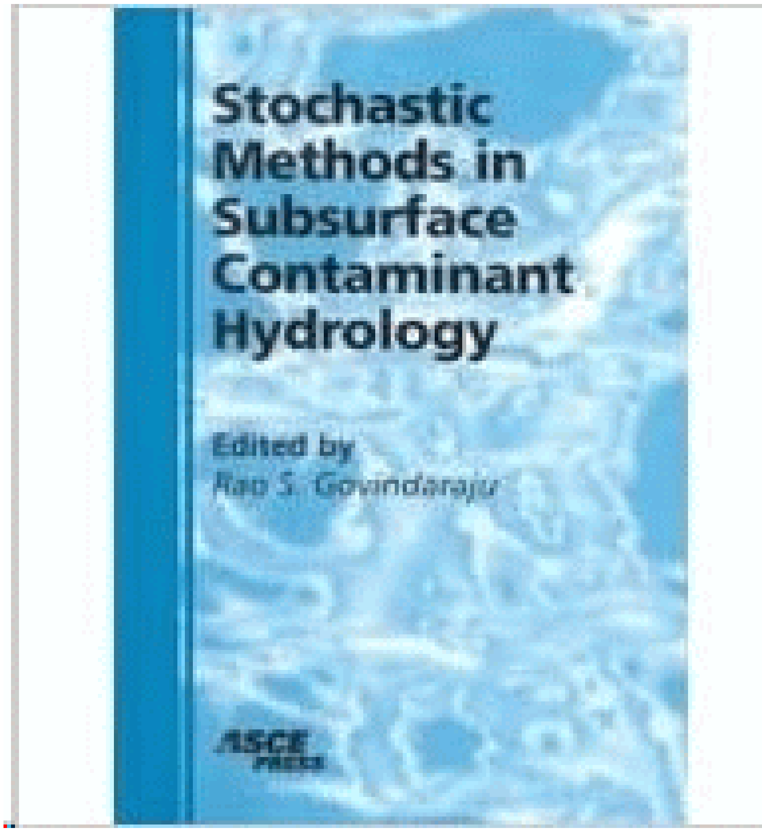

Stochastic Methods in Subsurface Contaminant Hydrology. Edited by R.S. Govindaraju. American Society of Civil Engineers, 2002. ISBN:9780784405321

A textbook for an advanced course in subsurface hydrology within a civil engineering curriculum. Researchers describe various approaches to using stochastic techniques to address the spatial heterogeneity of flow and transport parameters in problems of contaminant transport through the soil. Annotation

Stochastic Methods in Subsurface Contaminant Hydrology. Edited by R.S. Govindaraju. American Society of Civil Engineers, 2002. ISBN:9780784405321

8. SEMIGROUP AND DECOMPOSITION METHODS IN SOLVING STOCHASTIC SUBSURFACE CONTAMINATION PROBLEMS

Sergio E. Serrano
Department of Civil Engineering, Civil Engineering Building, University of Kentucky,
Lexington, Kentucky 40506-0281, U.S.A.

8.1 Introduction

This chapter summarizes the bases and the most important results obtained via the application of semigroup and decomposition methods in deriving and solving stochastic subsurface transport equations. These methods emphasize the application of fundamental physical laws to derive and solve solute transport differential equations in subsurface hydrology. In this process, the consideration of the regional hydrology is as important as the statistical representation of the aquifer hydrogeologic parameters. These methods also emphasize the utilization of mathematical procedures that rapidly converge to the true linear, or non-linear, solution. In other words, semigroup and decomposition methods aim at the definition of the appropriate mathematical model capable of considering the true physical conditions, rather than eliminating physical elements from consideration in order to fit a limited mathematical procedure (e.g., perturbation methods). In the following sections, we briefly describe the fundamentals of the approach with examples of applications to convection-dispersion models, the solution of scale-dependent transport equations in aquifers, the solutions for cases of non-point sources and spills originated in the unsaturated zone, and the definition of the functional form of the field-scale dispersion coefficient. Some notes on scale-dependent computer software for practical contaminant propagation forecasting are given. Also discussed are a few thoughts as to whether decomposition methods point towards an etiology of functional re-scaling of system parameters akin to today's fractal analyses.

Semigroup operators are related to fundamental solutions or Green's functions. Green’s functions are solutions to the differential equation when the initial condition is a delta function (i.e., an instantaneous point source) and the boundary conditions are zero. Semigroup operators are spatial integrals of the fundamental solution. They represent the output of a dynamical system subject to specific initial conditions, and permit the forecasting of the output function(s) subject to a variety of initial and boundary conditions. When the input functions or the boundary conditions are uncertain (i.e., random), the use of the semigroup operator offers a practical tool for the prediction of the state of a system with a great deal of notational economy and effort. When the system parameters are random, the semigroup operator may be approximated as a series expansion. The best approximation of the semigroup is via the method of decomposition.

The method of decomposition was developed by Dr. George Adomian (Adomian 1994, 1991, 1986, 1983). Originally, it was a procedure that allowed the solution of stochastic differential equations, particularly those with random coefficients, without resorting to small perturbation or hierarchical approximations. In other words, decomposition generated a series solution that converged rapidly to the true solution without eliminating terms of the differential equation on the subjective assumption that they were small (i.e., small perturbation assumptions), or without neglecting higher-order moments (hierarchical approaches). As the method evolved over the years, it became apparent that solutions to deterministic, stochastic, linear, non-linear, ordinary, partial, and integro-differential equations could be obtained in a systematic way. Each term in the series was analytical and for cases where a closed form solution was obtained, the solution was verifiable by direct substitution. Furthermore, in most dissipative systems the convergence rate is so fast, that only two or three terms in the series is necessary to approximate a solution consistent with the resolution of field measurement devices. Thus, whether or not the modeler obtains a closed-form solution built from an infinite set of terms, the method of decomposition provides a practical tool that allows the accurate simulation of a physical phenomenon. Decomposition has quickly extended to many fields of mathematical, physical, and engineering analysis (Adomian, 1994).

In subsurface contaminant hydrology, the method of decomposition has permitted the study of contaminant dispersion in heterogeneous media with the consideration of the aquifer regional hydrology, as well as the statistical properties of the hydrogeologic parameters. With decomposition, a return to the fundamental hydrology has been possible. The principle that aquifer hydrology and contaminant dispersion are inseparable can now be applied. This implies that the physical parameters of a contaminant transport equation should result from a solution to the underlying groundwater flow equation. The groundwater flow equation should be solved subject to the actual field boundary conditions, recharge from rainfall, and transient components in these functions. Although a good portion of this theory is already available (Serrano, 1996(2) 1995(1)), much work on the effects of transient components and seasonal hydrology remains to be done. In summary, the main advantages of decomposition methods are:

(1) It advocates the use, analysis, and solution of the transport differential equation, which results from the application of universal physical laws, such as mass conservation.

(2) It allows the consideration of the regional hydrology, and the aquifer hydraulics, as well as the aquifer heterogeneity (e.g., the effect of recharge from rainfall, aquifer boundary conditions, non-stationarity in the hydraulic conductivity, and transient components in these functions).

(3) It does not restrict the physics of the problem in order to fit a limited mathematical procedure. For example, it does not require small variances in the conductivity (small perturbation techniques), or a logarithmic transformation in the conductivity, or a Gaussian distribution in the parameters, or the arbitrary elimination of terms in the differential equations, or the exclusion of the underlying regional hydrology (see Serrano, 1996(3) for a comparison between decomposition and small perturbation techniques).

(4) It provides a systematic series procedure that rapidly converges to the true non-linear solution. Non-linear equations do not have to be linearized. Each term in the series is analytical, and verifiable by direct substitution.

We conclude this section with the inspiring words of Nobel Prize laureate Richard Feynman:

"*It is necessary for the very existence of science that minds exist that do not allow that nature must satisfy some preconceived notions.*"

8.2 Semigroup Operators in Subsurface Contaminant Hydrology

Application of the law of mass conservation to a contaminant propagating in the subsurface environment leads to particular forms of a class of an abstract evolution equation. Depending on the actual field conditions, this equation is subject to the hydrologic constraints imposed by the regional groundwater flow characteristics, the flow boundary conditions, the regime of the recharge from precipitation, the evapotranspiration time distribution, the biodegradability of the contaminant in question, the adsorption characteristics of the porous media, the spatial variability of the hydraulic conductivity and the storage coefficient, and the relationships between the solid, liquid, and vapor phases of the contaminant. The resulting equation may be classified as an abstract evolution equation of the form where u is the system output (e.g., contaminant concentration); g is a second-order stochastic process representing

$$\frac{\partial u}{\partial t}(X,\ t,\ \omega)\ +\ \boldsymbol{A}(X,\ t,\ \omega)u\ =\ g(x,\ t,\ \omega),$$
$$u(X,\ 0)\ =\ u_0(X),\quad (X,\ t,\ \omega)\ \in\ G\ \times\ [0,\ T]\ \times\ \Omega \qquad \textbf{(8.1)}$$

sources and sinks; G is a subset of $\Re^3$ with boundary ∂G on $(0 < T < \infty)$; X represents three-dimensional space; $\boldsymbol{A}$ is an m-th order random partial differential operator, whose parameters are in general time and space functions of the aquifer hydrology and the aquifer heterogeneity; $u_0(X)$ is the initial condition; T is the upper bound of the time coordinate; and Ω the upper bound of the probability variable, ω.

The solution to (8.1) is

$$u\ =\ \boldsymbol{J}_t u_0\ +\ \int_0^t \boldsymbol{J}_{t-t'}\, g dt' \qquad \textbf{(8.2)}$$

where $\boldsymbol{J}_t$ is the evolution operator associated with $\boldsymbol{A}$**.** If the operator $\boldsymbol{A}$ is time independent, and if $\boldsymbol{J}_t$ satisfies

(1) $\boldsymbol{J}_{t+t'}\ =\ \boldsymbol{J}_t \boldsymbol{J}_{t'}\ \geq\ 0$,

(2) $\boldsymbol{J}_{\boldsymbol{0}}\ =\ \boldsymbol{I}$, where $\boldsymbol{I}$ is the identity operator, and

(3) $\|\ \boldsymbol{J}_t u\ -\ u\ \|\ \to\ 0$ as $t\ \to\ 0$,

where $\|\ \|$ denotes the norm, then $\boldsymbol{J}_t$ is said to be the strongly continuous semigroup. From (8.1), one may derive moments equations which characterize the statistics of the output process. The first two moments define the mean and the correlation structure of the output.

Examples of semigroup operators in saturated groundwater flow are found in Serrano et al. (1985(1), 1985(2)) and in Serrano and Unny (1987(2)). These references illustrate the fundamental semigroup theory and its applications in cases of deterministic parameters and stochastic input and boundary conditions. Examples of semigroup operators in unsaturated zone hydrology are found Serrano (1990 (1), (2); 1998). These references focus on the solution of the infiltration equation when the ground-surface boundary condition is subject to time-stochastic rainfall and the soil-water functional relationships are subject to random hysteresis. The non-linear differential equation is transformed into a linear stochastic equation. However, recent refinements in the theory demonstrate that the solution to the non-linear equation could be obtained directly (see section 8.3, and Serrano, 1998). The approximation of the semigroup when the transmissivity is a random function is studied in Serrano and Unny (1987(1)). The approximation is attempted via the decomposition of the groundwater flow equation (Adomian, 1983).

Examples of semigroup operators in contaminant hydrology may be found in Serrano (1988(1)) along with illustrations of the form of the semigroup in cases of well contamination subject to measurement errors, the modeling of non-conservative contaminant migration, and the aquifer contamination subject to uncertain variability at a boundary source. Problems involving the approximation of the semigroup in cases of time or space stochastic variability in the parameters are studied in Serrano (1988(2)). Again, the approximation of the semigroup is approached via the decomposition of the differential equation. When the governing equation is the advective-dispersive equation in an infinite three-dimensional domain, the semigroup operator is the integral of the fundamental solution (i.e., the Green's function). For example, consider the one-dimensional advective-dispersive equation in an infinite aquifer:

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + v\frac{\partial C}{\partial x} = g(x,\ t),\ \ -\infty<x<\infty,\ \ 0<t$$
$$C(\pm\ \infty,\ t) = 0, \quad C(x\ ,\ 0) = f(x) \tag{8.3}$$

where C is the contaminant concentration in (*mg/L*); D is the dispersion coefficient ($m^2/month$); v is the pore velocity (*mm/month*); x is distance from the chemical spill (*m*); t is time after the initial spill (*month*); and g represents additional sources, sinks, adsorption, or contaminant loads from the unsaturated zone (*mg/L/month*); and $f(x)$ represents the initial spatial distribution of the contaminant plume (*mg/L)*.

From (8.2), the solution to this equation is

$$C(x,\ t) = \boldsymbol{J}_t f + \int_0^t \boldsymbol{J}_{t-t'}\ g(x,\ t')dt' \tag{8.4}$$

where the semigroup operator is given by

$$\boldsymbol{J}_t f(x) = \frac{1}{\sqrt{4\pi Dt}}\int_{-\infty}^{\infty} e^{-\frac{x-vt-x'}{4Dt}} f(x')dx' \tag{8.5}$$

Consider the classical case when $g=0$. If in addition the initial condition is $f(x) = C_i\delta(x)$, where C_i is the initial mass (*mg*) and $\delta(x)$ is the Dirac's delta function (i.e., an instantaneous point spill at the origin), then (8.4) reduces to the well-known Green's function of the homogeneous advective-dispersive equation:

$$C(x,\ t) = \boldsymbol{J}_t f(x) = \frac{e^{-\frac{x-vt}{4Dt}}}{\sqrt{4\pi Dt}} \tag{8.6}$$

Once the semigroup operator is available, it may be used to solve more general problems, such as chemical reactions, biological decay, spatially-variable source functions (i.e., non-point source problems), mass transfer between different contaminant phases or time-dependent boundary conditions. Thus, the forcing function, g , may be composed of several (deterministic or stochastic) terms representing the different possible scenarios. The semigroup operator may also be called in computational algorithms and used in combination with its intrinsic properties (1) through (3) described before. Furthermore, since the semigroup is analytic in form, there are obvious computational stability advantages. Extension to three-dimensional cases are straight forward (Serrano, 1988(1)). The semigroup operator is then given as a triple integral, one for each spatial coordinate.

8.3 Analytical Decomposition Methods in Subsurface Contaminant Hydrology

As stated in section 8.2, the study of contaminant transport problems subject to random spatial or temporal variability in the hydrogeologic parameters has been accomplished via a combination of semigroup operators with analytical decomposition of the transport equation. Until 1992, the fundamental semigroup associated with the operator A in (8.1) was used in each decomposition expansion term. However, recent advances in decomposition theory (Adomian, 1991, 1994; Adomian and Serrano, 1998; Serrano and Adomian, 1996) permitted a significant reduction in the form of each expansion term. The simplicity gained joined the usual advantages of decomposition (e.g., the ability to solve non-linear equations, fast convergence, the possibility to include large variances in the parameters, the inclusion of natural aquifer hydrology, etc.). This has generated new insight into complex problems, such as the scale-dependency of dispersion parameters, the solution of complex transport equations when the parameters are given as explicit functions of the underlying groundwater flow problem, and the solution when the parameters are non-stationary random functions. In this section we describe the general decomposition solution of (8.1).

Let us write (8.1) as

$$Lu = g - \boldsymbol{A}u \tag{8.7}$$

Using decomposition (Adomian, 1994; see Serrano, 1997(2) for a simple introduction to decomposition with numerical examples), we define L^{-1} as the definite integral from zero to *t*, with decomposition of *u* into $\sum_{n=0}^{\infty} u_n$ and identification of u_0 as *u(0)*, we have

$$\begin{aligned} L^{-1}Lu &= L^{-1}g - L^{-1}\boldsymbol{A}u, \\ u - u(t=0) &= L^{-1}g - L^{-1}\boldsymbol{A}u, \\ u &= u(t=0) + L^{-1}g - L^{-1}\boldsymbol{A}u \end{aligned} \tag{8.8}$$

Define $u_0 = u(t=0) + L^{-1}g$ and $u = \sum_{n=0}^{\infty} u_n$,

$$\begin{aligned} u &= u_0 - L^{-1}\boldsymbol{A}\sum_{n=0}^{\infty} u_n, \\ u_1 &= -L^{-1}\boldsymbol{A}u_0, \\ u_2 &= -L^{-1}\boldsymbol{A}u_1 = \left(-L^{-1}\boldsymbol{A}\right)^2 u_0, \\ &\vdots \\ u_n &= -L^{-1}\boldsymbol{A}u_{n-1} \end{aligned} \tag{8.9}$$

We can then write the “approximant”

$$\varphi_m[u] = u_0 - \sum_{n=0}^{m-2} L^{-1}\boldsymbol{A}u_n = \sum_{n=0}^{m-1}\left(-L^{-1}\boldsymbol{A}\right)^n u_0 \tag{8.10}$$

For example, consider the advective-dispersive equation

$$\frac{\partial u}{\partial t} = g - \boldsymbol{A}u, \tag{8.11}$$

where

$$\begin{aligned}
&\boldsymbol{A} = -D\frac{\partial^2}{\partial x^2} + v\frac{\partial}{\partial x},\\
&u = u(t = 0) + L^{-1}g,\\
&u_1 = -L^{-1}\left[-D\frac{\partial^2}{\partial x^2} + v\frac{\partial}{\partial x}\right]u_0 = L^{-1}D\frac{\partial^2}{\partial x^2}u_0 - L^{-1}v\frac{\partial}{\partial x}u_0\\
&\vdots
\end{aligned} \tag{8.12}$$

with D, v constant parameters. $\langle u \rangle$, where $\langle\ \rangle$ denotes the expectation operator, is found from $\langle \varphi_m[u] \rangle$:

$$\langle u_0 \rangle = \langle u(t = 0) \rangle + L^{-1}\langle g \rangle \ or \ u(t = 0) + L^{-1}\langle g \rangle, \tag{8.13}$$

depending on the given initial conditions,

$$\langle u_1 \rangle = L^{-1}D\frac{\partial^2}{\partial x^2}\langle u_0 \rangle - L^{-1}v\frac{\partial}{\partial x}\langle u_0 \rangle, \tag{8.14}$$

or even

$$\begin{aligned}
&\langle u_1 \rangle = L^{-1}\langle D \rangle\frac{\partial^2}{\partial x^2}\langle u_0 \rangle - L^{-1}\langle v \rangle\frac{\partial}{\partial x}\langle u_0 \rangle\\
&\vdots
\end{aligned} \tag{8.15}$$

if D, v are stochastic. g could be a general stochastic process. First and second-order statistics can be found easily. Because of the fast convergence of the series it is usually accurate to obtain $\varphi_4[t]$ and $\varphi_4[t']$ and average to derive the correlation function (the errors are discussed in Adomian, 1986). The results are easily generalized to three dimensions and, by assuming Gaussian behavior, to higher moments. Finally by using the Adomian polynomials (Adomian, 1994), the results can be extended to non-linear equations as well. For example, if (8.1) also has a term $f(u)$, the appropriate A_n polynomials for $f(u)$ are $f(u) = \sum_{n=0}^{\infty} A_n$ and proceeding exactly as with the u_n. The series $\sum_{n=0}^{\infty} A_n$ forms a generalized Taylor series about the function $u_0(x)$. For boundary value problems which are non-linear, evaluating the constants of integration must be done at each level of φ_m (Adomian, 1994).

A rigorous framework for the convergence of decomposition series has been developed by (Gabet, 1994, 1993, 1992) by connecting the method to well known formulations where classical theorems (fixed point theorem, substituted series, etc.) could be used. Other rigorous work on the convergence were published by Abbaoui and Cherruault (1994), Cherruault (1989), and Cherruault et al (1992). A convergence theorem on the advective-dispersive equation is found in Serrano (1992(2)).

8.4 Applications to Convection Dispersion Models

The convection dispersion equation (CDE) still is the heart of many dispersion models in porous media, at least at the laboratory scale. The CDE also constitutes the first approximation in some scale dependent equations, and is part of the kernel in some integral equation solutions. Therefore, the ability to accurately, and efficiently, estimate solutions to the CDE renders a tool useful in applications. Consider the case of a transient chemical spill in an infinite one dimensional aquifer governed by (8.3).

Now set $L_t C = \frac{\partial C}{\partial t}$ and rewrite the CDE as

$$L_t C = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x}, \tag{8.16}$$

or

$$C = DL_t^{-1}\frac{\partial^2 C}{\partial x^2} - vL_t^{-1}\frac{\partial C}{\partial x} \tag{8.17}$$

The decomposition series are $C = C_0 + C_1 + C_2 + ...,$ where the first term satisfies $LC_0 = 0,\ C_0(0) = f(x)$, and

$$\begin{aligned} C_0 &= f(x), \\ C_1 &= Dtf''(x) - vtf'(x), \\ &\vdots \\ C_n &= DL_t^{-1}\frac{\partial^2 C_{n-1}}{\partial x^2} - vL_t^{-1}\frac{\partial C_{n-1}}{\partial x}. \end{aligned} \tag{8.18}$$

Note that one may easily adjust the simulation time step to assure convergence, which would require that $\frac{Dt}{2} < 1$, or $\frac{vt}{2} < 1$. See Serrano (1998, 1992(2)) for a theorem with proof on the uniform convergence of the above series.

Without loss of generality, and as an example, let us assume an initial condition of the form

$$f(x) = C_0 = \frac{C_i}{\sqrt{4\pi}}e^{-\frac{x^2}{4}}, \tag{8.19}$$

which is a Gaussian distribution with plume variance $\sigma^2 = 2.0\ m$. As $\sigma^2 \to 0$, $f(x) \to C_i\delta(x)$, a Dirac's delta function of strength C_i, theoretically an instantaneous spill. From the above equations, the first terms in the series are

$$C_1 = \frac{tf(x)}{2}\left(D(\frac{x^2}{2} - 1) + vx\right),$$

$$C_2 = \frac{t^2 f(x)}{8}\{ 3D^2(1 - x^2 + \frac{x^4}{12}) \tag{8.20}$$

$$- vDx(6 - x^2) - v^2(2 - x^2) \}$$

$$\vdots$$

The exact solution of the CDE is, in this case,

$$C = \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} e^{-\frac{(x-vt-x')^2}{4Dt}} . \frac{C_i}{\sqrt{4\pi}} e^{-\frac{x'^2}{4}} dx'$$

$$= \frac{C_i}{\sqrt{4\pi(1+Dt)}} e^{-\frac{(x-vt)^2}{4(1+Dt)}} \tag{8.21}$$

Let us assume that $C_i = 100.0\ mg/l$, $D = 0.01\ m^2/month$, and $v = 0.1\ m/month$. Figure 8.1 illustrates a comparison between the exact solution of the CDE six months after the spill, and the decomposition solution as approximated by $\varphi_3[C]$ with the first three terms in the series. The accuracy of the decomposition with three terms is remarkable, and in this case only two terms would produce an acceptable approximation. Figure 8.2 is a graph of the individual terms, C_0, C_1, and C_2 as a function of distance for the same simulation time, which demonstrates numerically the fast and uniform convergence of the decomposition series.

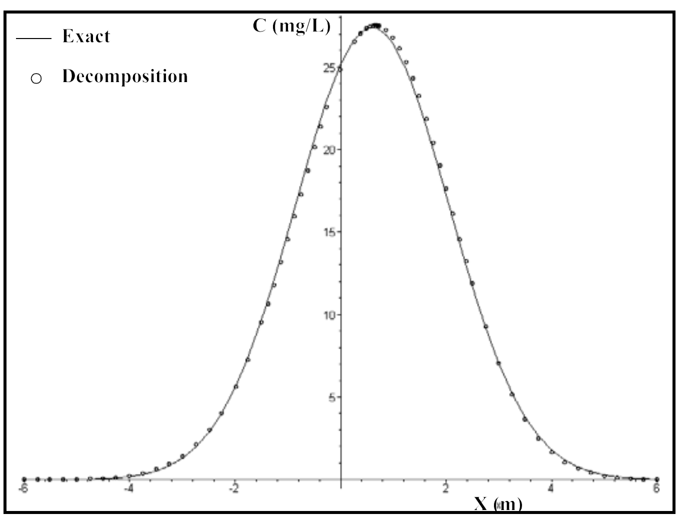

Figure 8.1: Comparison between Exact and Decomposition Solutions

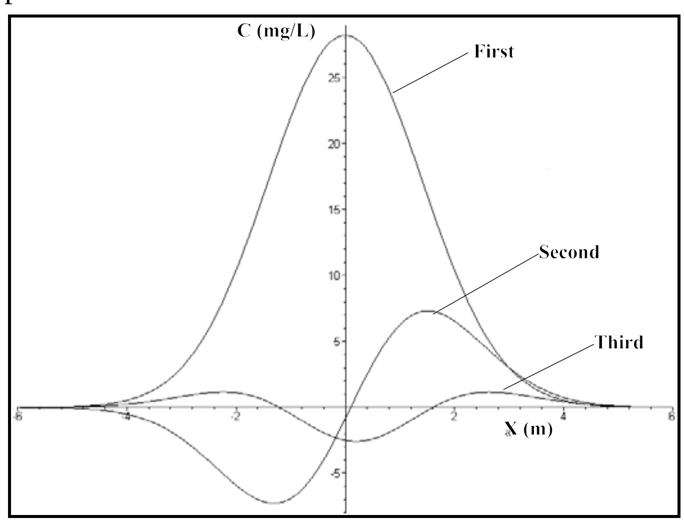

Figure 8.2: First Three Terms in the Decomposition Series

8.5 Applications to Scale Dependent Transport Models

Differential equations that account for the increase in the dispersion parameters with the scale of observation are beginning to appear in the hydrologic literature. Decomposition theory has attempted to define the dispersion parameters explicitly in terms of the underlying groundwater flow conditions. In this way, the dispersion model incorporates the hydrology of the aquifer (boundary conditions, recharge, etc.), as well as statistical properties in aquifer heterogeneity. In fact, even in a homogeneous aquifer with constant hydraulic conductivity, the simple addition of constant recharge in the analysis results in a transport equation with spatially-variable dispersion parameters (Serrano, 1992(1)). The resulting transport equations are difficult to solve with traditional analytic techniques. With decomposition some new solutions have been obtained. Consider the space variable dispersion equation (VDE) in a two dimensional heterogeneous phreatic aquifer with Dupuit assumptions subject to recharge from rainfall as given by (Serrano, 1996(1))

$$\frac{\partial \bar{C}}{\partial t} - h_1(x)\frac{\partial^2 \bar{C}}{\partial x^2} + h_2(x)\frac{\partial \bar{C}}{\partial x} + h_3\bar{C} - h_4(x)\frac{\partial^2 \bar{C}}{\partial y^2} = 0, \qquad (8.22)$$

$$-\infty < x < \infty, \quad -\infty < y < \infty, \quad 0 < t,$$

subject to the same boundary and initial conditions and

$$h_1(x) = \frac{\alpha_x}{nh_0}(Irx - h_0'\bar{T}),$$

$$h_2(x) = \frac{1}{nh_0}(Irx - h_0'\bar{T} - \alpha_x rI),$$

$$h_3 = \frac{Ir}{nh_0}, \qquad (8.23)$$

$$h_4(x) = \frac{\alpha_t}{nh_0}\left(Irx - h_0'\bar{T}\right), \quad r = 1 - \left(\frac{\sigma_T}{\bar{T}}\right)^2,$$

where $\bar{C}(x, y, t)$ is the mean solute concentration (mg/L); I is the mean monthly recharge from rainfall (*m/month*) responsible for the creation of non-uniform flow in the aquifer; n is the aquifer porosity; α_x is the small scale longitudinal dispersivity (m); α_y is the small scale transverse dispersivity (m); h_0' is the hydraulic gradient at the origin; h_0 is the mean saturated thickness(m); $\bar{T}$ is the mean aquifer transmissivity ($m^2/month$); σ_T is the transmissivity standard deviation ($m^2/month$); y represents plan view distance (m) perpendicular to x; and the rest of the terms as before.

Using a combination of Laplace and Fourier transforms, particular analytical solutions of (8.23) have been obtained (Serrano, 1996(1)). These solutions are stable for only a small range of values in the dispersion parameters. Using the original decomposition techniques (Adomian, 1983), series solution to (8.23) were also obtained. The results illustrated the fundamental properties of scale-dependent dispersion phenomena: plume non-symmetry and shifting. New contributions in decomposition theory (Adomian, 1994, 1991) have permitted better solutions to (8.23) (Serrano and Adomian, 1996).

For the purposes of illustration, let us consider the one dimensional version of the VDE in a heterogeneous aquifer (for the homogeneous case see Serrano, 1992(1)). Proceeding as in the previous sections we write the VDE as

$$C = h_1(x) L_t^{-1} \frac{\partial^2 C}{\partial x^2} - h_2(x) L_t^{-1} \frac{\partial C}{\partial x} - h_3 L_t^{-1} C, \tag{8.24}$$

and the individual terms in the decomposition series are given by

$$\begin{aligned}
C_0 &= f(x), \\
C_1 &= h_1(x) L_t^{-1} \frac{\partial^2 C_0}{\partial x^2} - h_2(x) L_t^{-1} \frac{\partial C_0}{\partial x} - h_3 L_t^{-1} C_0 \\
&= t h_1 f'' - t h_2 f' - t h_3 f, \\
C_2 &= h_1(x) L_t^{-1} \frac{\partial^2 C_1}{\partial x^2} - h_2(x) L_t^{-1} \frac{\partial C_1}{\partial x} - h_3 L_t^{-1} C_1 , \\
C_2 &= \frac{t^2}{2} \; [\; h_1 \left(h_1 f^{iv} + 2 h_1' f''' - h_2 f''' - 2 h_2' f'' - h_3 f'' \right) \\
&\quad - h_2 \left(h_1 f''' + h_1' f'' - h_2 f'' - h_2' f' - h_3 f' \right) \\
&\quad - h_3 \left(h_1 f'' - h_2 f' - h_3 f \right) \;] \\
&\;\vdots
\end{aligned} \tag{8.25}$$

For simulation examples and comparison with exact solutions in cases of large variances see Serrano and Adomian (1996).

8.6 Decomposition Theory of Non-Fickian Transport

The increase in magnitude of the dispersion parameters with the scale of observation, or the time after spill, has been a problem concern among hydrologists in the last two decades. It is generally accepted that the Fickian approximation is valid at the small scale (i.e., laboratory scale). According to decomposition theory, the scale effect is the result of hydrologic field conditions (i.e., recharge from rainfall, and flow boundary conditions), and aquifer heterogeneity at the field scale. The solute mass conservation equation is essentially valid at any scale. The Fickian approximation constitutes an initial condition to the evolution of the contaminant plume at large scales (Serrano, 1997(1)). Generalizations of this model to two dimensional and three-dimensional domains (Serrano, 1996(2)), and verification with limited tracer tests, confirm this hypothesis. This concept resonates with recent observations on the behavior of Fractal dynamical systems, where measures of system parameters repeat themselves and grow with the scale of observation. According to decomposition theory, this is reflected in the increase in magnitude of the variance of the output process and results solely from the initial condition input to a non-linear dynamical system.

Consider the solute continuity equation in an aquifer whose flow regime follows the Dupuit assumptions:

$$\begin{aligned}
&\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}\left(v_x C\right) + \frac{\partial}{\partial y}\left(v_y C\right) = 0 \\
&C(x, y, 0) = f(x, y),
\end{aligned} \tag{8.26}$$

where C, in this case, is the integrated over the vertical concentration. Thus, the large scale pore velocity in the x direction could be expressed as $v_x(x) = \bar{v}_x + v_{px}' + v_x'$, where v_{px}' represents the random component of the small scale pore velocity, and v_x' represents the random component of the large scale pore velocity. With the x coordinate coinciding with the (mean) regional groundwater pore velocity, the y (transverse) component of the pore velocity is defined as $v_y = v_{py}' + v_y'$, where v_{py}' represents the random component in the y direction of the pore velocity, and v_y' represents the random component of the large scale pore velocity in the y direction. Thus (8.26) becomes

$$\frac{\partial C}{\partial t}+\frac{\partial(\bar{v}_x C)}{\partial x}+\frac{\partial(v_{px}' C)}{\partial x}+\frac{\partial(v_x' C)}{\partial y}+\frac{\partial(v_{py}' C)}{\partial y}+\frac{\partial(v_y' C)}{\partial y}=0 \tag{8.27}$$

Adopting the Fickian approximation at the small scale, $v_{px}' C \simeq -D_x \frac{\partial C}{\partial x}$ and $v_{py}' C \simeq -D_y \frac{\partial C}{\partial y}$, where D_x and D_y are the small scale dispersion coefficients $(m^2/month)$ in x and y, respectively, defined as the product of a small (laboratory) scale dispersivity times the mean longitudinal pore velocity. Knowing the statistical properties of the regional groundwater flow velocity and using decomposition, (8.27) may be solved (Serrano, 1997(1); 1996(2)) to obtain the statistical properties of the concentration field. Each term in the decomposition series satisfies the same system differential equation forced by the previous term in the series.

Alternatively, the governing transport equation could be expressed in terms of an equivalent field dispersion coefficient:

$$\frac{\partial \bar{C}}{\partial t} - \bar{D}_x(t)\frac{\partial^2 \bar{C}}{\partial x^2} + \bar{v}_x \frac{\partial \bar{C}}{\partial x} - \bar{D}_y(t)\frac{\partial^2 \bar{C}}{\partial y^2} = 0, \tag{8.28}$$

where $\bar{D}_x(t)$ and $\bar{D}_y(t)$ are the longitudinal and transverse, time dependent, field dispersion coefficients, respectively. Knowing the functional form of the dispersion coefficients, the solution to this equation provides a practical tool to forecast groundwater pollution at the field scale (Serrano, 1996(2)). For simulation examples and comparison with exact solutions see Serrano and Adomian (1996).

8.7 The Form of the Field Dispersion Coefficient According to Decomposition

The longitudinal and transverse second-order moments of the solution to (8.28) constitute the longitudinal and transverse field dispersion coefficients (Serrano, 1997(1); 1996(2)):

$$\begin{aligned} \bar{D}_x(t) &= D_x + \sigma_{v_x}^2 t = D_x + \frac{\sigma_T^2 A^2}{n^2 h_0^2} t \\ \bar{D}_y(t) &= D_y + \sigma_{v_y}^2 t = D_y + \frac{2\rho\sigma_T^2 A^2}{n^2 h_0^2} t \end{aligned} \tag{8.29}$$

where $\sigma_{v_x}^2 = \overline{v_x^{\prime} v_x^{\prime}}$ is the variance of the longitudinal pore velocity; $\sigma_{v_y}^2 = \overline{v_y^{\prime} v_y^{\prime}}$ is the variance of the transverse pore velocity; σ_T^2 is the variance of the aquifer transmissivity; A is a parameter function of hydraulic gradient, aquifer dimensions and recharge; n is the aquifer mean porosity; h_0 is the aquifer mean hydraulic head; and ρ is the inverse of the transmissivity correlation length ("raw" , not log-transformed, transmissivity). (8.29) once again illustrates the principle that aquifer dispersion parameters are explicit functions of the aquifer hydrology, as well as aquifer heterogeneity in the transmissivity. For simple examples on the calculation of the field-scale dispersion coefficient in phreatic aquifers see Serrano (1997(2)).

Equations (8.29) describe the form of the field scale dispersion coefficients as functions of the aquifer hydrology, the statistical properties of the aquifer transmissivity, and time after the spill. According to this, the dispersion coefficients are not asymptotic functions of time, as the small perturbation theories propose. Instead, the dispersion coefficients keep evolving until the physical limits of the aquifer are found. The conceptual differences with the classical theories could be traced to the fundamental assumptions adopted by the different approaches, and the mathematical methods of solution used. The classical theories neglect the aquifer hydrology, use the logarithmic transformation of the hydraulic conductivity, and use the small perturbation approximation to the equations. The decomposition theory considers the aquifer hydrology as well as the statistical properties of the aquifer transmissivity, it uses the “raw” field transmissivity, and approaches to the true solution of the equation without restricting the size of the parameters.

8.8 Applications to Non-Point Sources and Spills Originated in the Unsaturated Zone

Most simulation models of groundwater pollution limit their attention to the solution of contaminant transport problems at either the unsaturated zone or the saturated zone. This is due in part to the conceptual difficulties in representing mass transfer at the interface between the saturated zone and the saturated zone, and the mathematics of subsequent propagation in the saturated zone subject to a non-point source at the interface. Yet an accidental chemical spill at the ground surface, which becomes a point source of contaminants in the unsaturated zone and eventually penetrate and propagate within the saturated zone, constitutes a frequent problem of practical importance.

In this section we attempt to extend the scale dependent fundamental solution of a point source problem in saturated media to the case of a distributed source coming from the unsaturated zone. First, a description of contaminant propagation in the unsaturated zone is needed in order to define the functional variability of the source concentration at the interface. For that purpose we focus our attention on the case of a shallow aquifer, that is one whose unsaturated zone depth is small as compared to the horizontal dimensions of the aquifer. In such case the large scale dependency of the dispersion parameters is controlled by the aquifer dimensions, rather than the unsaturated zone dimensions.

We assume that the source at the ground surface is instantaneous and punctual; the unsaturated soil is homogeneous and anisotropic in the dispersion coefficient; the contaminant loss through evapotranspiration is negligible; the concentration at the water table does not affect that of the unsaturated zone; the center of mass of contaminant plume moves as a result of mean percolation (recharge) rate from rainfall; and the dispersion in the horizontal direction is greater than that in the vertical direction.

The governing differential equation is (Serrano, 1992(3))

$$\frac{\partial C'}{\partial t} - D_x'\frac{\partial^2 C'}{\partial x^2} - D_x'\frac{\partial^2 C'}{\partial y^2} - D_z'\frac{\partial^2 C'}{\partial z^2} + \bar{v}_z\frac{\partial C'}{\partial z} = 0$$
$$-\infty<x<\infty;\ -\infty<y<\infty;\ -\infty<z<\infty;\ 0<t \qquad \textbf{(8.30)}$$

subject to

$$C'(\pm\infty,\pm\infty,\pm\infty,t)=0;\ C'(x,y,z,0)=C_i\delta(x)\delta(y)\delta(z), \qquad \textbf{(8.31)}$$

where C' is the solute concentration *(mg/Kg)*; *x, y* are the spatial horizontal coordinate axis (*m*), with *x* parallel to the regional saturated groundwater flow direction; *z* is the vertical spatial coordinate (*m*), positive downwards; *t* is the temporal coordinate (*months*); D_x' is the horizontal dispersion coefficient in ($m^2/month$); D_z' is the vertical dispersion coefficient in ($m^2/month$); $\bar{v}_z = \frac{I}{n}$ is the mean seepage velocity (*m/month*), where *I* is the mean monthly recharge rate from rainfall (*m/month*), and *n* is the soil porosity; and C_i is the initial solute concentration at the time of the spill *(mg/Kg)*.

The solution to (8.30) is (Serrano, 1995(2))

$$C'(x,y,z,t)=C_iX'(x,t)Y'(y,t)Z'(z,t), \qquad \textbf{(8.32)}$$

where

$$X'(x,t)=\frac{e^{-\frac{x^2}{4D_x't}}}{\sqrt{4\pi D_x't}},\ Y'(y,t)=\frac{e^{-\frac{y^2}{4D_x't}}}{\sqrt{4\pi D_x't}},\ Z'(z,t)=\frac{e^{-\frac{(z-\bar{v}_zt)^2}{4D_z't}}}{\sqrt{4\pi D_z't}} \qquad \textbf{(8.33)}$$

Equation (8.32), with the appropriate change in units, and with $z = w$, where *w* is the water table depth from the ground surface *(m)*, represents the space-time evolution of the contaminant concentration at the interface between the unsaturated and the saturated zone. If we interpret the transport problem of the saturated zone as one of a contaminant evolution due to a non-point source entering the water table, and using the results of the previous section, then the scale dependent differential equation governing solute dispersion in the saturated zone could be written as (Serrano, 1992(3))

$$\frac{\partial \bar{C}}{\partial t} - \bar{D}_x\frac{\partial^2 \bar{C}}{\partial x^2} + \bar{v}_x\frac{\partial \bar{C}}{\partial x} - \bar{D}_y\frac{\partial^2 \bar{C}}{\partial y^2} = g(x,y,t), \qquad \textbf{(8.34)}$$

$$-\infty<x<\infty,\ -\infty<y<\infty,\ 0<t,\ \bar{C}(\pm\infty,\pm\infty,t) = 0 = \bar{C}(x,y,0)$$

where $g(x,y,t)$ is the distributed source at the interface given from (8.32) as

$$g(x,y,t)=f'\ X'(x,t)Y'(y,t)Z'(w,t), \qquad \textbf{(8.35)}$$

and f' is a units conversion factor accounting for the change in concentration units (from *mg/Kg* in the unsaturated zone to *mg/L* in the saturated zone:

$$f' = \frac{\gamma_s}{1000n} \tag{8.36}$$

where γ_s is the soil dry bulk density. The solution to (8.34) may be written as (Serrano, 1995(2))

$$\bar{C}(x,\ y,\ t) = C_i\, f' \int_0^t \frac{e^{-\frac{(x-\bar{v}_x(t-t'))^2}{4[\bar{D}_x(t-t')(t-t')+D_x' t']}}}{\sqrt{4\pi[\bar{D}_x(t-t')(t-t')+D_x' t']}} \cdot \frac{e^{-\frac{y^2}{4[\bar{D}_y(t-t')(t-t')+D_y' t']}}}{\sqrt{4\pi[\bar{D}_y(t-t')(t-t')+D_y' t']}} \frac{e^{-\frac{(w-\bar{v}_z t')^2}{4D_z' t'}}}{\sqrt{4\pi D_z' t'}}\, dt' \tag{8.37}$$

An algorithm for a Gaussian quadrature may be easily constructed for the approximation of (8.37). KYSPILL (HydroScience Inc., 1998) is a practical computer software created for the purpose of predicting scale-dependent contaminant migration in random media. It incorporates several solutions of the VDE as described in this chapter with a friendly end-user interface, an automatic data diagnosis, a set of self-supported menus, graphics and windows, and a context-sensitive online help system. The model uses the solution of a differential equation that corresponds to the type of spill selected by the user (i.e., the initial condition): unsaturated zone or saturated zone spill, point or non point spill, and stationary or transient spill. In one screen, hydrologic and hydrogeologic data of the spill area is entered, including precipitation and air temperature that the model uses to estimate recharge, partition coefficients, and degradation rates for non-conservative contaminants. In the case of non-point sources, the user may enter an array of individual concentration sample values with their coordinates with respect to a selected origin. The model then interpolates to estimate an initial condition. Once the data is entered, the user has a variety of graphics to choose from a menu: surface or profile contours, time or space breakthrough curves, etc.

As an illustration, let us imagine that a small spill of a certain contaminant accidentally occurred at the ground surface and that we wish to forecast the contaminant concentration in the unsaturated zone and the saturated zone. The following parameters were measured: initial concentration, adjusted for the mass, is $500\ mg/kg$; small scale soil horizontal dispersivity 1.0 m; small scale soil vertical dispersivity 0.1 m; mean annual precipitation 1000 $mm/year$; mean annual air temperature 10^oC; water table depth $w = 1.0\ m$; soil dry bulk density $\gamma_s = 1500\ kg/m^3$; soil composition of 75% sand and 5% clay; soil porosity $n = 0.1$; aquifer mean hydraulic gradient 0.001 m/m; small scale aquifer longitudinal dispersivity 1.0 m; small scale aquifer transverse dispersivity 0.1 m; retardation factor 1.0; degradation constant $0.0\ month^{-1}$; aquifer mean hydraulic conductivity $\bar{K} = 100.0\ m/month$; conductivity standard deviation $\sigma_K = 30.0\ m/month$; and "raw" conductivity correlation length $\frac{1}{\rho} = 100.0\ m$.

Figures 8.3 and 8.4 show the unsaturated zone concentration contours 12 and 24 months after the spill, respectively. Figures 8.5 and 8.6 show the saturated zone plan view concentration contours 120 and 144 months after the spill. Note that due to the slow penetration of the source from the unsaturated zone, the saturated zone plume is not symmetrical with respect to the peak in the longitudinal direction. It is also interesting to observe that the maximum concentration remains somewhat close to origin, and that only after prolonged time, when most of the contaminant from the unsaturated zone has entered the saturated zone, the plume will tend to become symmetric. Finally if one attempts to model this problem with constant, rather than scale dependent, dispersion parameters, the calculated concentration values become unrealistic.

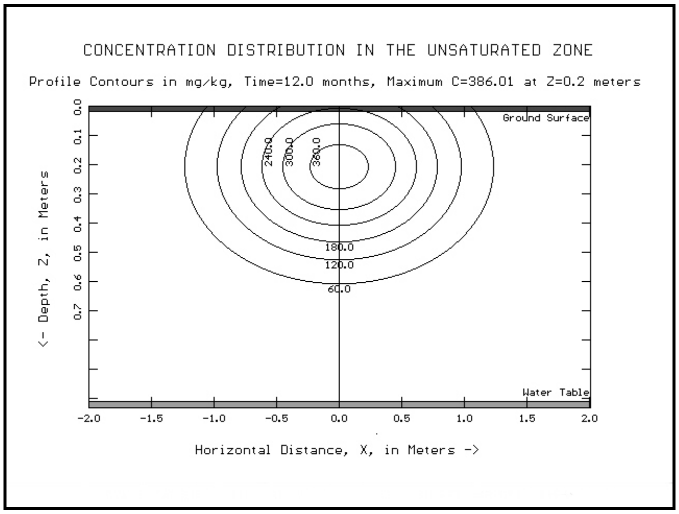

Figure 8.3: Concentration Distribution in the Unsaturated Zone

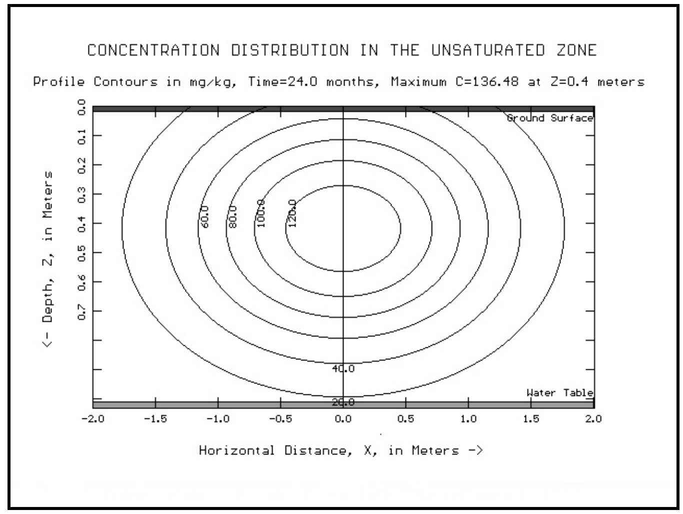

Figure 8.4: Concentration Distribution in the Unsaturated Zone

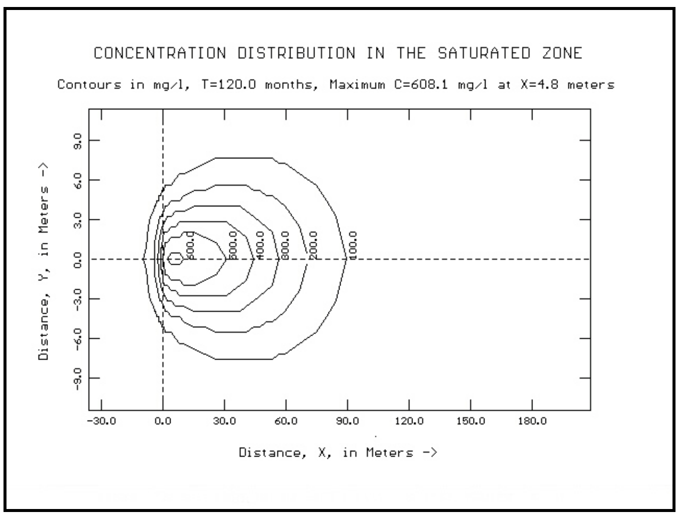

Figure 8.5: Concentration Distribution in the Saturated Zone

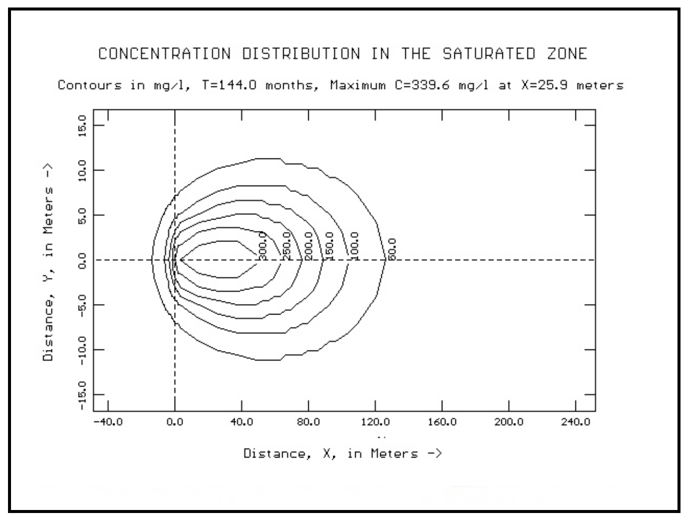

Figure 8.6: Concentration Distribution in the Saturated Zone

8.9. Conclusions and Recommendations

Semigroup and decomposition methods for the analysis and prediction of stochastic subsurface contamination problems have been presented. Emphasis has been given to the illustration of the methods and to the practical simulation of contamination problems in hydrology, such as the forecasting of soil and groundwater pollution, the simulation of scale-dependent phenomena, and the analysis of non-point sources. Decomposition methods offer the hydrologist a systematic and flexible tool to analyze and predict subsurface contaminant propagation.

Still remaining is an investigation on the use of the decomposition method in conjunction with numerical techniques to smooth uncertain initial conditions. Since most data bases are obtained from limited punctual information derived from isolated monitoring wells, the sensitivity of the decomposition solution to errors in the initial condition is a problem of practical significance. Another area to study is the development of sequential solutions for prolonged time simulations: as the variances in the random quantities increase, the maximum simulation time required for convergence decreases, and thus a combination of more terms in the approximant in concert with a cascade of successive solutions could be attempted. The consideration of transient boundary conditions and seasonal variability in precipitation is currently an active field of research.

8.10. References

Abbaoui, K., and Cherruault, Y., 1994. Convergence of Adomian's Method Applied to Differential Equations. Comp. Math. Applic., 28(5):103-109.

Adomian, G., 1994. Solving Frontier Problems of Physics-The Decomposition Method. Kluwer Acad. Pub.

Adomian, G., Non-Linear Stochastic Operator Equations. Academic Press, 1986

Adomian, G., 1991. A Review of the Decomposition Method and Some Recent Results for Nonlinear Equations. Computers Math. Applic., 21(5):101-127.

Adomian, G., 1986. Non-Linear Stochastic Operator Equations. Academic Press.

Adomian, G., 1983. Stochastic Systems. Academic Press, San Diego, California.

Adomian, G., and Serrano, S.E., 1998. Stochastic Contaminant Transport Equation in Porous Media. Appl. Math. Lett., 11(1):53-55.

Cherruault, Y., 1989. Convergence of Adomian's Method. Kybernetes, 18(2):31-38.

Cherruault, Y.,Saccomardi, G., and Some, B., 1992. New Results for Convergence of Adomian's Method Applied to Integral Equations. Math. Comput. Modelling, 16(2):85-93.

Gabet, L., 1992. Equisse d'une Théorie Décompositionnelle et Application aux Equations aux Dérivées Partialles. Dissertation, Ecole Centrale de Paris, France.

Gabet, L., 1994. The Decomposition Method and Distributions. Computers Math. Applic., 27(3):41-49.

Gabet, L., 1993. The Decomposition Method and Linear Partial Differential Equations. Math. Comput. Modelling, 17(6):11-22.

HydroScience Inc., 1998. KYSPILL, A Groundwater Pollution Forecasting System. HydroScience Inc., Lexington, Kentucky

Serrano, S.E., 1998. Analytical Decomposition of the Nonlinear Unsaturated Flow Equation. Water Resour. Res. 34(3):397-407.

Serrano, S.E., 1997(1). Non-Fickian Transport in Heterogeneous Saturated Porous Media. ASCE J. Engr. Mech., 123(1):70-76.

Serrano, S.E., 1997(2). Hydrology for Engineers, Geologists, and Environmental Professionals. An Integrated Treatment of Surface, Subsurface, and Contaminant Hydrology. HydroScience Inc., Lexington, Kentucky.

Serrano, S.E., 1996(1). Towards a Nonperturbation Transport Theory in Heterogeneous Aquifers. Mathl. Geology, 28(6):701-721.

Serrano, S.E., 1996(2). Hydrologic Theory of Dispersion in Heterogeneous Aquifers. ASCE J. Hydrol. Engr., 1(4):144-151.

Serrano, S.E., 1996(3). Comment on "Operator and Integro-Differential Representations of Conditional and Unconditional Stochastic Subsurface Flow." Stochastic Hydrol. Hydraul., 10:151-161.

Serrano, S.E., 1995(1). Analytical Solutions of the Non-Linear Groundwater Flow Equation in Unconfined Aquifers and the Effect of Heterogeneity. Water Resour. Res., 31(11):2733-2742.

Serrano, S.E., 1995(2). Forecasting Scale-Dependent Dispersion from Spills in Heterogeneous Aquifers. J. Hydrol., 169:151-169.

Serrano, S.E., 1992(1). The Form of the Dispersion Equation Under Recharge, and Variable Velocity and its Analytical Solution. Water Resour. Res., 28(7):1801-1808.

Serrano, S.E., 1992(2). Semianalytical Methods in Stochastic Groundwater Transport. Appl. Math. Modelling, 16:181-191.

Serrano, S.E., 1992(3). Migration of Chloroform in Aquifers. ASCE J. Envr. Engr., 118(2):167-182.

Serrano, S.E., 1990(1). Stochastic Differential Equations Models of Erratic Infiltration. Water Resour. Res., 26(4):703-711.

Serrano, S.E., 1990(2). Modeling Infiltration in Hysteretic Soils. Adv. Water Resour., 13(1):12-23.

Serrano, S.E., 1988(1). General solution to Random Advective-Dispersive Transport Equation in Porous Media, 1, Stochasticity in the Sources and in the Boundaries. Stochastic Hydrol. Hydraul., 2(2):79-98.

Serrano, S.E., 1988(2). General solution to Random Advective-Dispersive Transport Equation in Porous Media, 2, Stochasticity in the Parameters. Stochastic Hydrol. Hydraul., 2(2):99-112.

Serrano, S.E., and Adomian, G., 1996. New Contributions to the Solution of Transport Equations in Porous Media. Mathl. Comput. Modelling, 24(4):15-25.

Serrano, S.E., and Unny, T.E., 1987(1). Semigroup Solutions to Stochastic Unsteady Groundwater Flow Subject to Random Parameters. Stochastic Hydrol. Hydraul., 1(4):281-296.

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

Serrano, S.E., Unny, T.E., and Lennox, W.C., 1985(1). Analysis of Stochastic Groundwater Flow Problems, 1, 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, 2, Stochastic Partial Differential Equations in Groundwater Flow, A Functional-Analytic Approach., J. Hydrol., 82(3-4):265-284.

Acknowledgements

The support and encouragement of the National Science Foundation, Grant Number BES 9710587 is greatly appreciated.