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Stochastic Hydrology and Hydraulics

General solution to random advective-dispersive equation in porous media

Part 1: Stochasticity in the sources and in the boundaries

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Abstract: This series of articles present general applications of functional-analytic theory to the solution of the partial differential equation describing solid transport in aquifers, when either the evolution of the system, the sources, the parameters and/or the boundary conditions are prescribed as stochastic processes in time or in space. This procedure does not require the restricting assumptions placed upon the current particular solutions on which today's stochastic transport theory is based, such as "small randomness" assumptions (perturbation techniques), Montecarlo simulations, restriction to small spatial stochasticity in the hydraulic conductivity, use of spectral analysis techniques, restriction to asymptotic steady state conditions, and restriction to variance of the concentration as the only model output among others. Functional analysis provides a rigorous tool in which the concentration stochastic properties can be predicted in a natural way based upon the known stochastic properties of the sources, the parameters and/or the boundary conditions. Thus the theory satisfies a more general modeling need by providing, if desired, a systematic global 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. Part I of this series of articles presents the main relevant results of functional-analytic theory and individual cases of applications to the solution of distributed sources problems, with time as well as spatial stochasticity, and the solution subject to stochastic boundary conditions. It was found that the stochastically-forced equation may be a promising model for a variety of random source problems. When the differential equation is perturbed by a time and space stochastic process, the output is also a time and space stochastic process, in contrast with most of the existing solutions which ignore the temporal component. Stochastic boundary conditions seems to quickly dissipate as time increases.

Key words: Stochastic groundwater transport, semigroups, stochastic partial differential equations.

1 Introduction

A very serious problem in water resources today is the difficulty to predict the spatial distribution and time evolution of a contaminant plume in a system of aquifers responding to a particular source. The difficulty comes from the inaccuracy or insufficiency of hydrogeological and hydrochemical information, and from the several uncertainties in the physical and chemical processes occurring in the phenomenon of contaminant transport. Studies have shown that calibrated field dispersion coefficients are orders of magnitude larger than those found in small-scale laboratory tests (Fried 1975; Anderson 1979; Smith and Schwartz 1980; Matheron and De Marsily 1980; Dagan and Bresler 1979). Field observations have shown that the dispersion coefficient increases with displacement distance at a given site (Sudiky and Cherry 1979; Dieulin et al. 1980). Summaries of field observations demonstrate the wide range of dispersivities encountered (Lallemand-Barres and Peaudecerf 1978; Anderson 1979). Stochastic fluctuations in flow velocity caused by media heterogeneities and failure of Fick's diffusion law to describe hydrodynamic dispersion at field scale are reasons cited for the inappropriateness of the advective-dispersive equation to describe mass transport in porous media at field scale. Thus except for very special cases, the true transport process does not satisfy the advective-dispersive equation at the field scale (Cushman 1987a).

Efforts to understand this scale dependence of the dispersion process have focused on the effects of the heterogeneity of the hydraulic conductivity in natural formations. Several theoretical studies have analyzed the effects of such heterogeneity using various stochastic descriptions of spatial variability (Warren and Skiba 1964; Heller 1972; Schwartz 1977; Gelhar et al. 1979; Smith and Schwartz 1980; Matheron and Demarsily 1980; Simmons 1982; Tang et al. 1982; Dagan 1982; Gelhar and Axness 1983; Dagan 1984; Winter et al. 1984). All of these works have provided considerable insight on the phenomenon of mass transport in aquifers. However several inconsistencies and deficiencies have been noted.

As noted in the recent survey article by Sposito and Jury (1986) on the problems and inconsistencies of the approaches to solve the contaminant transport equation, the existing solutions of the stochastic advective- dispersive equation have not yet proved useful in shedding fundamental light on the scale effect of the dispersion coefficient nor do they provide information on the transient behaviour of solute concentration with a clear predictive value. The main difficulties with the existing solutions may be summarized as follows:

(i) A significant limitation of the existing solutions is the assumption of small randomness required by the perturbation expansion solutions (Gelhar and Axness 1983; Dagan 1984). Adomian (1971) has demonstrated that the perturbation solution in a stochastic differential equation is accurate only if the stochastic processes have small variance. If the stochastic processes involved in the differential equation are insignificant in importance, then a deterministic model could be a sufficient as an appropriate forecasting tool. For an in depth analysis of the Gelhar and Axness (1983) approach the reader is referred to Cushman (1987a).

(ii) Most of the existing solutions have assumed the hydraulic conductivity as the only source of uncertainty. In many cases, however, the large-scale hydraulic conductivity can safely be described by well defined deterministic functions and other sources of uncertainty may be more important. The effect of stochasticity in the time or spatial distribution of the sources, stochasticity in the boundary conditions, or the stochasticity in the environmental evolution of the system has largely been ignored.

(iii) Some of these solutions are strictly applicable only to steady state asymptotic conditions of the concentration field (i.e., Gelhar and Axness 1983).

(iv) Cushman (1987a) has shown that stochasticity is a function of the scale of observation, that is, it is a function of the scale of the instrumentation used in the experiment. By decreasing the instrumentation scale we may observe randomness at a degree not previously noticed, but at the same time we may improve resolution (Cushman 1987a). In many circumstances regional groundwater pollution problems may be approached with corresponding large scale measurement strategies which minimize the stochasticity. However some of the field validations to the perturbation solution of the advective-dispersive equation generate the stochasticity in the hydraulic conductivity by small scale measurement approaches, and their unavoidable errors, to large scale contaminant migration Sudiky (1986).

(v) Some of the approaches use Montecarlo simulations. This procedure may give preliminary information on the first two moments of the concentration. However the procedure is expensive.

(vi) Some of the existing solutions only provide information about the concentration variance. Authors do not give specifics on the procedure to obtain sample functions, different correlation functions and higher order moments.

(vii) Some of the existing solutions assume that the hydraulic conductivity tensor is ergodic. It is clear that the ergodicity in the conductivity field does not imply ergodicity in the concentration field. This raises an important modeling difficulty, which is the inability to validate the stochastic solutions of the advective-dispersive equation against one sample function of the concentration distribution measured in the field.

From above it is clear that the existing solutions of the advective-dispersive equation in porous media are subject to very special circumstances. There is a need for a general theory capable of solving this equation and predicting the time and space evolution of the contaminant migration in aquifers subject to any form or any size of stochasticity. This theory should be rigorous, general and capable of describing the stochastic properties of the concentration given the stochastic properties of the dominant processes. This would provide the hydrologist with a more realistic modeling tool for forecasting purposes. It is the main objective of this series of articles to introduce this solution procedure in the field of groundwater pollution and to present some preliminary examples of possible applications.

In what follows I assume that it is possible to model some field cases of regional groundwater pollution with the advective-dispersive equation subject to stochasticity in the sources, the parameters or the boundaries. I will not discuss the physical validity of this equation. Methodologies which are in use to develop groundwater transport equations are treated in detail elsewhere (see Cushman 1987a, for a review of these methods).

The mathematics of a complex dynamic process, such as the one involving solute advection and dispersion in porous media, can be best represented within the general framework of functional-analytic theory. In the field of groundwater transport, functional analysis has been used by Cushman (i.e., 1986, 1985, 1983a, 1982), and Tang and Pinder (1979). Serrano, et al. (1985a, b, c) used functional analysis to solve stochastic groundwater flow equations. They demonstrated that the solution of the stochastic groundwater flow equation may be only obtained after fundamental questions concerning the existence and uniqueness of a solution have been resolved. This is done by posing the problem in an abstract functional- analytic context which will provide the desired rigor, notational economy and generality. By following this procedure, some of the limitations presented by classical mathematics when attempting to solve a stochastic partial differential equation are avoided. Furthermore, by using the topological properties of the identified solution space, a series of approximations towards an explicit solution can be obtained. This is the ultimate aim from the purely applied point of view, that is the hydrologic modeling problem.

Therefore, knowing the importance of functional analysis and following the current trend of mathematical analysis and modeling in most scientific disciplines, I use the language of functional analysis in Section 2. Since this article is mainly concerned with the geohydrological applications, I will concentrate only on the main results of interest and I will not repeat here the fundamental concepts behind this tool or the proofs of the theorems. However, I do advice the open-minded and interested hydrologist to read the references I mention throughout the article, with the hope that this tool of the future will help in the solution of increasingly complex problems.

Section 3 presents some examples of the application of the theory to the solution of distributed source problems, both when spatial or time stochasticity are specified, and the solution for the case of random boundary conditions. I consider these types of models to have enormous potential for applications to cases of uncertainty in reactive non-conservative pollutants. I chose the classical one-dimensional advective-dispersive equation in the examples for simplicity in the presentation. However, the reader should bear in mind that the development in Section 2 applies to n- dimensional domains. It will be clear in Part II that the extension of some of the examples in Section 3, Part I, to three-dimensional cases is straight forward. I use a well-known stochastic process in the examples, namely the white Gaussian process. 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 that this is not a limitation of the theory and that the following development bases the solution of the stochastic partial differential equation on the known properties of the forcing processes. Any known stochastic process in $L_2(\Omega)$ could be used. Since the present research did not involve field measurements, I chose a process with known properties for the illustrations. At some point in the research, an attempt was made to use field data. However I was faced with the insurmountable fact that the existing long-term groundwater quality data banks have been taken under a deterministic conception of the mass transport process, making difficult their use in the validation of a stochastic model. Future measurement efforts will have to be reoriented towards a more realistic stochastic conception. In particular, the stochastic properties of field concentration distributions should be defined for different instrumentation scales (Cushman 1987a). At each scale level, several simultaneous long-term sample functions of the concentration should be measured in order to define the correlation structure of the concentration process and to observe for possible ergodicity. The implementation of these measurement strategies would be more expensive than the existing ones, but important insight on the groundwater pollution phenomenon would be gained.

2 The mathematical theory

The general three-dimensional stochastic advective-diffusive equation in porous media may be treated as a stochastic evolution equation of the form

$$\frac{\partial u}{\partial t}(x, t, \omega) + A(x, t, \omega)u = g(x, t, \omega), \qquad (x, t, \omega) \in G \times [0, T] \times \Omega \tag{1}$$

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

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

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; $G \subset I\!R^3$ 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 the space $H^m(G)$ and it is given by

$$Au = \sum_{|k|,|l| \leq m} (-1)^{|k|} D^k(p_{kl}(x, t, \omega)D^l u), \tag{2}$$

where D is weak 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

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

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 $\|\cdot\|_V$; V' is the dual of V; $g \varepsilon L_2(0, T; V')$; and $u_0 \varepsilon H \times \Omega$ 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., Serrano, et al. 1985a, b; 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. (1) have been extensively treated in Sawaragi et al. 1978; Bensoussan 1977; Chow 1979; and Curtain and Falb 1971 among others.

In a complex system like the one described by Eq. (1), the randomness may enter 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. To this author's knowledge, only a few limited problems in the category (iv) have been treated in the hydrologic literature. Basically the efforts have been focused on solving the advective-dispersive equation for the specific case in which the parameters are defined as spatial stochastic quantities. The effect of stochasticity in the sources and/or the boundaries has not received attention. In Part II of this series of articles (this issue), I will describe a general methodology for treating the case (iv) of random parameters which is not subject to the limitations of small randomness appearing in the previous literature on the subject.

Closely related work involving cases (i) through (iv) in groundwater flow equations has been recently presented in the literature. The groundwater flow equation subject to random initial conditions (case (i)) has been solved by Serrano et al. 1985b. The problem of random forcing terms (case (iii)) has been solved by Serrano, Unny and Lennox 1985b; Serrano, Unny and Lennox 1986; and Serrano and Unny 1987c. Practical field applications of the above cases appear in Serrano and Unny 1986; and Serrano and Unny 1987b. In these two articles the authors developed two models describing the stochastic nature of the groundwater potential in the Twin Lake aquifer at the Chalk River Nuclear Laboratories, Ontario, Canada: The first one was the one-dimensional stochastic Boussinesq equation, whose solution was obtained by applying the concepts of semigroups and expressing the Wiener process as an infinite basis in a Hilbert space composed of independent unidimensional Wiener processes with incremental variance parameters. A process of this style was found to successfully explain the stochastic nature of field measurements of groundwater level. The second model was the two-dimensional Laplace's equation with stochastic free-surface boundary condition. Moments equations for the potential at any point inside the aquifer were obtained by applying a representation of the Itő's Lemma in a Hilbert space. The solution of the moments equations was obtained by applying the boundary integral equation method.

A general solution of groundwater flow equations subject to spatial or time stochasticity in the parameters (case (iv)) appears in Serrano and Unny 1987a. The success of the above results has motivated the extension of the techniques to the solution of the stochastic advective-dispersive equation in porous media.

One important difference between groundwater flow equations and contaminant transport equations is that whereas in groundwater flow equations the spectrum is discrete and the eigen functions are orthogonal, in mass transport equations the spectrum is continuous. This stems from the physical nature of the groundwater flow process, which exhibits a marked dependency on the boundary conditions, whereas the hydrodynamic dispersion process does not present the same degree of dependency from relatively distant non-source boundaries. This allows in many cases the mathematical treatment of the mass transport process in infinite and semi-infinite domains.

As stated in Section 1, the objective of the present research is to investigate the different sources of stochasticity affecting the process of mass transport, their individual effects on the behaviour of the output concentration of the system, and the development of a systematic methodology to solve the mass transport equation subject to either form of stochasticity. In part I of this series of articles, cases (ii) and (iii) will be solved. In part II, case (iv) will be solved. The problem of random initial conditions, case (i), will not be treated since it does not offer much potential for modeling applications. Most applications of the mass transport equation involve the case of a contaminated regional aquifer subject to a single realization of the initial condition and the stochasticity is concentrated in the boundaries, the parameters or the time evolution of the system.

Thus for cases (ii) and (iii), the operator A is deterministic and in some practical applications it is a time-independent operator. then J_t is said to be a strongly continuous semigroup. Moreover, if we transform the functional spaces in Eq. (1) into an equivalent one in which the system has homogeneous boundary conditions, we will have

$$\frac{\partial v}{\partial t}(x, t, \omega) + A(x)v = h(x, t, \omega), \quad v\,|_{\partial G} = 0, \quad v(x, 0) = v_0(x), \tag{3}$$

where $v \;\varepsilon\; L^2(0, T; V)$ 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; and $v_0(x)$ includes $u_0(x)$. Without loss of generality we assume hereafter that $h(x, t, \omega)$ is a zero mean stochastic process.

The general solution of Eq. (3) is

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

where $J_t \;\varepsilon\; l(H, H)$ is the semigroup associated with A (Curtain and Pritchard 1978; Ladas and Lakshmikantham 1972; Butzer and Berens 1967). If a transformation of spaces is not done, it is clear that the semigroup operator must satisfy the prescribed boundary conditions. In General, if the operator A is time dependent and will not generate a semigroup. For the practical cases when A is time independent 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) $\| J_t v - v \|_H \to 0$ as $t \to 0$ for all $v \;\varepsilon\; H$, where $\| \cdot \|$ 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 represent more than what 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. The first two moments give considerable information about the joint probability density function of v. Thus

$$E\{v(x,t)\} = J_t v_0 + \int_0^t J_{t-s} E\{h(x,s,\omega)\} ds = J_t v_0 \tag{5}$$

$$\begin{aligned} E\{v(t_1)v(t_2)\} &= E\{ [J_{t_1} v_0 + \int_0^{t_1} J_{t_1-s} h(s) ds] \cdot [J_{t_2} v_0 + \int_0^{t_2} J_{t_2-\xi}\, h(\xi) d\xi] \}, \\ &= J_{t_1+t_2} v_0 + \int_0^{t_1} \int_0^{t_2} J_{t_1+t_2-s-\xi} E\{h(s)h(\xi)\} ds d\xi, \end{aligned} \tag{6}$$

where $E\{\cdot\}$ denotes the expectation operator and ω has been omitted for convenience. Note that the calculation of Eq. (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.

In the following sections I shall illustrate the application of the above theory to the solution of the advective-dispersive equation in porous media subject to either time stochasticity as a source term, spatial stochasticity as a source term, and time stochasticity in the boundary conditions.

3 Solution for the stochastically-forced equation

3.1 General

To begin the illustration on the applications of the theory presented in Section 2, I have chosen the differential equation of longitudinal dispersion in a semi-infinite aquifer subject to a plane source at the origin. Assuming that the porous media is homogeneous and isotropic, that no mass transfer occurs between the solid and liquid phases, 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):

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} = g(x,t,\omega), \tag{7}$$

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

where $C(x,t,\omega)$ is the stochastic process representing the contaminant concentration in the fluid $[M/L^3]$; D is the aquifer dispersion coefficient $[L^2/T]$; u is the average pore velocity, that is the flux velocity divided by the average porosity of the media $[L/T]$; x is the coordinate parallel to the flow; t is the time coordinate; $k(t,\omega)$ is the time-dependent concentration process at the origin $[M/L^3]$; $f(x)$ is the initial concentration distribution across the aquifer $[M/L^3]$; and $g(x,t,\omega)$ represents a stochastic source or sink disturbing the system.

We assume that it is possible to separate the solution to Eq. (7) into a deterministic function and a random function satisfying Eq. (7) and its boundary conditions. If the decomposition exists, we may express the concentration C as the superposition of two problems:

$$C(x, t, \omega) = C_1(x, t, \omega) + C_2(x, t), \tag{8}$$

where C_1 is the solution to the problem

$$\frac{\partial C_1}{\partial t} - D\frac{\partial^2 C_1}{\partial x^2} + u\frac{\partial C_1}{\partial x} = g(x,t,\omega); \quad C_1(0,t)=0;\ C_1(\infty,t)=0;\ C_1(x,0)=f(x), \tag{9}$$

and C_2 is the solution to the problem

$$\frac{\partial C_2}{\partial t} - D\frac{\partial^2 C_2}{\partial x^2} + u\frac{\partial C_2}{\partial x} = 0; \quad C_2(0,t)=k(t,\omega);\ C_2(\infty,t)=0;\ C_2(x,0)=0. \tag{10}$$

Let us study the problem described by Eq. (9). The operator A, such that

$$AC_1 = (-D\frac{\partial^2}{\partial x^2} + u\frac{\partial}{\partial x})C_1$$

generates a strongly continuous semigroup J_t given by (see Appendix A)

$$J_t f(x) = \frac{1}{(4\pi Dt)^{1/2}} \int_0^\infty \{\exp[-\frac{(x-ut-s)^2}{4Dt}] - \exp[-\frac{(x-ut+s)^2}{4Dt}]\} f(s)ds. \tag{11}$$

Thus, according to Eq. (4), the solution to Eq. (9) is simply

$$C_1(x, t, \omega) = J_t f(x) + \int_0^t J_{t-\tau} g(x, \tau)ds. \tag{12}$$

From this expression we can generate sample functions of the process C_1 if sample functions of the process g 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. (5) and (6), as we shall show in the following examples. The remarkable feature here is that after a semigroup operator has been explicitly defined and its properties studied (see Appendix A), a variety of more complex deterministic and stochastic problems may be solved.

The solution to the deterministic problem described by Eq. (10) may be approached in two ways: As stated in Section 2, We may transform the problem described by Eq. (10) into an equivalent one with homogeneous boundary conditions by defining C_1 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. Thus the solution to Eq. (10) is (Ogata and Banks 1961)

$$C_2(x, t) = \frac{x}{(4\pi D)^{1/2}} \int_0^t \exp[-\frac{x - u(t-\tau))^2}{4D(t-\tau)}] \frac{k(\tau, \omega)}{(t-\tau)^{3/2}} d\tau. \tag{13}$$

We will use this equation to study the case of stochastic boundary conditions. For the particular case in which $k(t, \omega) = C_0 =$ a constant, Eq. (13) becomes (Li 1972; Willis and Yeh 1987; Marinño 1974)

$$C_2(x, t) = \Phi(x, t) = \frac{C_0}{2}\{erfc[\frac{x-ut}{(4Dt)^{1/2}}] + \exp(\frac{ux}{D})erfc[\frac{x+ut}{(4Dt)^{1/2}}]\}, \tag{14}$$

where $erfc(\cdot)$ denotes the "error function complement". In the following sections we will develop the explicit solutions of equations (7), (9) and (10) for cases when the statistical properties of the input stochastic processes are known. Equations for the first two moments will also be developed.

3.2 Case 1: A distributed source problem. Time stochasticity

The stochastically-forced equation may be used to model the effect of unknown environmental quantities affecting the concentration distribution, errors generated in the development of the model, errors in the estimation of parameter values, and/or uncertain chemical reactions between the porous matrix and the fluid. In this section we study the kind of problems when a time-stochastic distributed source dominates the uncertainty of the system.

Let us consider the case in which the random function g in Eq. (7) is a white Gaussian noise process in time and smooth in space, the boundary condition k is a constant source function in time C_0, and the initial condition $f(x)$ is zero. The use of a white Gaussian noise in this example is not a limitation of the theory, but a convenient tool for illustrative purposes. It is clear, however, that the statistical properties of the forcing process must be known and that the measurement strategy should be concentrated on the evaluation of these quantities. Although a white Gaussian process is a common residual of a good deterministic model, I am not claiming that this particular random process actually disturbs the advective-dispersion phenomenon in an aquifer. Future field research should be focused on the identification of the stochastic processes affecting the dispersion phenomenon. The existing groundwater pollution data bases have been constructed under a deterministic conception of the physics of dispersion and in no way may help in the assessment of the validity of specific random processes.

With these considerations Eq. (7) becomes

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} = \frac{d\beta(t)}{dt}; \quad C(0,t)=C_0,\ C(\infty,t)=0,\ C(x,0)=0, \tag{15}$$

where $d\beta(t)/dt = w$ is a white Gaussian process with the properties

$$E\{w(t)\} = 0, \qquad E\{w(t_1)w(t_2)\} = q\,\delta(t_2 - t_1), \tag{16}$$

where q is the variance parameter $[M/(L^3 \cdot T)]$.

Simplifying the inner integral in Eq. (12) (see Appendix A), and using Eq. (8) we find the general solution of Eq. (15):

$$C(x, t, \omega) = \Phi(x, t) + \int_0^t erf[\frac{x-u(t-\tau)}{(4\pi D(t-\tau))^{1/2}}]w(\tau, \omega)d\tau. \tag{17}$$

By generating sample functions of w we may obtain sample functions of C. Now taking expectations on both sides of Eq. (17) and using Eq. (16) we find the mean concentration to be

$$E\{C(x, t)\} = \Phi(x, t). \tag{18}$$

Now following Eqs. (6), (11) and (16), the second moment of C is

$$E\{C(x,t_1)C(x,t_2)\} = \Phi(x,t_1)\Phi(x,t_2)$$

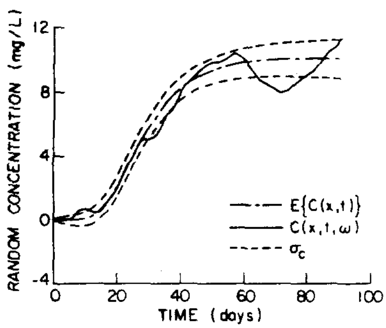

Figure 1

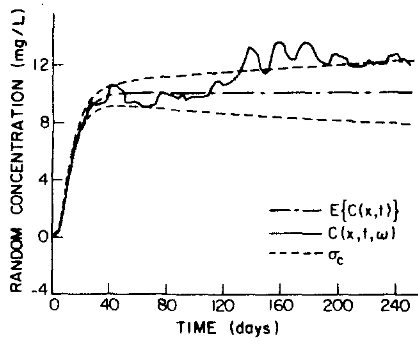

Figure 2

Figure 1. Stochastic concentration with time at $X = 6.0$ m (Case 1)

Figure 2. Stochastic concentration with time at $X = 3.0$ m (Case 1)

$$+ q\int_0^{t_1}\int_0^{t_2} erf\left[\frac{x-u(t_1-\tau)}{(4D(t_1-\tau))^{1/2}}\right] erf\left[\frac{x-u(t_2-\xi)}{(4D(t_2-\xi))^{1/2}}\right]\delta(t_1-t_2)d\xi d\tau. \quad (19)$$

If we let $t_1 = t_2 = t$ the variance of C becomes:

$$\sigma_c^2 = q\int_0^t erf^2\left[\frac{x-u(t-\tau)}{(4D(t-\tau))^{1/2}}\right]d\tau. \quad (20)$$

As an example of the application of the above solution, Eqs. (17), (18) and (20) where 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 evaluated using the trapezoidal rule for this particular case. Figure 1 is a digital plotter output of the program for a point in space $x = 6.0$ m from the origin. 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. Figure 2 shows another simulation when $x = 3.0$ m and the calculations are prolonged up to 240 days. 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. (12).

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 (Sposito and Jury 1986) as one of the difficulties in using the existing models. Thus we may conclude that a model such as the one presented in this section may partially explain the stochastic nature of the concentration in an aquifer. A similar phenomenon is observed when one has evolving heterogeneities and no stochastic forcing function. Potential applications of the stochastically-forced equation include the situation of groundwater pollution monitoring at a particular well. The information collected may help in the identification and parameter estimation of the stochastic process involved, and the model could be used to forecast the statistical properties of the concentration at another well down the field where contamination is feared. The applicability of this Case 1 is more understood when one realizes that groundwater pollution data bases are collected at individual wells in the aquifer. Another most promising application is the possibility of handling uncertain chemical reaction terms in the differential equation by using a solution of the randomly-forced equation.

Extensions of Case 1 type of models to two-dimensional and three-dimensional domains are straight forward. In Part II of this series of articles a generalization to three-dimensional domains is presented.

3.3 Case 2: A distributed source problem. Time and space stochasticity

A very interesting case arises when the function g in Eq. (7) is a stochastic process in space and smooth in time. An example of this occurs when a source is randomly distributed in time and space, or a reaction term poses a random in time and space behaviour. Let us explore the situation in which $g(x, \omega)$ is a white Gaussian process in space. Eq. (7) becomes

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} = \frac{d\beta(x)}{dx}; \quad C(0,t)=C_0,\ C(\infty,t)=0,\ C(x,0)=0. \tag{21}$$

Now we split our problem as before and let C be described by Eq. (8) as the summation of C_1 and C_2, where C_1 satisfies

$$\frac{\partial C_1}{\partial t} - D\frac{\partial^2 C_1}{\partial x^2} + u\frac{\partial C_1}{\partial x} = w(s,\omega); \quad C_1(0,t)=0,\ C_1(\infty,t)=0,\ C_1(x,0)=0, \tag{22}$$

and C_2 satisfies Eq. (10) with $C_2(0, t) = C_0$. According to Eq. (12), the solution of Eq. (22) is

$$C_1(x,t,\omega) = \int_0^t \frac{1}{(4\pi D(t-\tau))^{1/2}} \int_0^\infty \{ \exp[-\frac{(x-u(t-\tau)-s)^2}{4D(t-\tau)}] - \exp[-\frac{(x-u(t-\tau)+s)^2}{4D(t-\tau)}]\} w(s,\omega) ds d\tau. \tag{23}$$

The solution for C_2 is given by Eq. (14). Eq. (23) may be simplified for the calculation of sample functions after conceiving 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. (23) may be written as

$$C_1(x, t, \omega) = \sum_{k=0}^{k=t} \sum_{i=1}^{N} w_i M_i(t - k), \tag{24}$$

where N is a suitable truncation index, The function M_1 for example is given by

$$M_1(t-k) = \frac{1}{(\pi b)^{1/2}} \int_0^1 \{\exp[-\frac{(a - s)^2}{b}] - \exp[-\frac{(a + s)^2}{b}]\} ds, \tag{25}$$

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

$$M_1(t-k) = \frac{1}{\pi^{1/2}} \{ \int_{-a/b^{1/2}}^{(1-a)/b^{1/2}} e^{-\xi^2} d\xi - \int_{a/b^{1/2}}^{(1+a)/b^{1/2}} e^{-\xi^2} d\xi \}.$$

$$= \frac{1}{2} \{ erfc(-\frac{a}{b^{1/2}}) - erfc(\frac{1-a}{b^{1/2}}) - erfc(\frac{a}{b^{1/2}}) + erfc(\frac{1+a}{b^{1/2}}) \}. \tag{26}$$

The general from of the function M_i for any i is

$$M_i(t-k) = \frac{1}{2} \{ erfc(\frac{i-1-a}{b^{1/2}}) - erfc(\frac{i-a}{b^{1/2}}) - erfc(\frac{i-1+a}{b^{1/2}}) + erfc(\frac{i+a}{b^{1/2}}) \}. \tag{27}$$

Now the mean concentration is given by Eq. (18), and the concentration variance for the case when $x_1 = x_2 = x$ can be deduced from Eqs. (6), (11) and (16) to be

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

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

$$\cdot \{\exp[-\frac{x - u(t-\rho) - \xi)^2}{4D(t-\rho)}] - \exp[-\frac{x - u(t-\rho) + \xi)^2}{4D(t-\rho)}]\} \delta(s-\xi) ds d\xi d\tau d\rho. \tag{28}$$

Integrating with respect to ξ and solving the product of exponentials,

$$\sigma_c^2 = q \int_0^t \int_0^t \frac{1}{\pi (bd)^2} [\int_0^\infty \exp(-\frac{(a-s)^2}{b} - \frac{(c-s)^2}{d}) ds - \int_0^\infty \exp(-\frac{(a-s)^2}{b} - \frac{(c+s)^2}{d}) ds$$

$$- \int_0^\infty \exp(-\frac{(a+s)^2}{b} - \frac{(c-s)^2}{d}) ds + \int_0^\infty \exp(-\frac{(a+s)^2}{b} - \frac{(c+s)^2}{d}) ds] \, d\rho d\tau, \tag{29}$$

where $a = x - u(t - \tau)$, $b = 4D(t - \tau)$ as before, $c = x - u(t - \rho)$, and $d = 4D(t - \rho)$. Each of the spatial integrals may be manipulated into an integral of an exponential of a second degree polynomial whose solution is exact (Spiegel 1968). Thus Eq. (29) becomes

$$\sigma_c^2 = q \int_0^t \int_0^t \frac{1}{(4\pi b d m_1)^{1/2}} \{\exp(\frac{m_2^2 - 4m_1 m_3}{4m_1})$$

$$erfc[\frac{m_2}{(4m_1)^{1/2}}] - \exp(\frac{g_2^2 - 4m_1 m_3}{4m_1}) erfc[\frac{g_2}{(4m_1)^{1/2}}] - \exp(\frac{h_2^2 - 4m_1 m_3}{4m_1})$$

$$erfc[\frac{h_2}{(4m_1)^{1/2}}] + \exp(\frac{p_2^2 - 4m_1 m_3}{4m_1}) erfc[\frac{p_2}{(4m_1)^{1/2}}]\}, \tag{30}$$

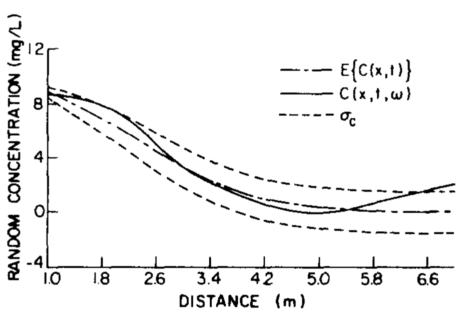

Figure 3

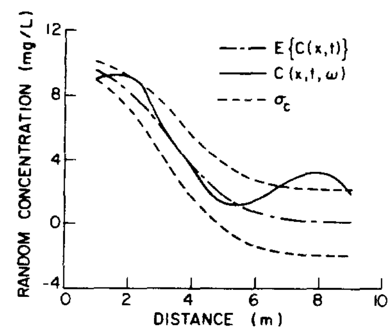

Figure 4

Figure 3. Stochastic concentration in space at $t = 10$ days (Case 2)

Figure 4. Stochastic concentration in space at $t = 15$ days (Case 2)

where $m_1 = (b+d)/(bd)$, $m_2 = (-2cb-2da)/(bd)$,
$m_3 = (da^2+bc^2)/(bd)$, $g_2 = (2bc-2da)/(bd)$,
$h_2 = (2da-2bc)/(bd)$, and $p_2 = (2ad+2bc)/(bd)$.

Equations (18), (24), (27) and (30) 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 Eqs. (24) and (27) 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. (27) 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 in Section 3.2. Figures 3 and 4 show two examples of the simulations carried out at $t = 10$ days and $t = 15$ days respectively. 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 Case 1 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 figures 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 be useful in explaining the stochastic nature of a set of field data. However the most important result here indicates a direct increase in the statistical dispersion of the concentration around the mean with time. This indicates that by disturbing the system with a time and space stochastic process, the time component is as important as the spatial component. This may be easily observed by studying the form of Eq. (23). 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 inaccurate.

We may conclude that the problem of time stochasticity is a most interesting one and that much future research should be devoted to the analysis and

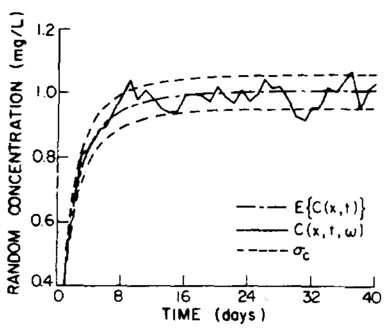

Figure 5

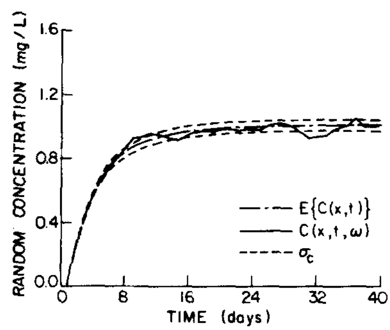

Figure 6

Figure 5. Stochastic concentration with time at $X = 0.5$ m (Case 3)

Figure 6. Stochastic concentration with time at $X = 1.0$ m (Case 3)

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.

3.4 Case 3: Stochasticity in the boundary conditions

Another important case of the stochastically-forced advective-dispersive equation is the one described by Eq. (10), when the boundary condition is a random function in time. This practical case appears in situations when there is a high degree of uncertainty associated with the history of deposition of solid or liquid wastes in the groundwater system. Usually some sort of deterministic function could be associated with the boundary source, but there is always a totally unpredictable component derived from the illegal nature of waste dump sites. In this section a general methodology for treating this case will be presented. To this author's knowledge, there is only one solution of the advective-dispersive equation subject to time stochastic boundary source (Duffy and Gelhar 1985). This solution is an application of a very similar work published by Gelhar in 1974 and it involves a perturbation expansion of the differential equation and a spectral representation of the perturbed equation to obtain the input-output variance. While the frequency domain analysis gives some valuable information, it has been long recognized that spectral techniques of hydrologic signals provide at best only a qualitative description of stochastic quantities (Kottegoda 1980). The direct solution I present here is considerably simpler since it does not require any form of transformation or inversion,where information is inevitably lost, and it is capable of providing much more information, such as sample functions, other forms of correlation functions and higher-order moments.

Let us consider the case of Eq. (10) when the function $k(t,\omega)$ is described by a white Gaussian process in time $w(t)$ with the properties described by Eq. (16):

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} = 0; \quad C(0,t) = w(t,\omega);\ C(\infty,t) = 0;\ C(x,0) = 0. \tag{31}$$

The solution of this equation is easily found from Eq. (13) to be

$$C(x, t) = \frac{x}{(4\pi D)^{1/2}} \int_0^t \exp[-\frac{(x - u(t - \tau))^2}{4D(t - \tau)}] \frac{w(\tau, \omega)}{(t - \tau)^{3/2}} d\tau. \tag{32}$$

The mean concentration is $E\{C(x, t)\} = 0$. By following a procedure similar to the above section one finds the variance of the concentration at time t to be given by

$$E\{C^2(x, t)\} = \sigma_c^2 = \frac{qx^2}{4\pi D} \int_0^t \frac{1}{(t - \tau)^3} \exp[-\frac{(x - u(t - \tau))^2}{2D(t - \tau)}] d\tau. \tag{33}$$

As in the previous sections, Eqs. (32) and (33) 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 staircase function for an interval of one day and solving Eq. (32). The singularity was treated by splitting the integral as

$$C = \int_0^{t-1} \cdots + \int_{t-1}^{t} \cdots,$$

where the first integral was solved by using the trapezoidal rule and the second integral was very accurately calculated by using a Gauss-Legendre quadrature for 24 points (Hornbeck 1975). Equation (33) was similarly solved.

Figures 5 and 6 show the stochastic evolution of the concentration with respect to time for $x = 0.5$ m and $x = 1.0$ m, respectively. The stochastic solution was superimposed to a deterministic solution where the concentration at the source was $C_0 = 1.0$ 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. 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.

4 Conclusions

General applications of functional-analytic theory to the solution of the partial differential equation describing solid transport in aquifers were presented. The applications presented in this Part I included new solutions to the advective-dispersive equation when either the evolution of the system, the sources, and/or the boundary conditions are prescribed as stochastic processes in time or in space. It was found that functional analysis presents considerable advantages over the existing methods of solution. Functional analysis provides a rigorous tool in which the concentration stochastic properties can be predicted in a natural way based upon the known stochastic properties of the sources, and/or the boundary conditions. Thus the theory satisfies a more general modeling need by providing, if desired, a systematic global 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.

The example on the application of the theory included the solution of distributed source problems, with time as well as spatial stochasticity, and the solution subject to stochastic boundary conditions. It was found that once the semigroup operator is known, the solution to a large variety of problems becomes simple. The stochastically-forced equation seems to be a promising model for a variety of random source problems currently being investigated in hydrology. When the differential equation is disturbed by a time and space stochastic process, the output is also a time and space stochastic process, in contrast with most of the existing solutions which ignore the temporal component. There is much to be learned about the stochasticity in time and in space of a contamination field. Stochastic boundary conditions seems to quickly dissipate as time increases and source stochasticity seems to be relatively more important.

Future geohydrologic research should be devoted to the field identification of the kinds and properties of other dominant environmental sources of uncertainty, not just hydraulic conductivity uncertainty.

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Appendix A Derivation of the fundamental semigroup operator for the advective-dispersive equation in porous media

We begin by writing the deterministic advective-dispersive equation in an infinite aquifer:

$$\frac{\partial C}{\partial t} - D\frac{\partial^2 C}{\partial x^2} + u\frac{\partial C}{\partial x} = 0, \qquad C \in L^2(0, T; V),\ V = H_0^1(-\infty, \infty), \tag{A1}$$

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

where the first order in the Sobolev space H_0^1 comes from the concept that a smooth functional (Spiegel 1971) whose first-order derivative exists and whose magnitude vanish at the boundaries, is a distributional solution to Eq. (A1). Let us define $\hat{x} = x - ut$, $\hat{t} = t$, and $v(\hat{x}, \hat{t}) = C(x, t)$. Equation (A1) is reduced to

$$\frac{\partial v}{\partial \hat{t}} - D\frac{\partial^2 v}{\partial \hat{x}^2} = 0, \; v(\pm\infty, t) = 0; \; v(\hat{x}, 0) = C(x, 0) = f(x). \tag{A2}$$

This equation has received much attention among engineers, mathematicians and scientists in the last centuries. For an excellent summary of all the mathematical aspects of this equation, the reader is referred to Cannon (1984). The classical references for the engineering applications are Carslaw and Jaeger (1971) and Crank (1970). The solution to Eq. (A2) thus gives (Zauderer 1983)

$$v(\hat{x}, \hat{t}) = \frac{1}{(4\pi D\hat{t})^{1/2}} \int_{-\infty}^{\infty} \exp[-\frac{(\hat{x} - s)^2}{4D\hat{t}}] f(s) ds. \tag{A3}$$

We finally obtain an expression for the semigroup operator for the partial differential operator A:

$$C(x, t) = J_t f(x) = \frac{1}{(4\pi Dt)^{1/2}} \int_{-\infty}^{\infty} \exp[-\frac{(x - ut - s)^2}{4Dt}] f(s) ds. \tag{A4}$$

With the substitution $s = x - ut + (4Dt)^{1/2}\xi$. Equation (A4) becomes:

$$C = \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} e^{-\xi^2} f(x - ut + (4Dt)^{1/2}\xi) d\xi. \tag{A5}$$

In this expression we note that as $t \to 0$, $C \to \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} e^{-\xi^2} f(x) d\xi = f(x)$. Now, it is easy to show that the semigroup property also holds:

$$\begin{aligned} J_t J_\tau f(x) &= \frac{1}{(4\pi Dt)^{1/2}} \frac{1}{(4\pi D\tau)^{1/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp[-\frac{(x - ut - s)^2}{4Dt}] \exp[-\frac{(x - u\tau - \rho)^2}{4D\tau}] f(s, \rho) ds d\rho \\ &= \frac{1}{(4\pi D(t + \tau))^{1/2}} \int_{-\infty}^{\infty} \exp[-\frac{(x - u(t + \tau) - s)^2}{4D(t + \tau)}] f(s) ds = J_{t+\tau} f(x). \end{aligned} \tag{A6}$$

This property permits the calculation of the concentration at time $t + \tau$, knowing some intermediate concentration at time τ. It is easy to show that the third property of semigroups, that is "strong continuity", also holds. Butzer and Berens (1967) show the strong continuity of the semigroup of the transformed Eq. (A3). Hence the evolution operator described by Eq. (A4) follows all of the properties characterizing a strongly continuous semigroup stated in Section 2. By knowing the form of the semigroup, we may solve a large variety of more complex problems involving sources, sinks, and different boundary conditions in both the deterministic and the stochastic domain.

Most of the applications discussed in this article deal with the case of a semi-infinite aquifer. In this case, we may assume that the aquifer extends to the negative side and that at $-x$ for $x > 0$, $C = -f(x)$ and $f(0) = 0$. Therefore, from Eq. (A4) we have,

$$C = \frac{1}{(4\pi Dt)^{1/2}} \int_0^{\infty} \{ \exp[-\frac{(x - ut - s)^2}{4Dt}] - \exp[-\frac{(x - ut + s)^2}{4Dt}] \} f(s) ds. \tag{A7}$$

For the particular case in which $f(x) = C_i =$ constant, we make $s = x - ut + (4Dt)^{1/2}\xi$ in the first integral, and $s = -x + ut + (4Dt)^{1/2}\xi$ in the second integral. Thus Eq. (A7) becomes

$$C = C_i erf[\frac{x - ut}{(4Dt)^{1/2}}],$$

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

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