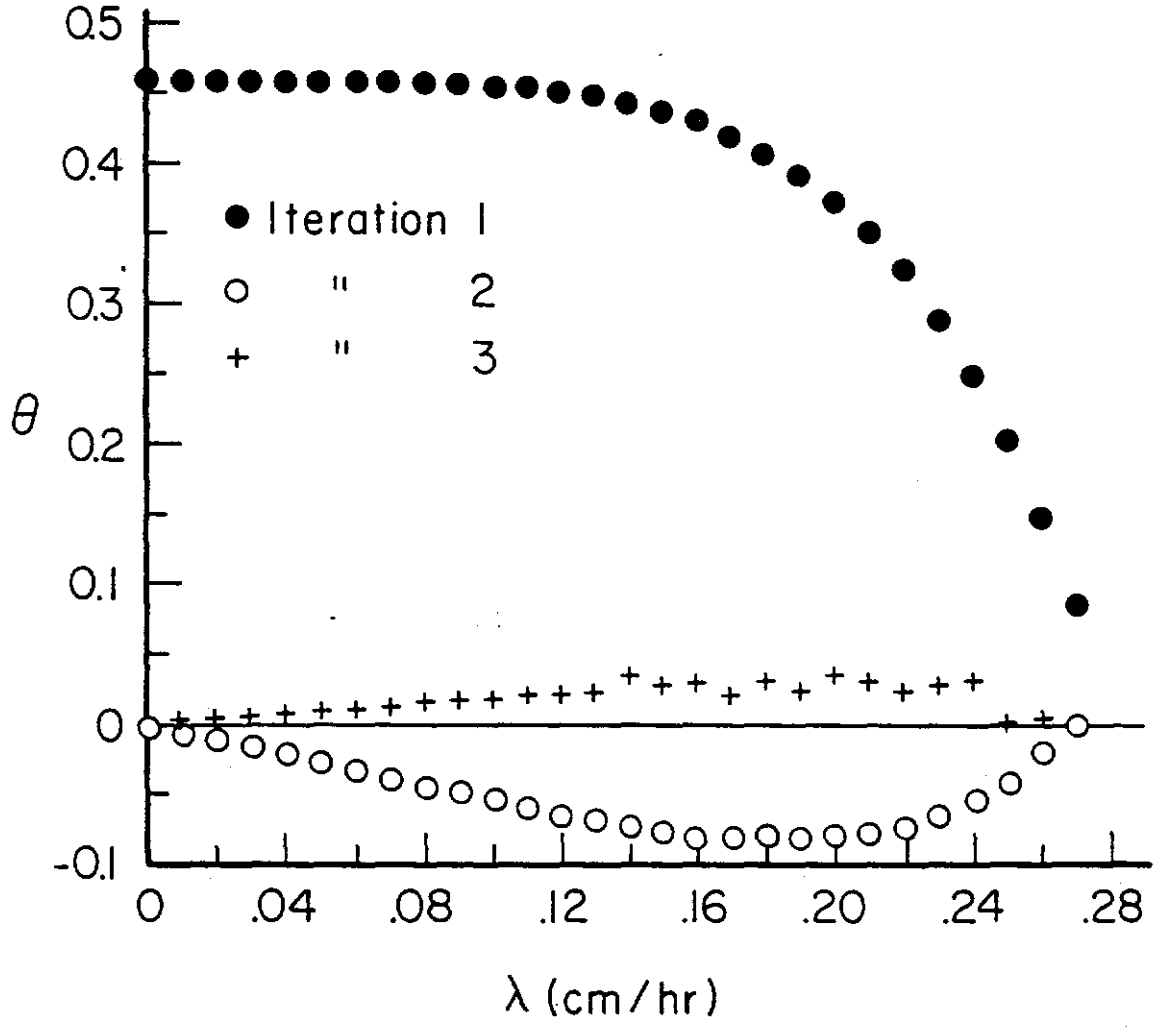

Fig. IV.3: First Three Iterations of Water Content versus λ

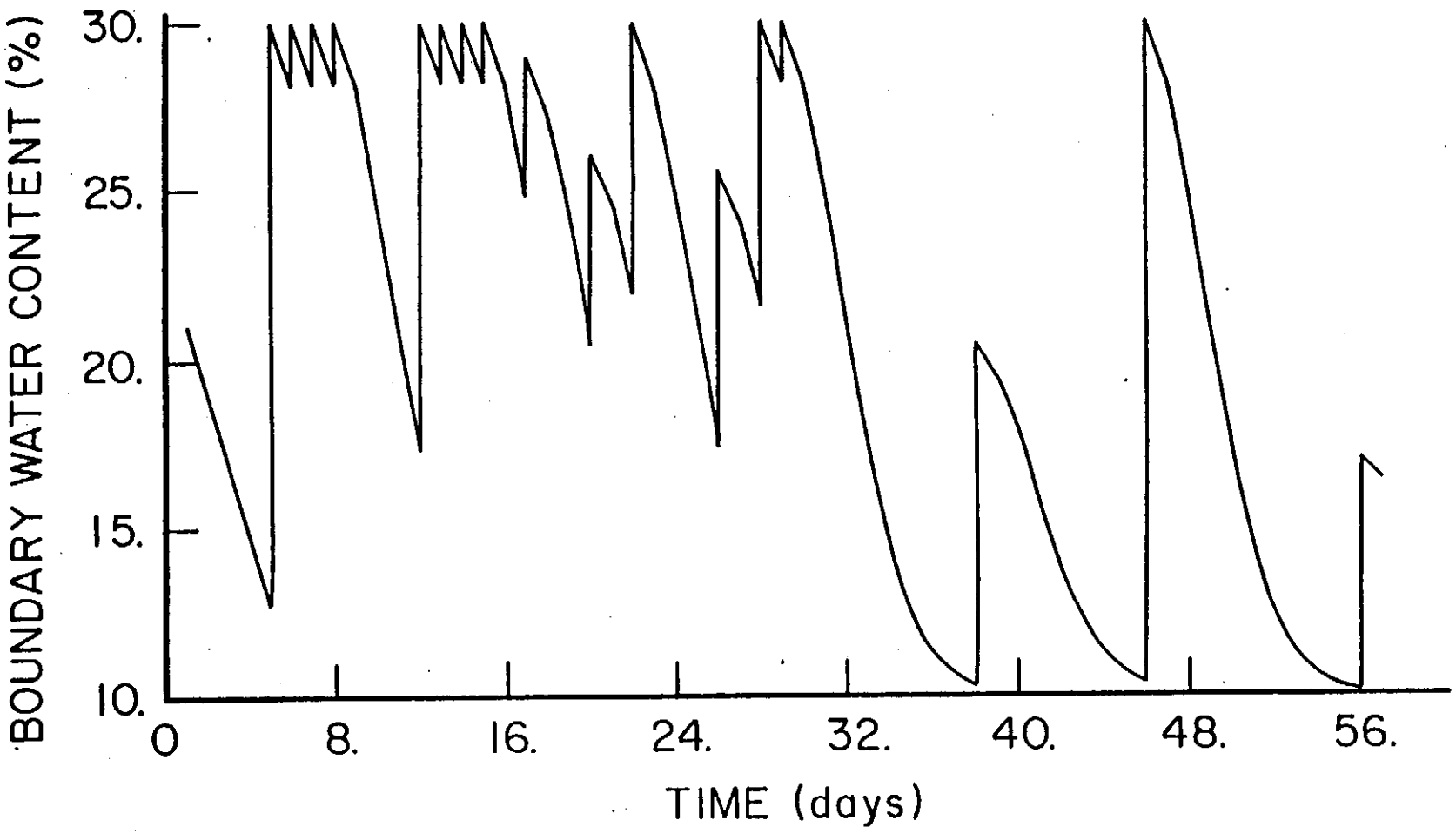

Fig. IV.4: Water Content at the Upper Boundary versus Time

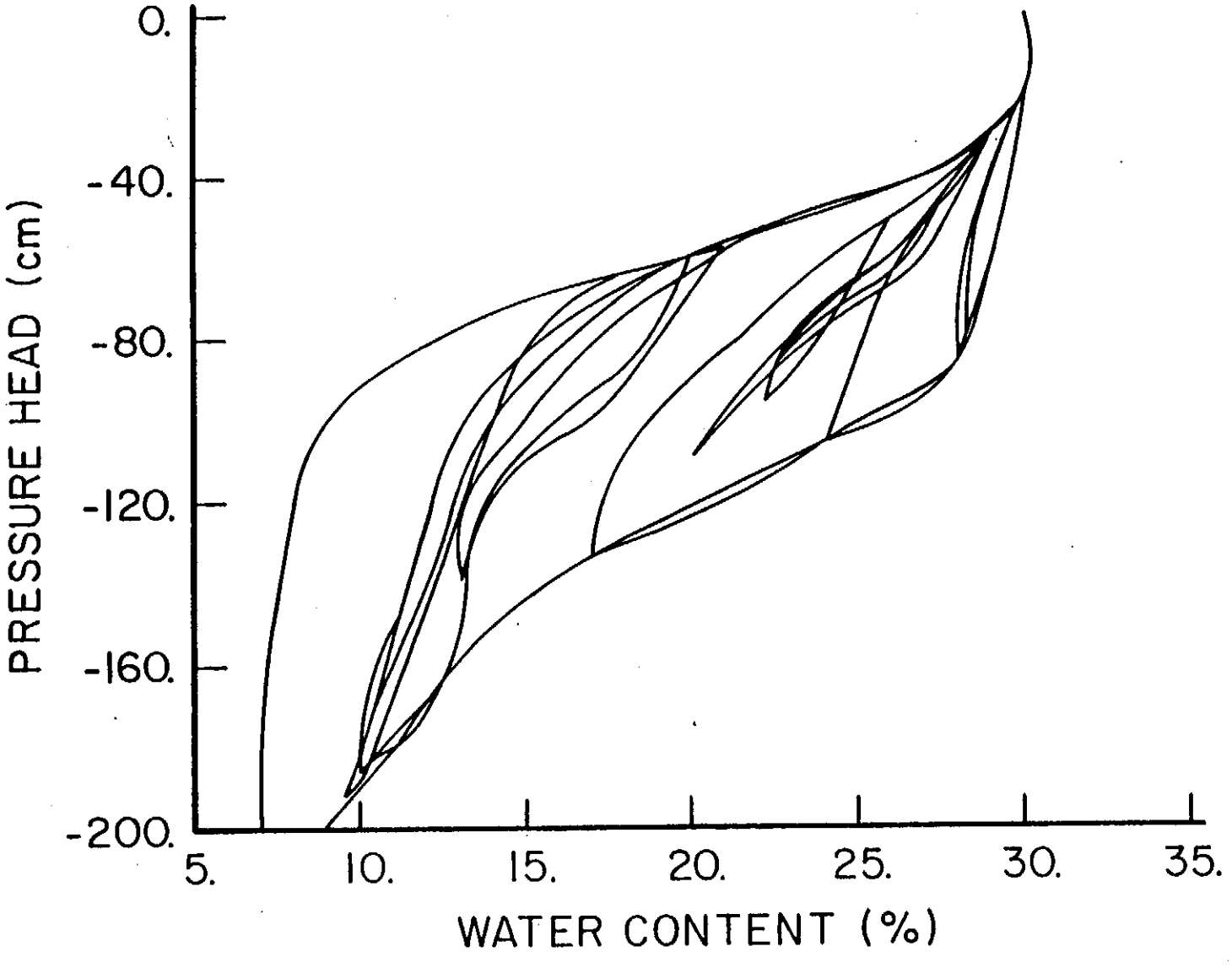

Fig. IV.5: Water Content versus Pressure Head Relationship

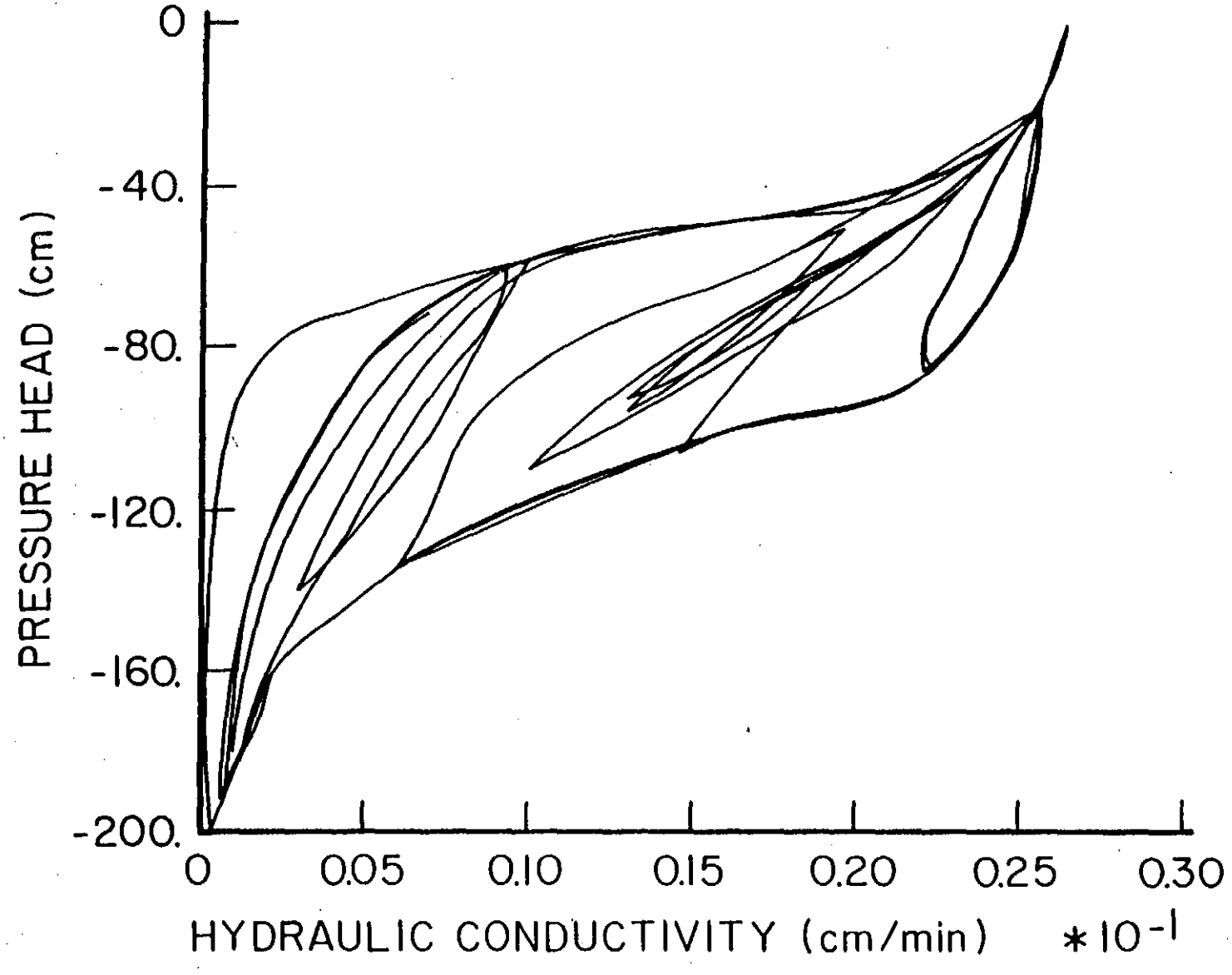

Fig. IV.6: Hydraulic Conductivity versus Pressure Head Relationship

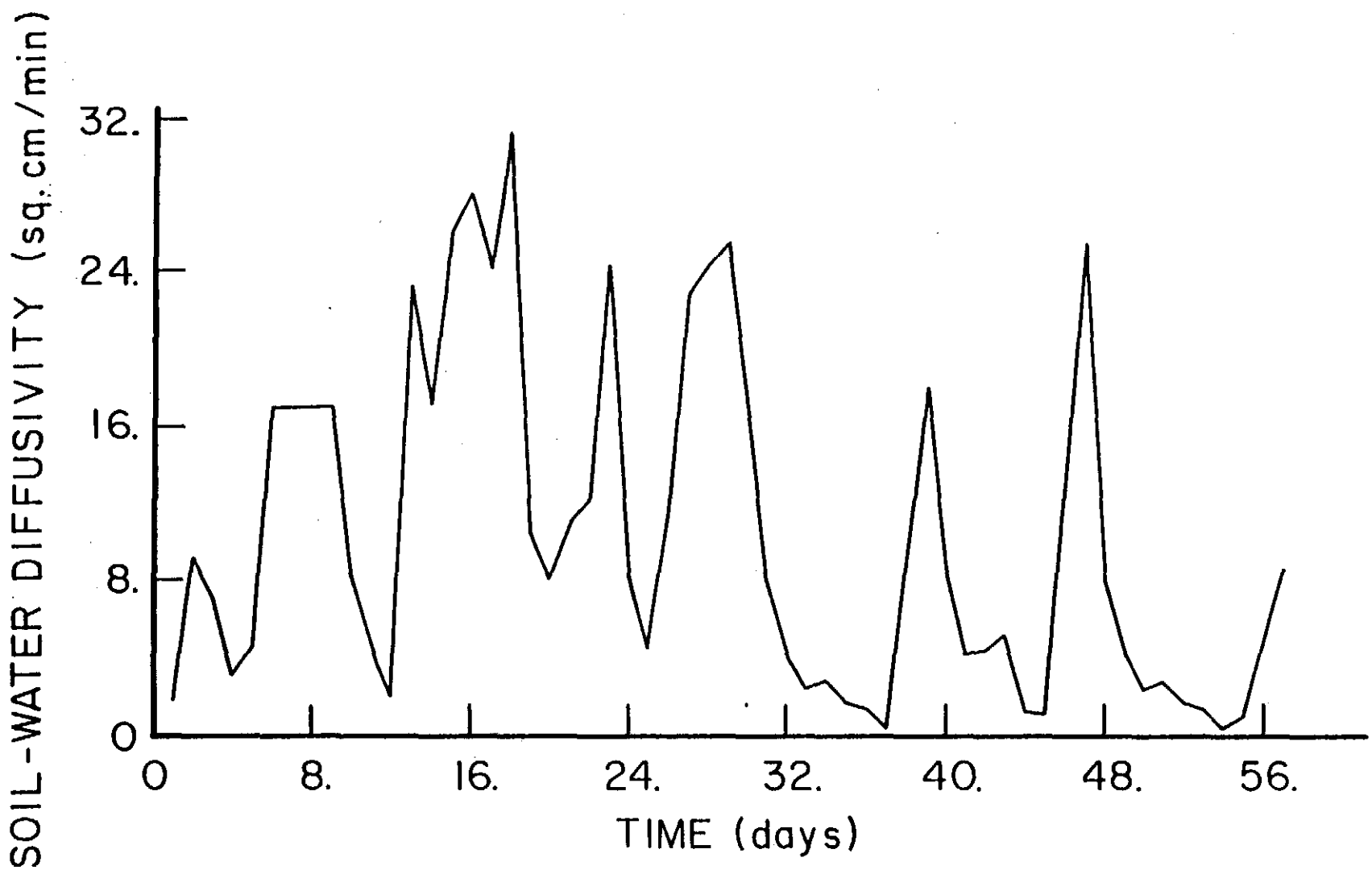

Fig.IV.7: Soils-Water Diffusivity time series for the Root Zone

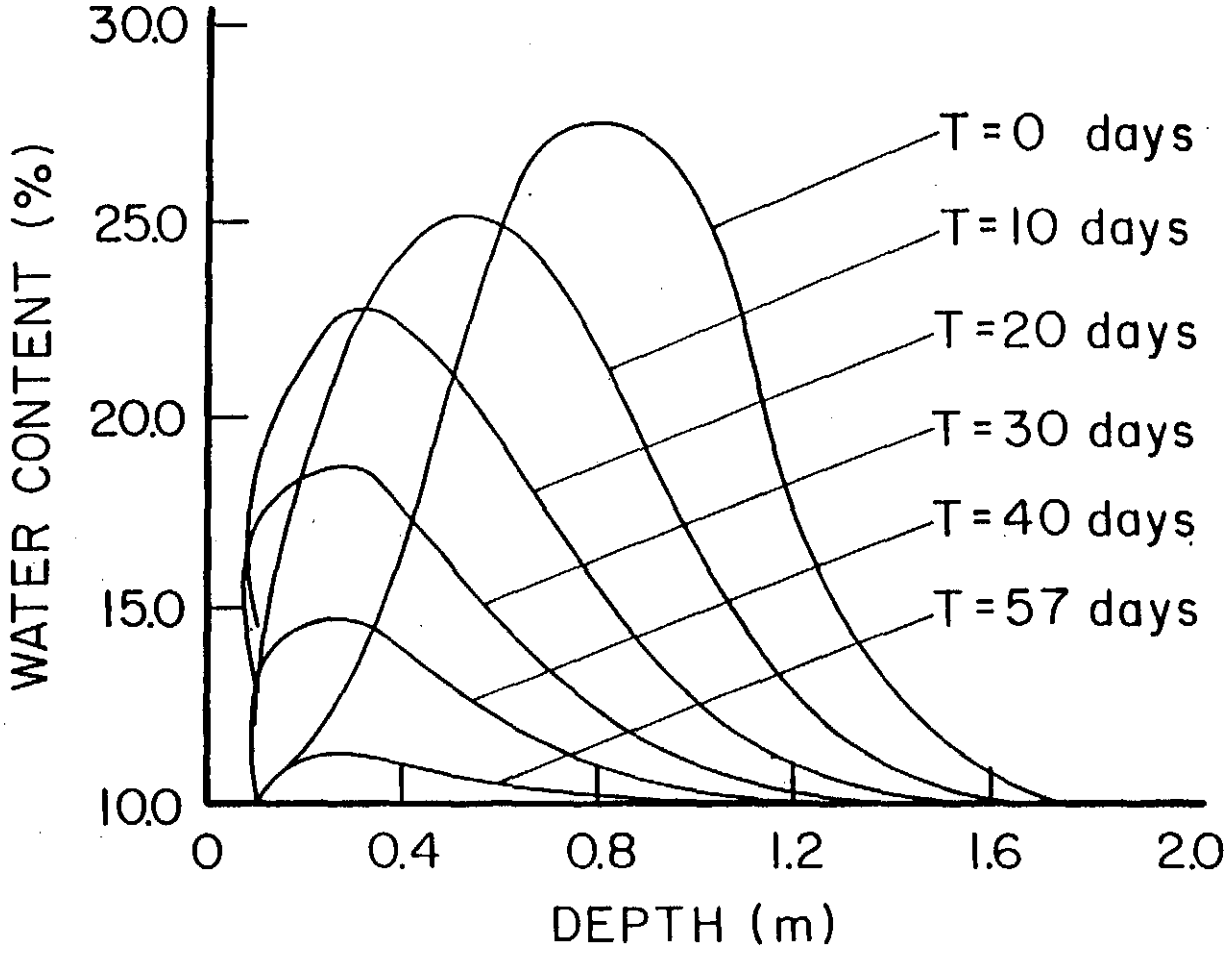

Fig. IV.8: Deterministic Component of Water Content Versus Depth

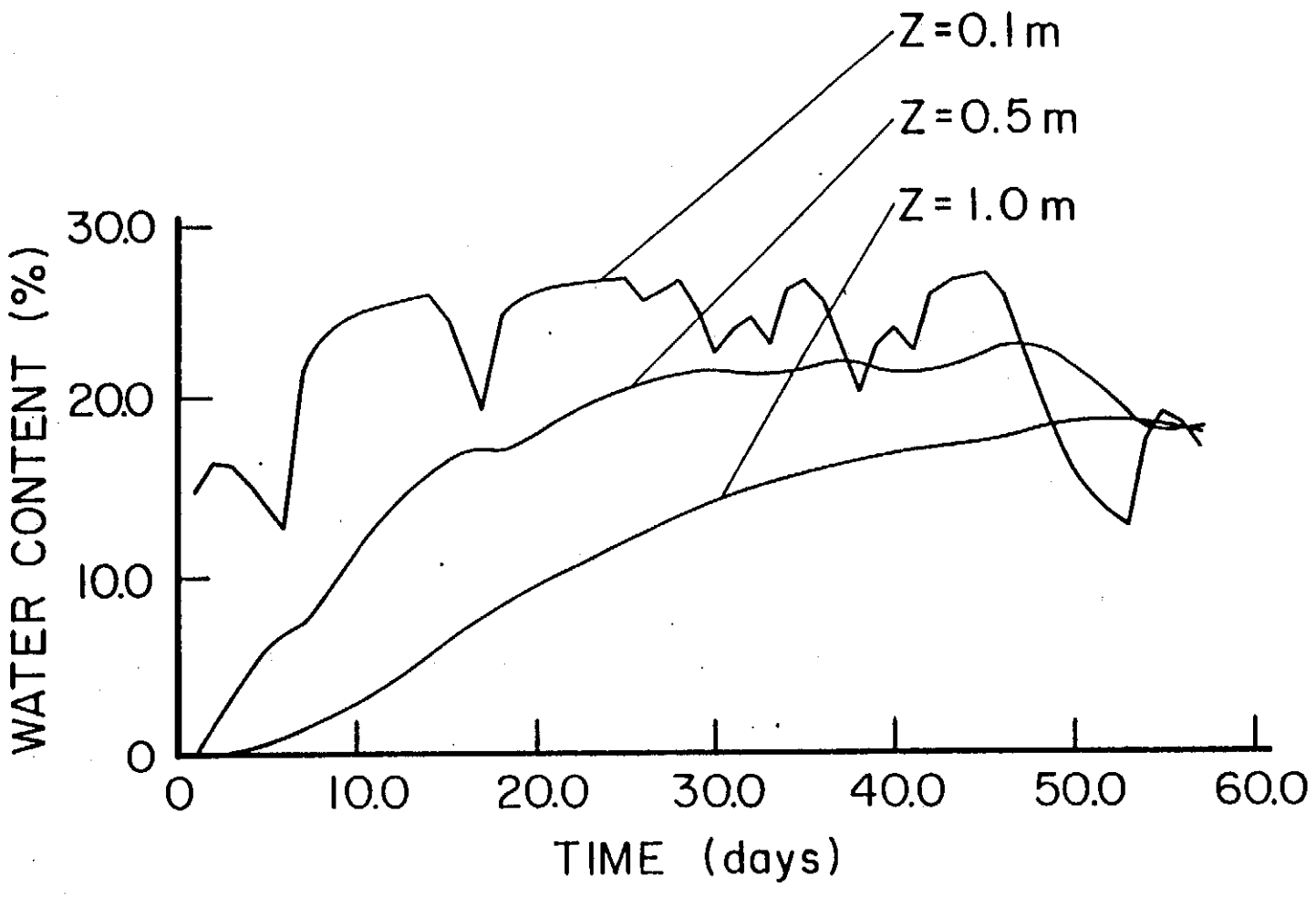

Fig. IV.9: Sample Functions of the Boundary Component of Water Content versus Time at Different Depths

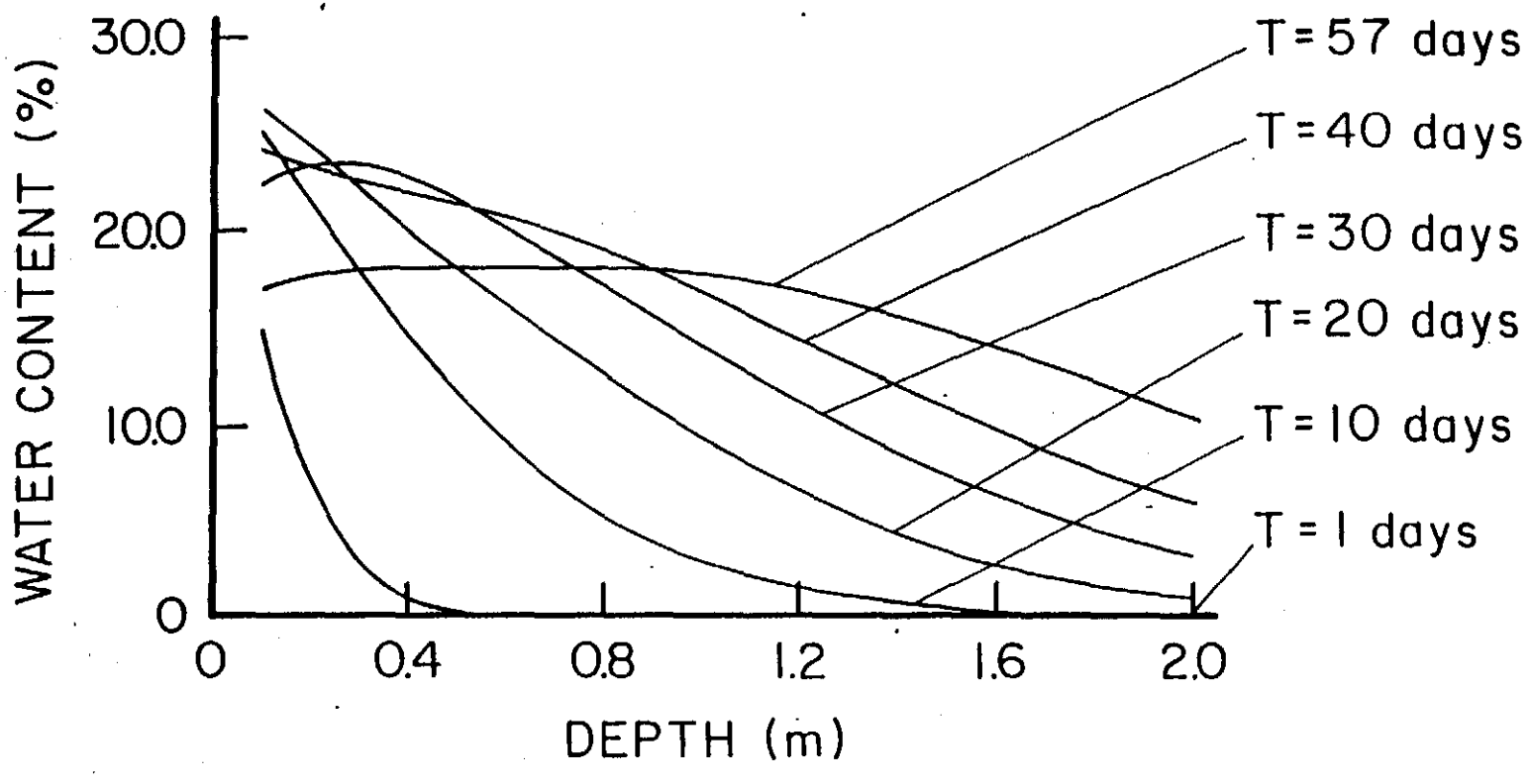

Fig. IV.10: Sample Functions of the Boundary Component of Water Content versus Depth at Different Times

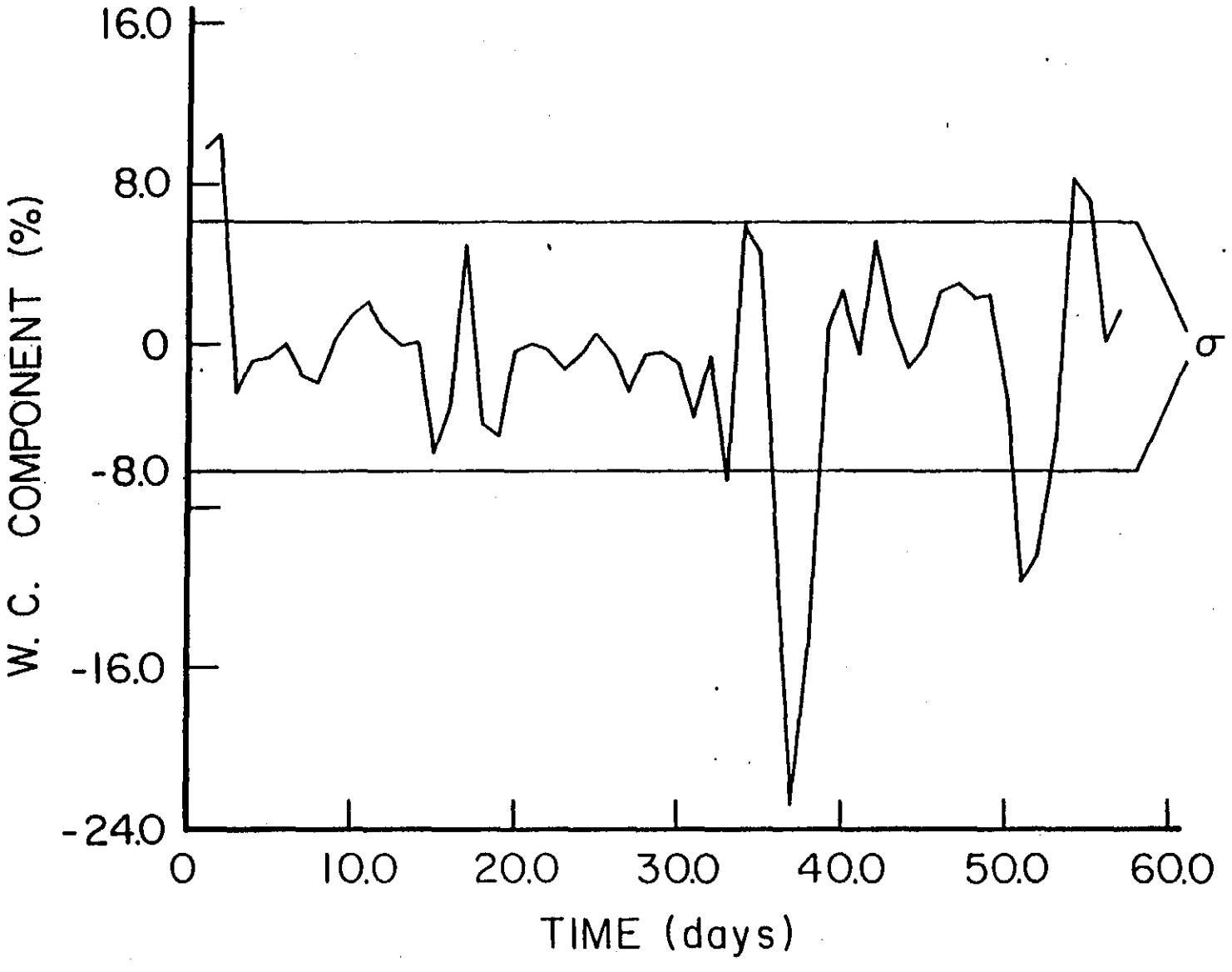

Fig. IV.11: Sample Function of the Component Due to D' of Water Content versus Time and Standard Deviation

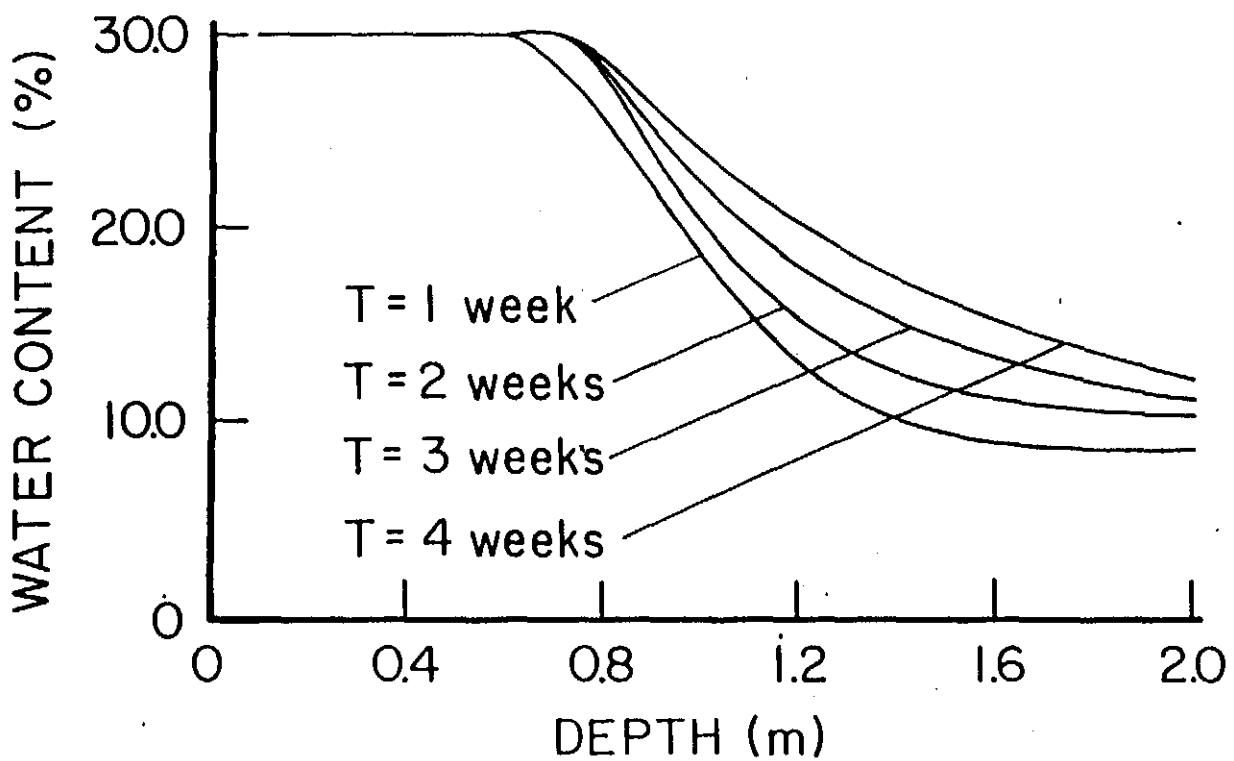

Fig. IV.12: Sample Water Content Versus Depth at Different Times

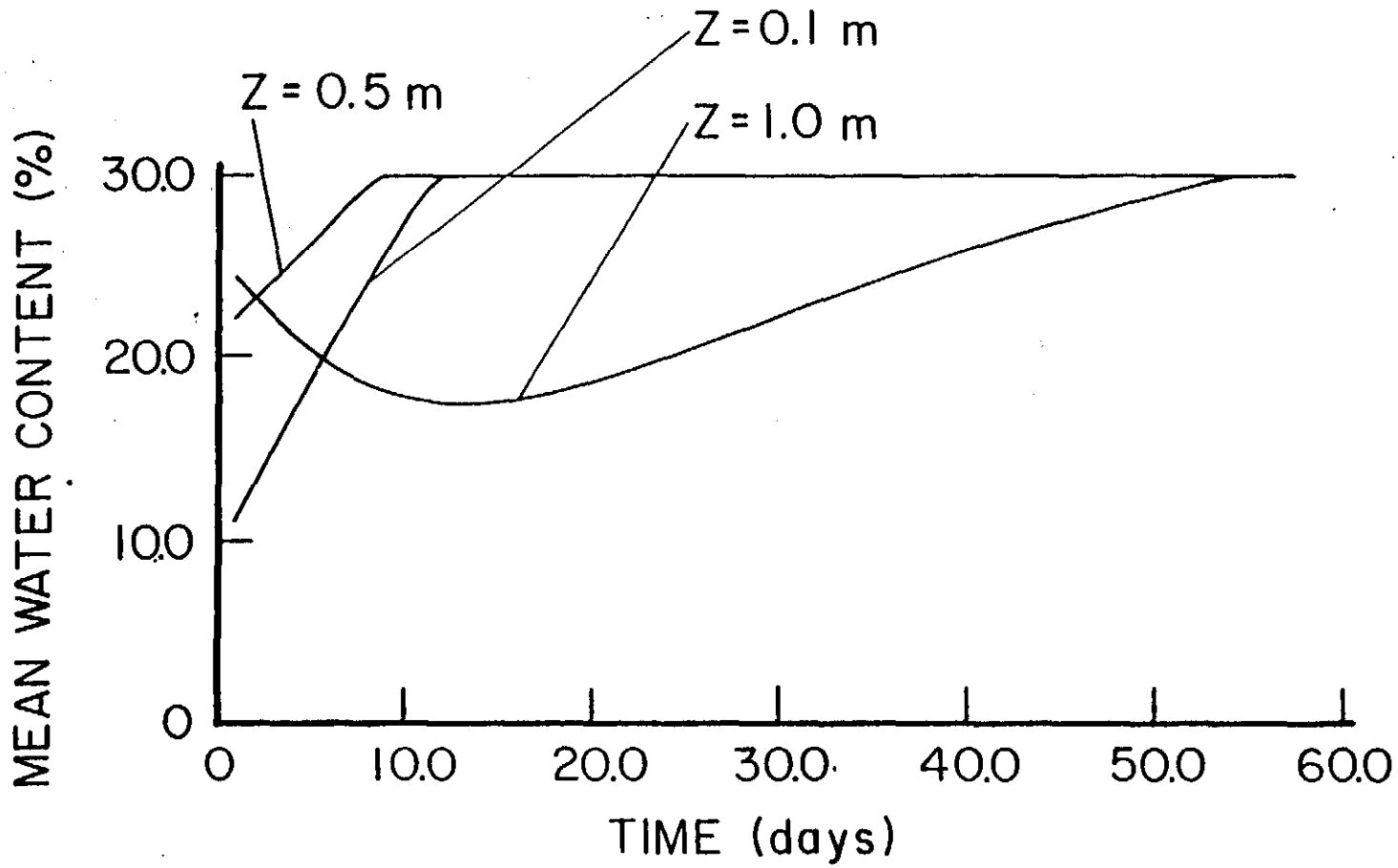

Fig. IV.13: Mean Boundary Component of the Water Content Versus Time at Different Depths

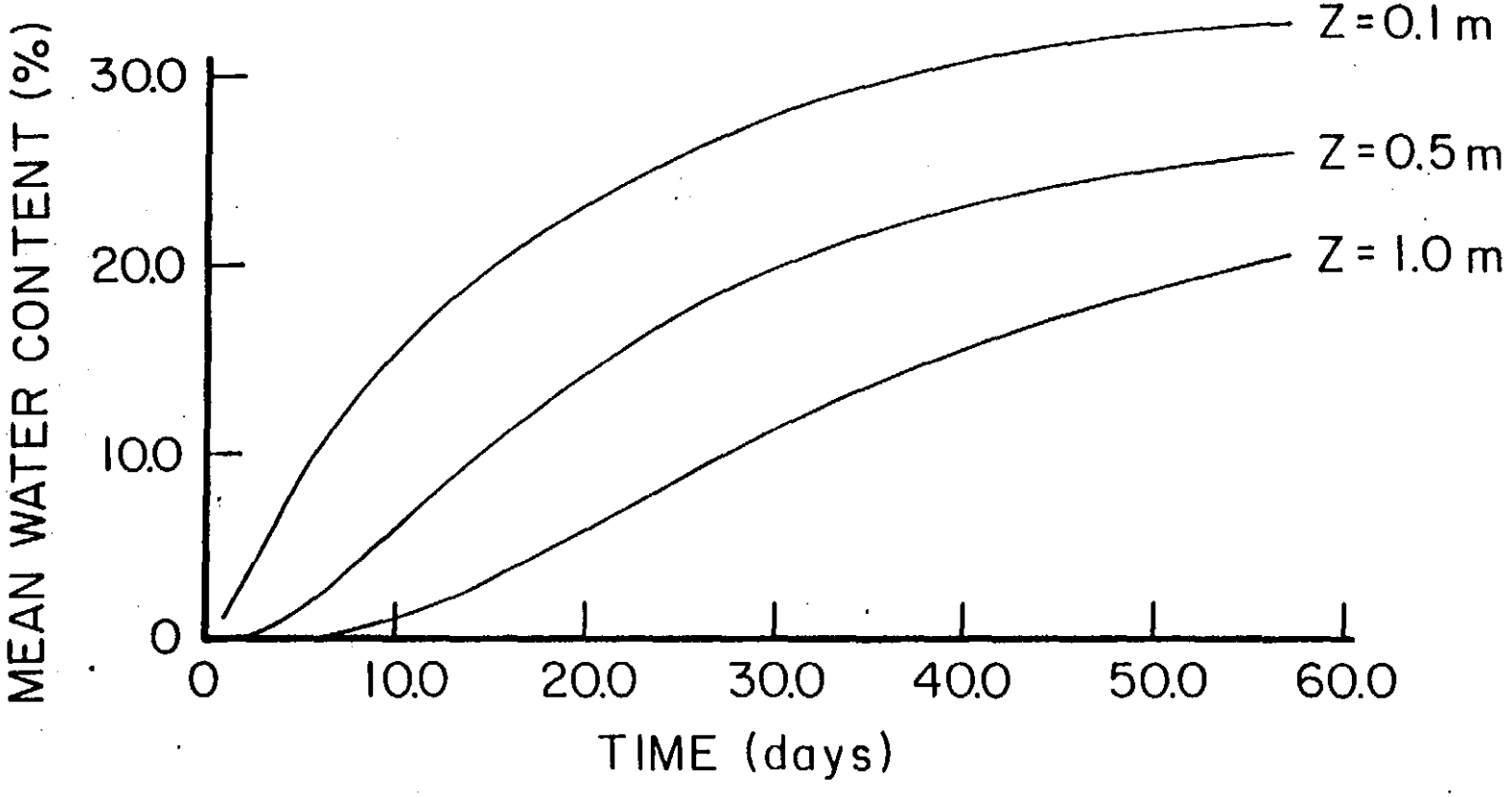

Fig. IV.14: Mean Water Content versus Time at Different Depths

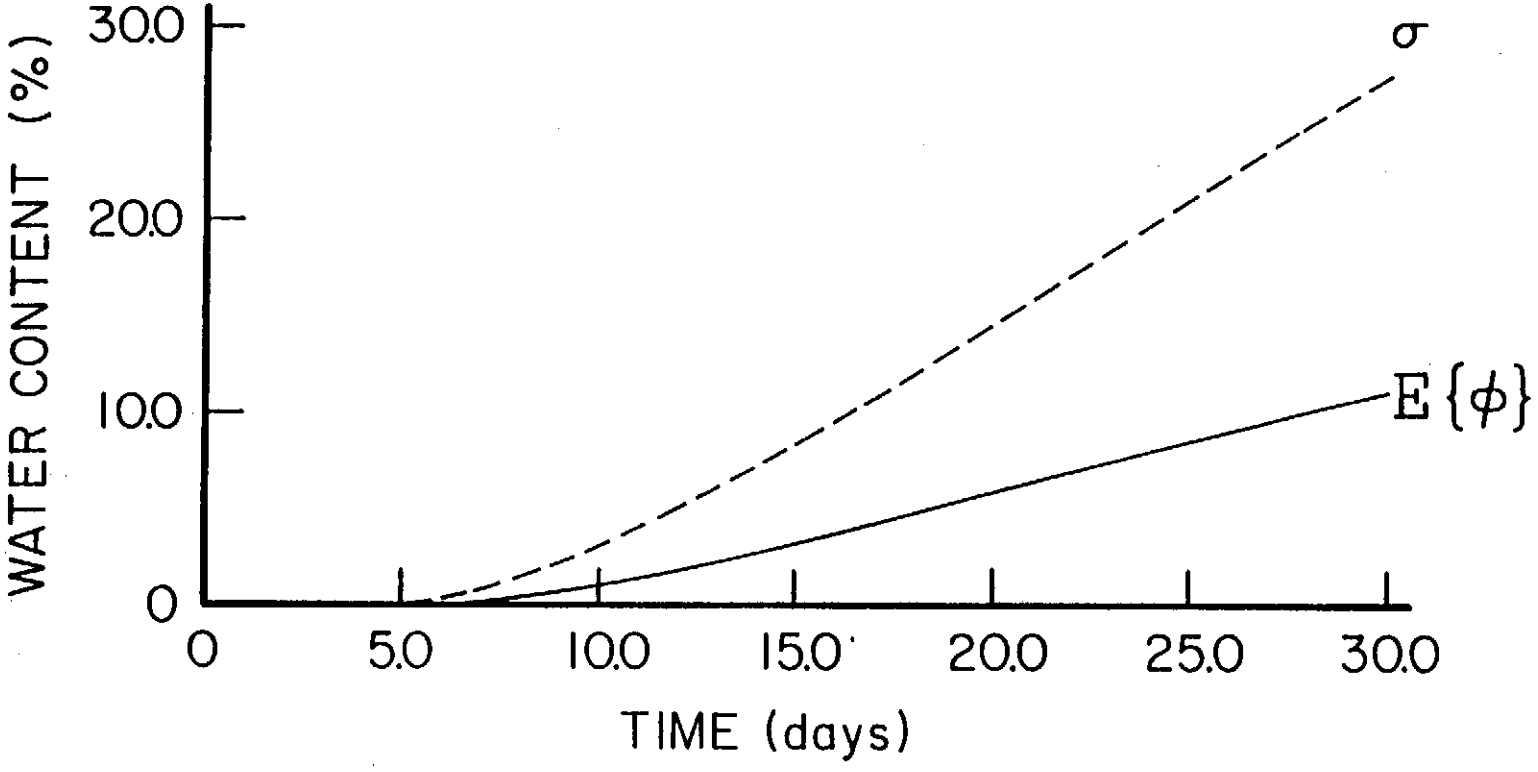

Fig. IV.15: Mean and Standard Deviation of the Boundary Component of the Water Content versus Time at One Meter Depth

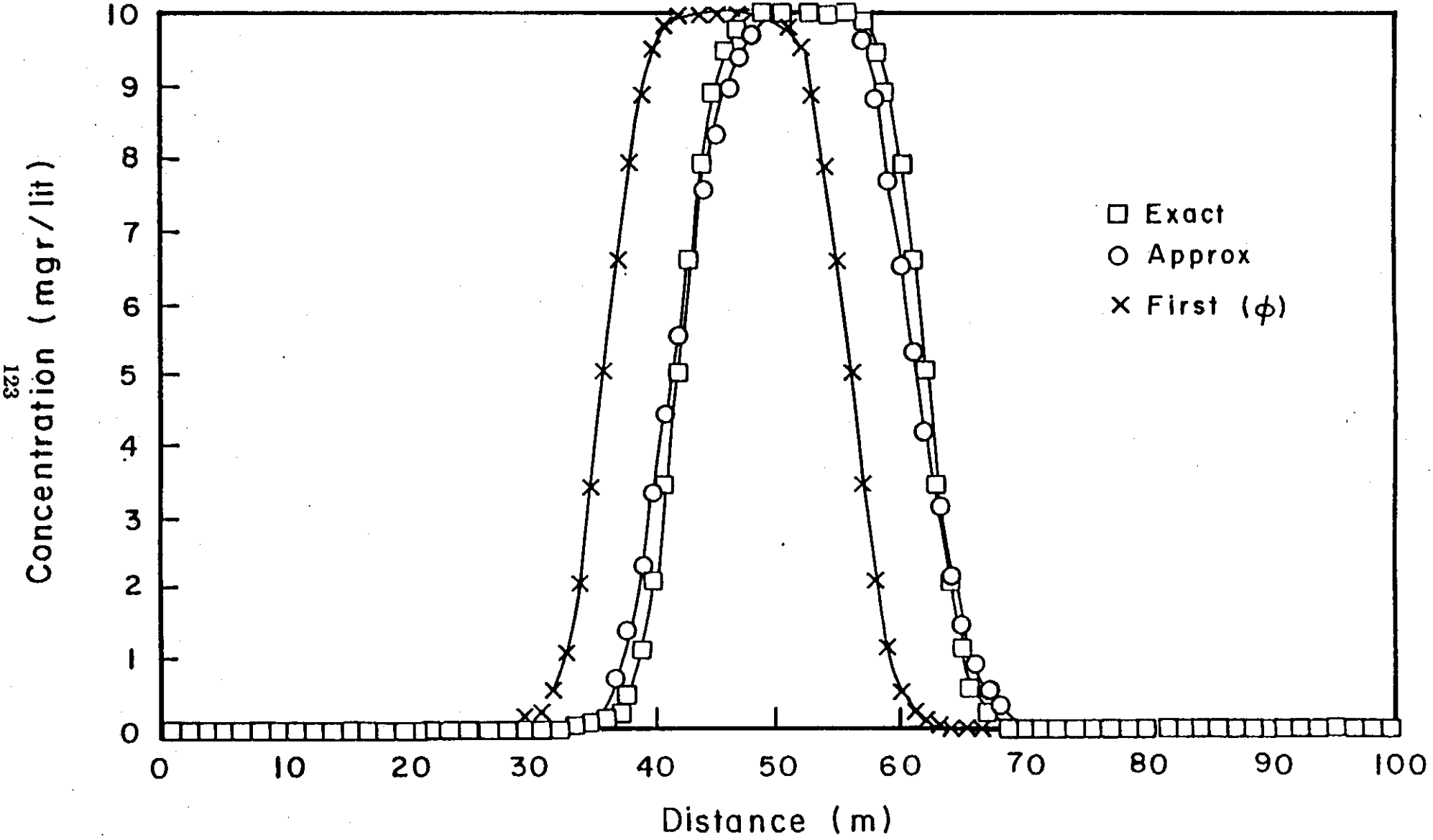

Fig.41: Concentration Breakthrough Curves After a 100% Increase in the Velocity

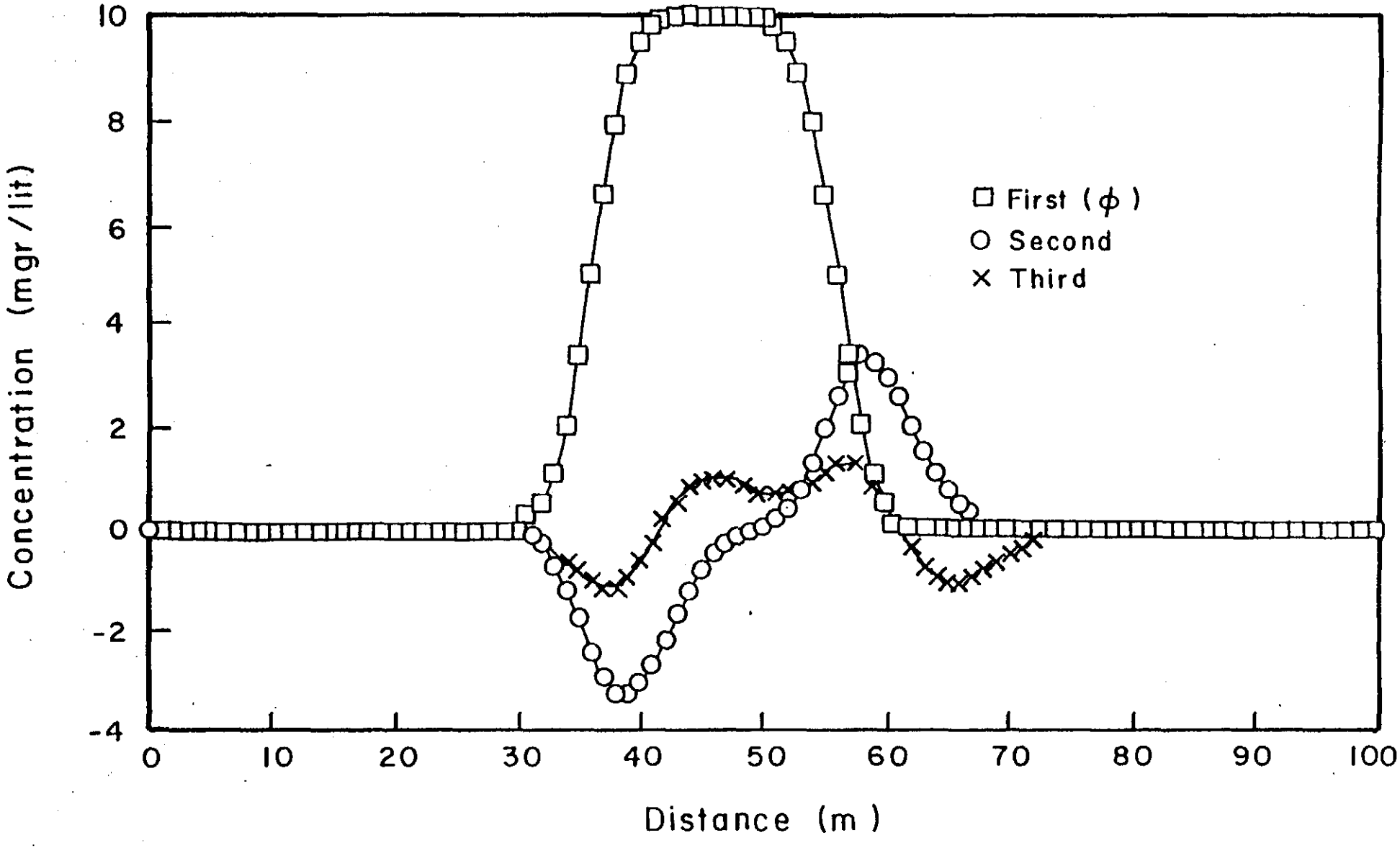

Fig 2: First Three Individual Approximations Versus Distance

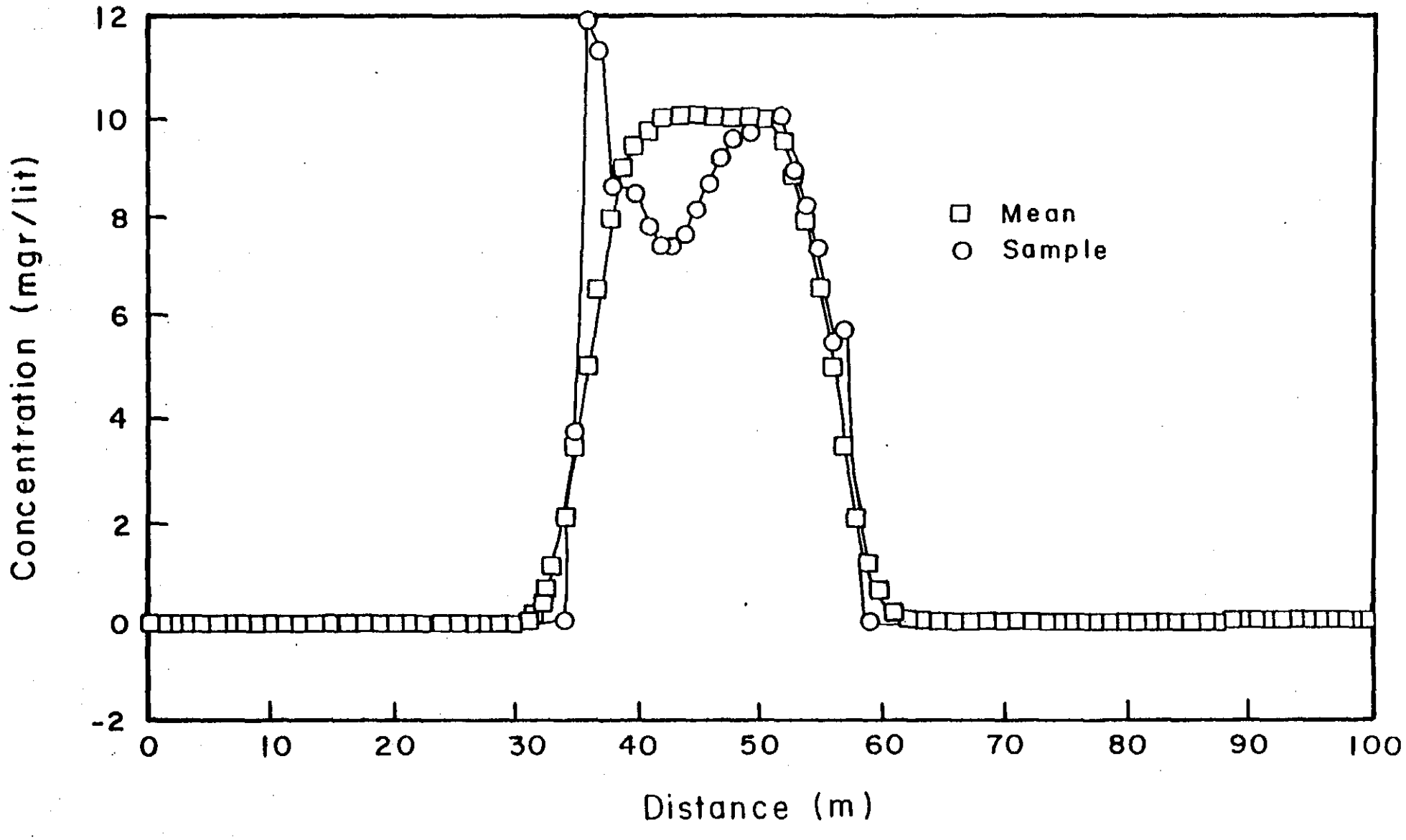

Fig.3: Mean and One Sample Concentration Versus Distance

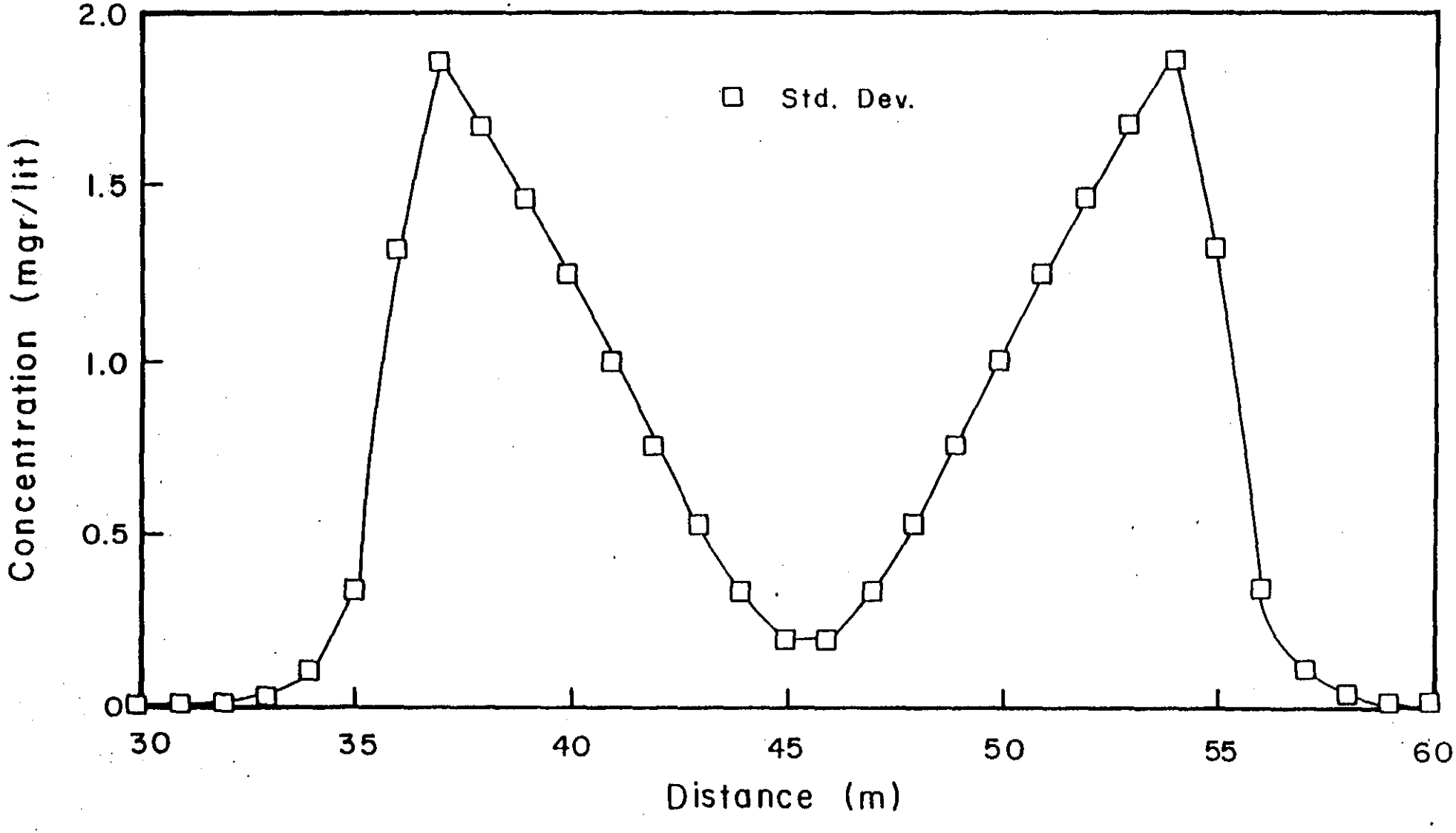

Fig V.4: Standard Deviation of Concentration Versus Distance

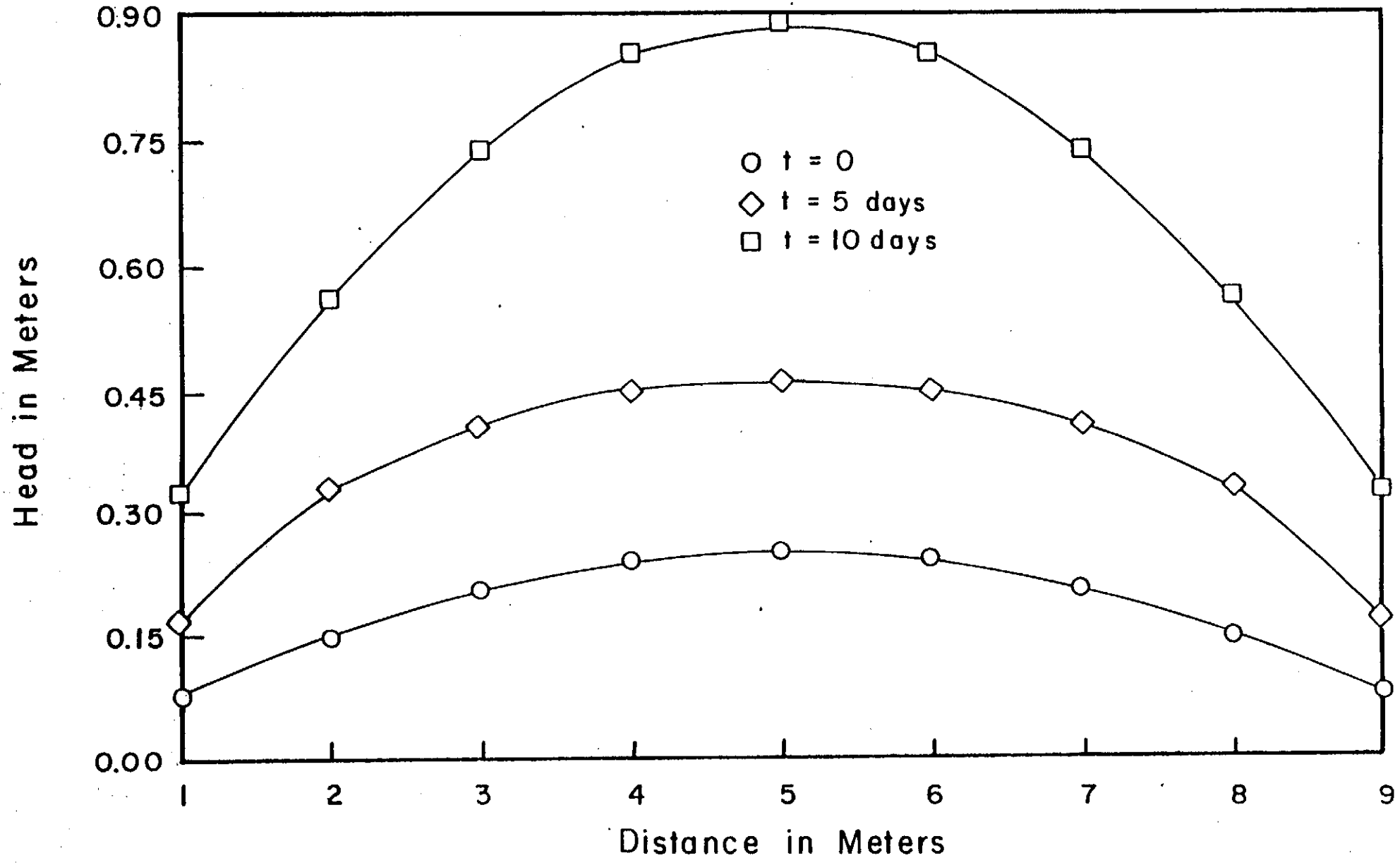

Fig V.5: Sample Groundwater Head with Distance

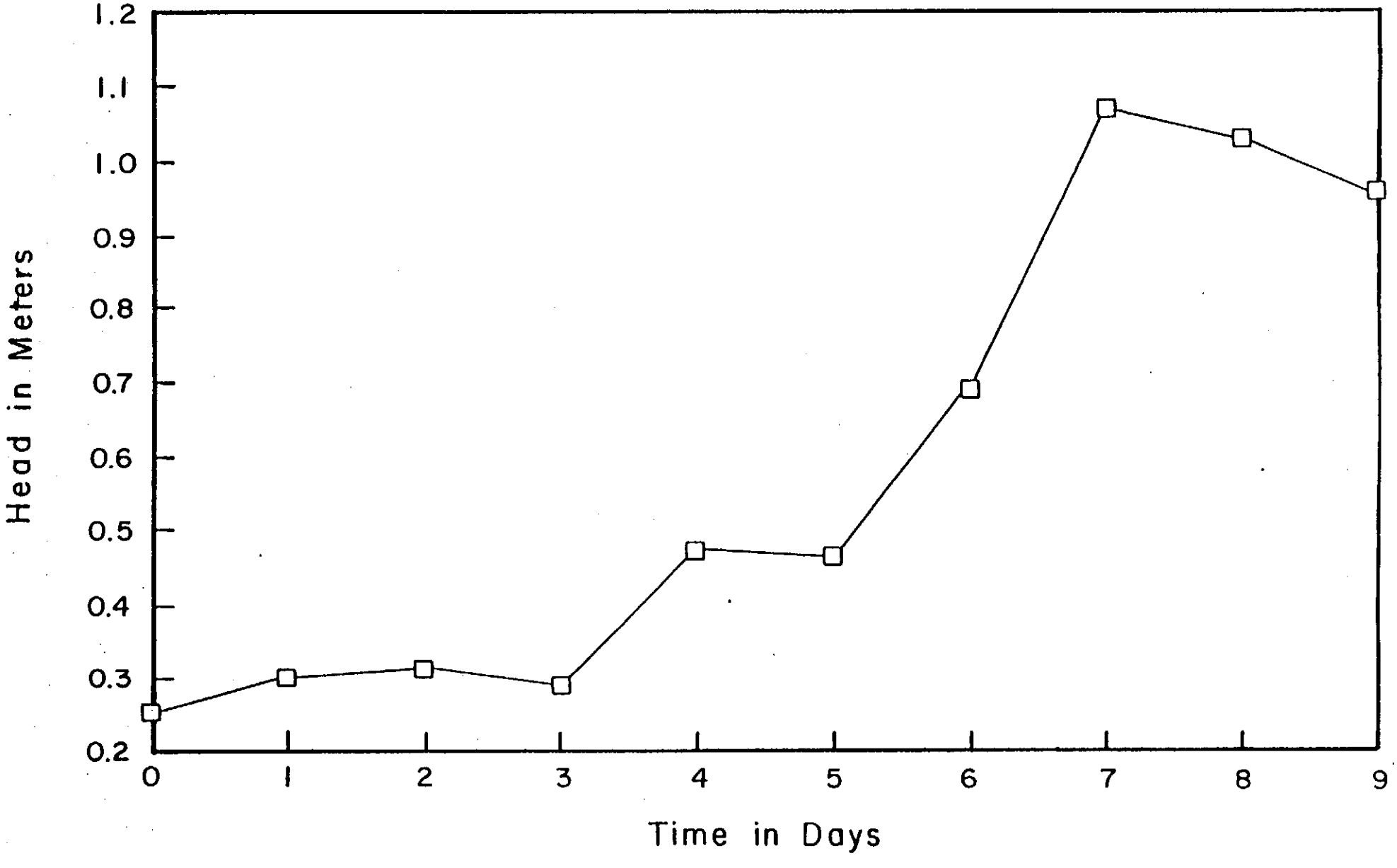

Fig 6: Sample Groundwater Head with Time at x=5 m

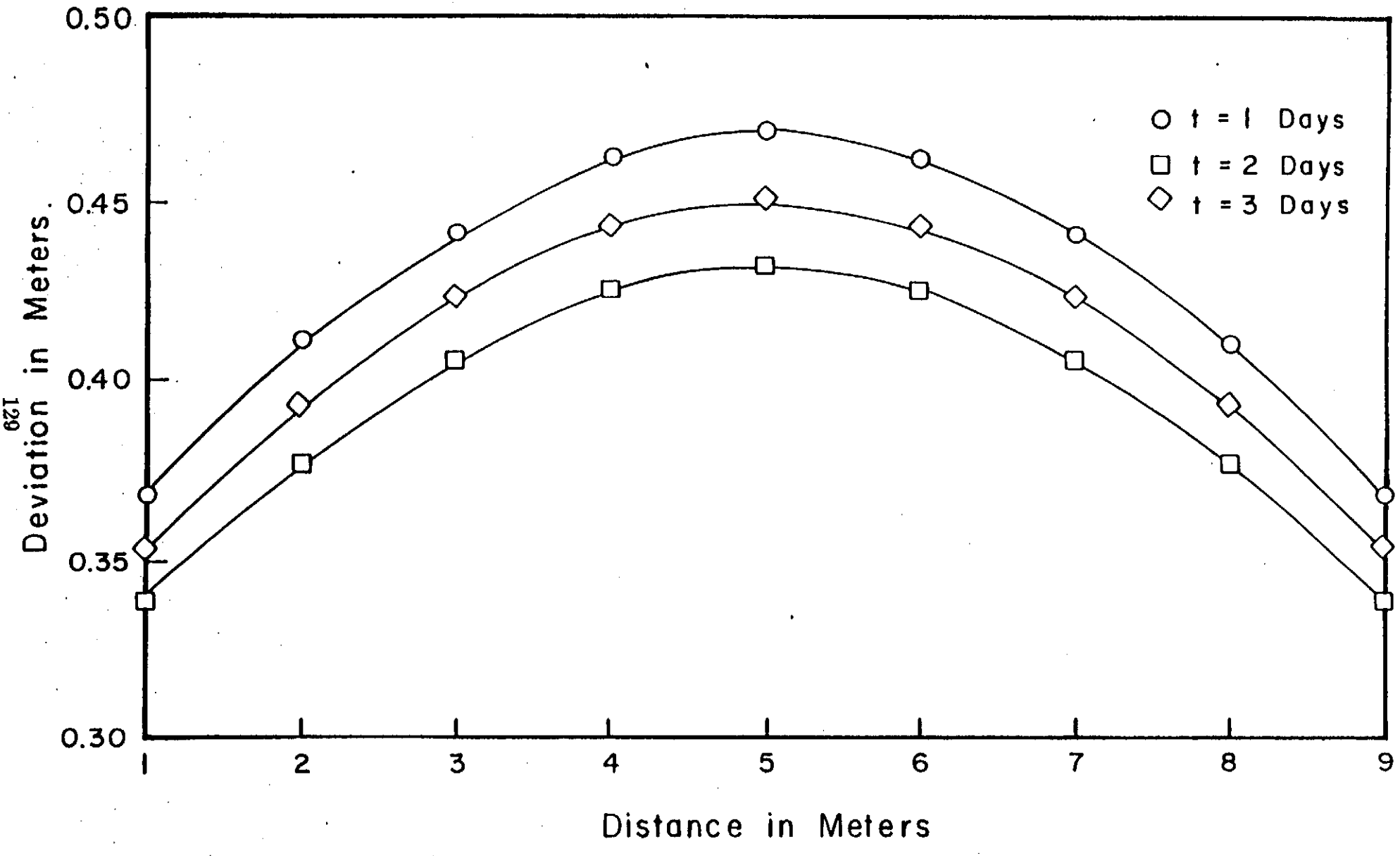

Fig 7: Head Standard Deviation with Distance

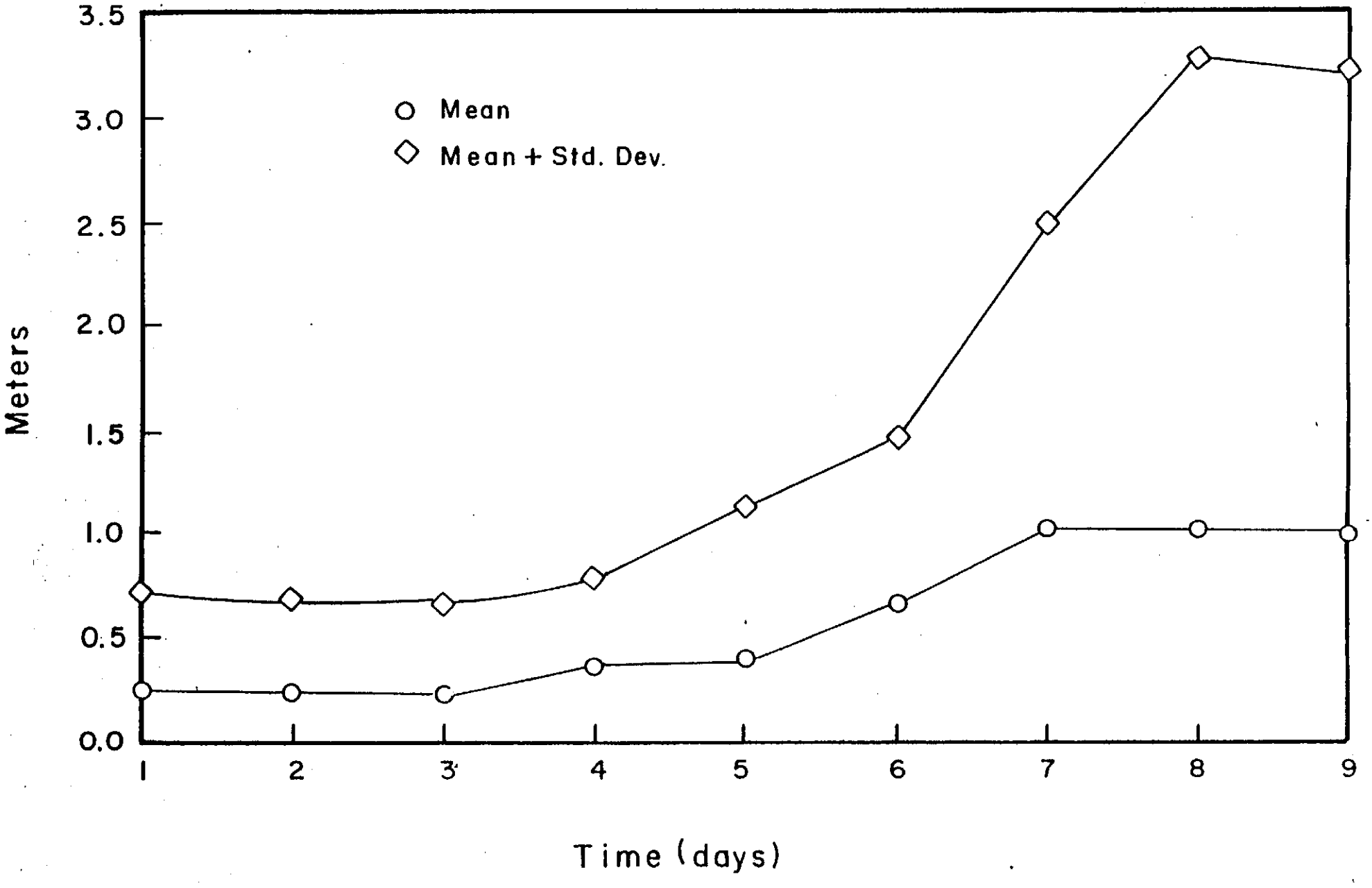

Fig. 8: Mean Head and Mean Plus One Standard Deviation with Time at X=5 m

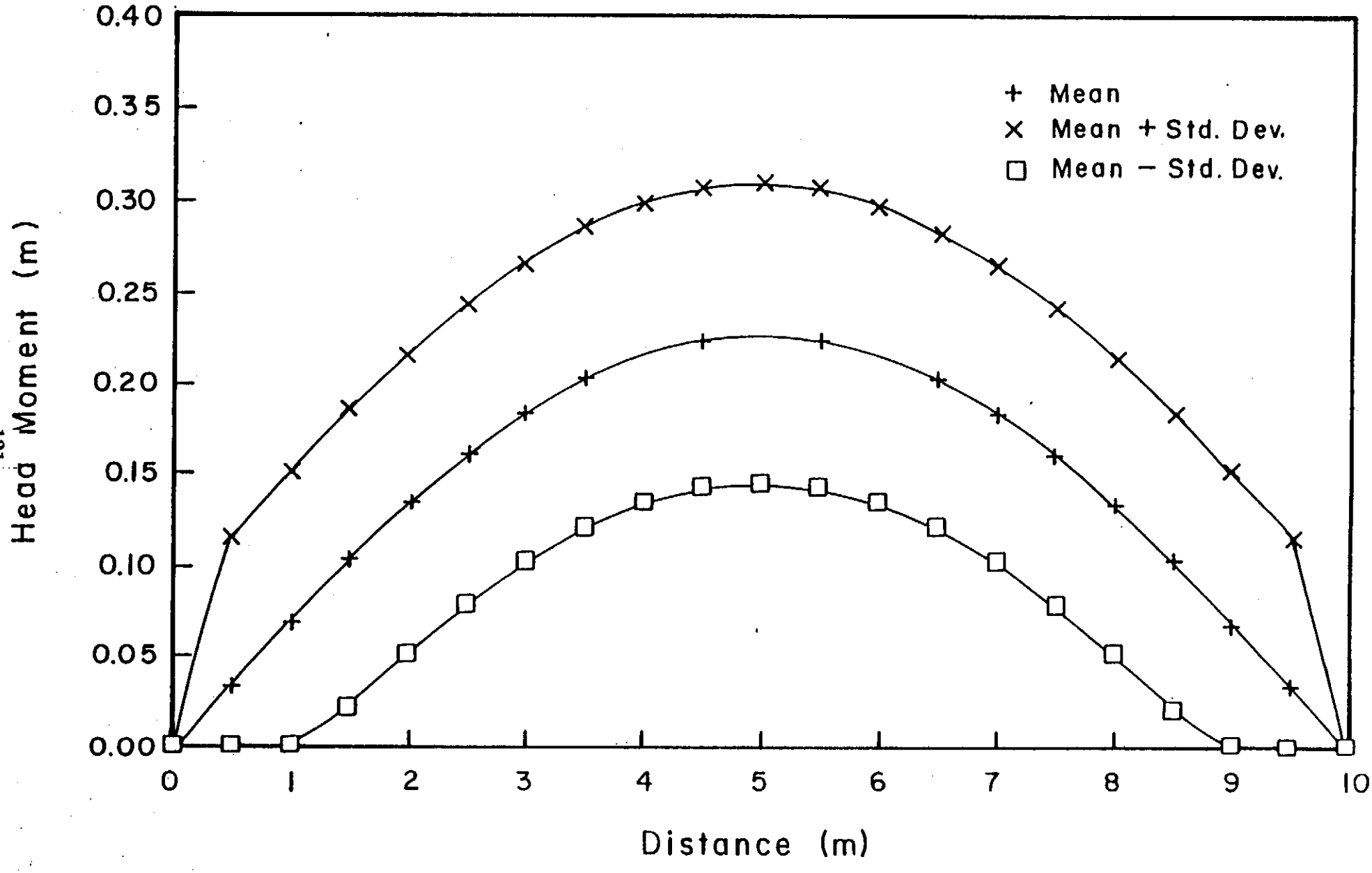

Fig. 9: Mean Head and Mean Plus and Minus One Standard Deviation With Distance