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A new approach in modelling groundwater pollution under uncertainty

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This article presents a new methodology to model the time and space evolution of a contaminant in a system of aquifers when certain components of the model, such as the geohydrologic information, the boundary conditions, the magnitude and variability of the sources or physical parameters are uncertain and defined in stochastic terms. The method is based on applications of modern mathematics to the solution of the resulting stochastic transport equations. This procedure exhibits considerable advantages over the existing stochastic modelling techniques. In particular, the semigroup solutions are not restricted to small variances in the stochastic elements (perturbation technique), unsteady dynamic conditions are specifically considered, time and space randomness may be considered in the sources, the boundary conditions or the parameters, and the methodology reflects a well-posed functional-analytic theory. Several basic example problems are presented in order to illustrate the application of the methodology to the modelling of complex spatially and temporally distributed sources of interest in engineering hydrology today. Further potential applications of the method are very promising.

Key Words: stochastic groundwater transport, semigroups, evolution equations.

1. MODELLING GROUNDWATER POLLUTION UNDER UNCERTAINTY

Practical engineering problems involving groundwater pollution modelling today require the prediction of the time and space evolution of a principal contaminant in an aquifer due to a particular contamination source. The accurate forecast of the concentration magnitude facilitates the design of appropriate preventive or remedial measures. The time and space evolution of a contaminant plume in a system of aquifers is theoretically, and ideally, predicted by a solution of the advective-dispersive partial differential equation in porous media subject to an appropriate set of boundary conditions and source functions. Solving this equation for the concentration distribution subject to the several physical and chemical uncertainties in the phenomenon of mass transport in aquifers and the insufficiency of hydrogeological and hydrochemical information is one of the main difficulties in engineering hydrology today. The literature reports the inaccuracy of deterministic models in predicting contamination in situations when the parameters, the boundary conditions, and the pollution sources are difficult to measure or when they vary erratically in space and time. Modelling of reactive transport poses serious difficulties to the hydrologic community because of the inability of deterministic functions to represent the wide spectrum of variability of a nonconservative contaminant. It has also been reported the large differences between laboratory-measured dispersion coefficients and the corresponding field scale values. This discrepancy tends to increase as time or distance from the source increases.

As a result of the above difficulties, some limited stochastic modelling techniques attempting to describe an uncertain quantity in stochastic terms have emerged. While these stochastic methods have provided insight on the phenomenon of mass transport in aquifers, several inconsistencies and deficiencies have been noted, which can be related to the limitations of the mathematical procedures employed.

The main limitation of the existing stochastic methods relates to the assumption of small randomness required by the perturbation expansion solutions. The existing methods can only handle randomness in one quantity, and as a result the hydraulic conductivity has been assumed as the only source of uncertainty. The effect of randomness in the time or spatial distribution of the sources, randomness in the boundary conditions, or the randomness in the environmental evolution of the system has not been studied. In some cases the applications are limited to steady state asymptotic conditions of the concentration field and the dynamic features of the system have not been considered. Some of the apparent stochasticity in the hydraulic conductivity may be generated by small scale measurement approaches, and their unavoidable errors, to large scale contaminant migration as may be seen in the recent field work. Some of the approaches use Monte Carlo simulations, which are expensive and empirical. Some of the existing modelling methods only provide information about the concentration variance, without a description of the form...
of sample functions, different correlation functions and higher order moments, which would give a better information of the stochastic properties of the concentration process. Finally, the existing methods are in a sense parameter estimation techniques rather than methods to obtain explicit solutions for engineering forecasting purposes.

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

The proposed methodology is based on the application of modern mathematics to the solution of stochastic transport equations (Refs 5, 9, 12, and 35 among others). The solutions are obtained by blending some developments on the theory of stochastic partial differential equations in Hilbert spaces, the theory of stochastic evolution equations, and the theory of semigroups of operators with some classical results on the heat flow (diffusion) equation. These works have defined a functional-analytic framework to study many stochastic equations in mathematical physics. Applications of these concepts to the modelling of stochastic groundwater flow have generated important results. It is the objective of the present article to present a modelling procedure for the more complex problem of solid transport in aquifers subject to uncertainty.

In what follows we assume that the advective-dispersive equation subject to some form of stochasticity is an appropriate form of modelling the dispersion phenomenon in porous media for certain regional-scale pollution problems. We do not discuss here the methods to derive transport equations, which are treated in detail elsewhere. In section 2, a general mathematical statement of the groundwater pollution modelling problem subject to general uncertainty is made. The relevant functional-analytic results leading to a new general solution of the differential equations is presented. The emphasis is on applications and the description is concentrated on main results. Therefore, theoretical aspects of existence and uniqueness of solutions, topological properties of solutions spaces and theorems have been omitted. In section 3, several application cases of modelling groundwater pollution subject to different forms of uncertainty are shown in detail. These applications are chosen to satisfy the current needs in groundwater pollution modelling and to illustrate the potentially of the method in more complex cases.

2. MATHEMATICAL STATEMENT AND SOLUTION OF GROUNDWATER POLLUTION UNDER UNCERTAINTY

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

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

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

subject to

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

where \(C(x, t, \omega)\) is the stochastic process representing the concentration of the principal contaminant in the fluid (mg/L); \(D(t, \omega)\) is the random process representing the aquifer dispersion coefficient (m²/day); \(u\) is the average pore velocity, that is the flux velocity divided by the average porosity of the media (m/day); \(x\) is the coordinate parallel to the flow; \(t\) is the time coordinate; \(k(t, \omega)\) is the time-dependent concentration at the origin (mg/L); \(f(x)\) is the initial concentration distribution across the aquifer (mg/L); and \(g(x, t, \omega)\) is the stochastic function representing the reaction term. Assume that the stochastic components are well-behaved and obtained after repetitive sampling in the aquifer and the pond.

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

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

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

\[
Q(x,t,\omega)u = F(\omega), \quad (x,t,\omega) \in \mathcal{D}G \times [0, T] \times \Omega
\]

\[
u(x,0,\omega) = u_0(x,\omega), \quad (x,\omega) \in G \times \Omega
\]  \hspace{1cm} (2)

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; \(G \subset R^3\) is an open domain subset of the three-dimensional real space with boundary \(\partial G\); \(0 < T < \infty\); \(\Omega\) is a boundary operator; \(\mathcal{D}G\) is the basic probability sample space of elements \(\omega\); \(L^2(\Omega, B, P) = L^2(\Omega)\) is the complete probability space of second-order random functions with probability measure \(P\) and \(B\) borel field or class of \(\omega\) 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

\[
Au = \sum_{k,l=0}^m (-1)^k D^k(p_k(\xi_1,\xi_2)D^l\xi_1)u
\]

where \(D\) is differentiation; \(p_k(\xi_1,\xi_2)\) are random-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 \(L^2(0, T; V)\) is the Sobolev space of order \(m\) of \(L^2(\Omega)\)-valued functions; \(V \subset H \subset V'\), \(V\) is dense in \(H\), where \(H = H^{0}\); the norm on \(V\) is denoted by \(\|\|\); \(V'\) is the dual of \(V\); \(g \in L^2(0, T; V')\); and \(u_0 \in H \times \Omega\) is the system initial condition. For a more complete description of the above definitions the reader is referred to the available functional-analytic literature\(^2,\,\,17,\,\,19,\,\,24,\,\,30,\,\,38\).

Theorems and proofs concerning the existence and uniqueness of the solution to a system given by equation (1) have been extensively treated in Refs 5, 7, 9, and 30 among others.

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

\[
v(t) = v_0 + \int_0^t J_{\tau, t} h(x, s, \omega) ds
\]  \hspace{1cm} (3)

where \(v \in L^2(0, T; V)\) is the system output; \(V = H^{0}\) is a closed subspace of \(H^2\); \(H^{0}\) is the closure of \(C^0(\Omega; G; L^2(\Omega))\) in \(H^2\), that is, \(H^{0}\) is the \(m\)th order Sobolev space of second-order random functions with compact support; \(h(x, t, \omega)\) includes the function \(g(x, t, \omega)\) and the appropriate function(s) resulting from the space transformation, including the boundary conditions; \(v_0(x)\) includes \(u_0(x)\); \(J_{\tau, t} \in (H, H)\) is the evolution operator associated with \(A\) (Refs 2, 4, 6, 8, 16, 20, 23 and 24). If a transformation of spaces is not done, it is clear that the operator must satisfy the prescribed boundary conditions. If the operator \(A\) is time independent and if the evolutional operator \(J_{\tau, t}\) in the Hilbert space \(H\) satisfies:

(i) \(J_{\tau, t} = J_{0, \tau} J_{0, t} \geq 0\),

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

(iii) \(\|J\|_{H \rightarrow H} = 0\) as \(\tau \rightarrow 0\) for all \(v \in H\),

where \(\|\|\) denotes the norm, then \(J_{\tau, t}\) is said to be a strongly continuous semigroup. Properties (i) and (ii) above give the semigroup structure, whereas property (iii) is topological and defines the 'strong continuity'.

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

The mean value of \(v\) is given by

\[
E[v(x, t)] = J_{0, t} v_0 + \int_0^t J_{\tau, t} E[h(x, s, \omega)] ds
\]  \hspace{1cm} (4)

where \(E[\,\,\,]\) denotes the expectation operator.

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Now the second moment of \( v \) in equation (3) is given by

\[
E[v(t_1)v(t_2)] = E \left[ \int_0^{t_1} J_{t_1-t} h(s) \, ds \right] \times \left[ \int_0^{t_2} J_{t_2-t} h(\xi) \, d\xi \right]
\]

where \( \omega \) has been omitted for convenience. Without loss of generality we assume that \( h \) is a zero mean stochastic process. This is the result after a deterministic model has been optimized. Thus the second term in equation (4) is equal to zero and equation (5) becomes

\[
E[v(t_1)v(t_2)] = J_{t_1+t_2} v_0^2 + \int_0^{t_1} \int_0^{t_2} J_{t_1-t} h(s) \, ds \, J_{t_2-t} h(\xi) \, d\xi \, \, ds \, d\xi
\]

(6)

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

If the operator \( A \) in equation (2) is stochastic because one or more of the parameters is defined as a stochastic process, then it is a nonlinear stochastic partial differential equation which in general has no exact solution. We follow in this case a procedure similar to the one used in Ref. 1 to decompose an ordinary stochastic differential operator into an infinite series in order to approximate the corresponding stochastic Green's function. We shall present a semigroup formulation for a general stochastic partial differential operator, such as the one introduced in Ref. 37 for the groundwater flow equation subject to stochastic transmissivity.

Let us write the operator \( A \) as

\[
A(x, t, \omega) = A(x) + R(t, \omega)
\]

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

\[
v = J_{t_1} v_0 + \int_0^{t_1} J_{t_1-t} h(s) \, ds - \int_0^{t_1} J_{t_1-t} R v(s) \, ds
\]

(8)

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

\[
v = J_{t_1} v_0 + \int_0^{t_1} J_{t_1-t} h(s) \, ds - \int_0^{t_1} J_{t_1-t} R v_1 + v_2 + v_3 + \ldots \, ds
\]

(9)

where the semigroup \( J \) is now deterministic. Identifying \( v_1 \) as the preceding term \( \int_0^{t_1} J_{t_1-t} h(s) \, ds \), we can determine each \( v_i \) in terms of the preceding \( v_{i-1} \). Thus

\[
v = J_{t_1} v_0 + \int_0^{t_1} J_{t_1-t} h(s) \, ds + \int_0^{t_1} \int_0^{t_1} J_{t_1-t} R J_{t_1-s} h(\tau) \, d\tau \, ds
\]

\[- \int_0^{t_1} \int_0^{t_1} \int_0^{t_1} J_{t_1-t} R J_{t_1-s} R J_{t_1-r} h(\tau) \, d\tau \, d\xi \, ds \ldots
\]

(10)

where the last term in the series contains \( v \). The basic idea here is that a random semigroup operator, which may be difficult to derive in particular cases, can be determined in an easily computable series by decomposition of the differential operator \( A(x, t, \omega) \) into a deterministic operator \( A(x) \) whose semigroup is known or found with little effort, and a random operator \( R(t, \omega) \) whose contribution to the total semigroup \( J_{t_1} \) modification can be found in series form. The convergence question will not be treated here, since it has been discussed elsewhere.

The mean value of \( v \) is obtained by truncating equation (13) and taking expectations:

\[
E[v] = J_{t_1} v_0 + \int_0^{t_1} \int_0^{t_1} J_{t_1-t} h(s) \, ds
\]

\[- \int_0^{t_1} \int_0^{t_1} \int_0^{t_1} J_{t_1-t} R J_{t_1-s} h(\tau) \, d\tau \, ds \ldots
\]

(11)

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

Similarly, the correlation function is given by

\[
E[v(t_1)v(t_2)] = E \left[ \int_0^{t_1} J_{t_1-t} h(s) \, ds \right]
\]

\[- \int_0^{t_1} \int_0^{t_1} J_{t_1-t} R J_{t_1-s} h(\tau) \, d\tau \, ds \ldots
\]

\times J_{t_2-t} R J_{t_2-s} h(\xi) \, d\xi \, ds
\]

(12)

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

\[
E[v(t_1)v(t_2)] = J_{t_1+t_2} v_0^2
\]

\[+ \int_0^{t_1} \int_0^{t_2} J_{t_1-t} J_{t_2-s} E[h(s)h(\rho)] \, ds \, d\rho
\]

\[- \int_0^{t_1} \int_0^{t_2} \int_0^{t_2} J_{t_1-t} R J_{t_1-s} E[h(s)h(\gamma)] \, dy \, d\beta \, ds
\]

\[+ \int_0^{t_1} \int_0^{t_2} \int_0^{t_2} \int_0^{t_2} J_{t_1-t} J_{t_2-s} E[R J_{t_2-s} R J_{t_2-\gamma}] \times E[h(\tau)h(\gamma)] \, d\tau \, ds \, d\gamma \, d\beta
\]

(13)

These are the results obtained by considering one term \( v_1 \) in the series of equation (9). Obviously calculations can be extended up to a desired degree of accuracy by considering more terms. However, it is known that the
series converges rapidly and that in some circumstances considering one term is sufficiently accurate, as demonstrated by the sensitivity analysis on the semigroup for the stochastic boussinesq equation in groundwater flow presented in Ref. 37.

In the following sections we shall illustrate the application of the above theory to the modelling of groundwater pollution in engineering problems. The example problems show the solution of special cases of equation (1) which appear in applications. The emphasis is on the illustration of the methodology rather than on the routine modelling steps, we use a well-known stochastic process in the applications, namely the White Gaussian Noise. This is done for simplicity and because the properties of this process closely resemble many physically-realizable processes after the deterministic trend has been removed. It is clear, however, that any process in $L_2(\Omega)$ could be used, the properties of which should be derived from sample field measurements followed by an estimation algorithm.

3. APPLICATION PROBLEMS

3.1 Modelling contamination at a well subject to measurement errors

In section 2 we described a contamination problem in a shallow phreatic aquifer due to a pond receiving industrial waste. Suppose the facility is new and that due to budgetary restrictions, only one monitoring well was drilled. After studying the average amplitude of the chloride concentration in the pond it was decided to locate this well at a distance from the pond $X$ such that the random variations in the boundary condition could be neglected and replaced by their average value $C_0$. Assume also that the uncertainty in the dispersion coefficients is minimum, and that the reaction term is negligible. However, the instrumentation used in measurement concentration is rudimentary and the individuals performing the measurement are not experienced, in which case there are important errors in the concentration. The modelling problem reduces to predicting the concentration at the well over time. The modelling equation will be equation (1) with a constant source boundary condition $k=C_0$, an initial condition $C(x,0)=0$ and a forcing term at the well $g(X,t,\omega)=w(t)$.

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

$$C(x,t,\omega) = C_1(x,t,\omega) + C_2(x,t)$$ (14)

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

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

generates a strongly continuous semigroup $J$, given by

$$Jf(x) = \frac{1}{(4\piDt)^{1/2}} \int_0^\infty \left\{ \exp\left[\frac{(x-ut-s)^2}{4Dt}\right] \right\} f(s) ds$$ (15)

This is easy to see by analogy of equation (1) with the classical heat flow (diffusion) equation. It is easy to show that $J$, in this case is a strongly continuous semigroup with the properties of semigroups described in section 2. These properties permit the calculation of the concentration at time $t+\tau$, knowing some intermediate concentration at time $t$. Most importantly, knowing the form of the semigroup we may obtain the solution of our differential equation. For the random component of the solution we have, according to equation (3),

$$C_1(x,t,\omega) = Jf(x) + \int_0^t \int_0^\infty \exp\left[\frac{(x-ut-\tau-s)^2}{4D(\tau-\tau)}\right] \frac{w(\tau,\omega)}{(4\pi D(\tau-\tau))^1/2} ds d\tau$$ (16)

or

$$C_1(x,t,\omega) = \frac{w(t,\omega)}{(4\pi D(t-\tau))^1/2} \int_0^\infty \exp\left[\frac{(x-ut-\tau+s)^2}{4D(t-\tau)}\right] ds d\tau$$ (17)

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

Now the solution of the deterministic component in equation (14) may be approached in two ways: As stated in section 2, we may transform our functional space $H^1(0,\infty)$ into a Sobolev space with compact support $H^1(0,\infty)$ by defining $C_2$ in terms of a smooth function satisfying the boundary conditions and replacing it into the differential equation. This procedure will generate a forcing term and the problem can be solved 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:

$$C_2(x,t) = \frac{x}{(4\pi D)^{1/2}} \int_0^\infty \exp\left[\frac{(x-ut-\tau)^2}{4D(t-\tau)}\right] \frac{C_0}{(t-\tau)^{1/2}} dt$$ (18)

Since $C_0$ is a constant, equation (18) becomes:

$$C_2(x,t) = \Phi(x,t) = \frac{C_0}{2} \left[ \text{erfc} \left( \frac{x-ut}{(4Dt)^{1/2}} \right) + \exp\left( \frac{ux}{D} \right) \text{erfc} \left( \frac{x+ut}{(4Dt)^{1/2}} \right) \right]$$ (19)

where erfc() denotes the 'error function complement' given by

$$\text{erfc}(z) = \frac{2}{\pi^{1/2}} \int_z^\infty e^{-s^2} ds$$

Simplifying the inner integral in equation (17), and replacing equations (17) and (19) into equation (14) we
find the general solution of our model differential equation:

\[ C(x, t, \omega) = \Phi(x, t) + \int_{0}^{t} \text{erf} \left[ \frac{x - u(t - \tau)}{4\pi D(t - \tau)} \right] w(\tau, \omega) \, d\tau \]  \hspace{1cm} (20)

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

\[ E\{w(t)\} = 0, \quad E\{w(t_1)w(t_2)\} = q \delta(t_2 - t_1) \] \hspace{1cm} (21)

where \( q \) is the variance parameter (mg/lit/day) and \( \delta(\cdot) \) is the Dirac's delta function. This would indicate that the randomness in the system comes from nonsystematic measurement errors due to the limitations of the instrumentation and the data processing.

Now taking expectations on both sides of equation (20) and using equation (21) we find the mean concentration to be

\[ E\{C(x, t)\} = \Phi(x, t) \] \hspace{1cm} (22)

Now following equations (6), (20) and (21), the second moment of \( C \) is

\[ E\{C(x, t_1)C(x, t_2)\} = \Phi(x, t_1)\Phi(x, t_2) + q \int_{0}^{t_1} \int_{0}^{t_2} \text{erf} \left[ \frac{x - u(t_1 - \tau)}{4D(t_1 - \tau)} \right] \text{erf} \left[ \frac{x - u(t_2 - \xi)}{4D(t_2 - \xi)} \right] \delta(t_1 - t_2) \, d\xi \, d\tau \]  \hspace{1cm} (23)

If we let \( t_1 = t_2 = t \) and subtract the square of the mean, equation (23) becomes the variance of \( C \):

\[ \sigma_c^2 = q \int_{0}^{t} \text{erf} \left[ \frac{x - u(t - \tau)}{4D(t - \tau)^{1/2}} \right] d\tau \] \hspace{1cm} (24)

In order to have a quantitative observation of the above solution, equations (20), (22) and (24) were programmed in the micro-computer and numerical values of the mean concentration, a sample function and the standard deviation of the concentration with time where computed. An average pore velocity \( u = 0.2 \) m/day, a dispersion coefficient \( D = 0.1 \) m²/day, a concentration at the origin \( C_0 = 10.0 \) mg/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 Ref. 19). The integrals were solved numerically. Fig. 1 is a digital plotter output of the program for a well located \( X = 6.0 \) m from the pond. The solid line represents the evolution with time of the mean concentration, the continuous sinuous line represents the sample concentration, and the dotted lines represent the mean concentration plus and minus one standard deviation respectively. For high values of \( t \), the calculations are more efficient if the differential equation is solved step wise with the output from one step becoming the initial condition to the next one. This procedure could be easily adapted to equation (20).

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 an 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

\[ E\{C(x, t)\} \]

\[ C(x, t, \omega) \]

\[ \sigma_c \]

**Fig. 1.** Stochastic concentration with time at \( X = 6.0 \) m

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\textsuperscript{47,48} as one of the difficulties in using the existing models. Thus we may conclude that a model such as the one presented replicates concentration distribution values with the same characteristics of the ones measured in the field.

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

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

3.2 Modelling of non-conservative contaminant migration

Consider the groundwater modelling problem depicted in section 2 and assume that the most important source of uncertainty comes from the difficulty in identifying a fixed deterministic function representing the spatial erratic variation in the main contaminant concentration due to the reaction between the main contaminant and the chemical constituents of the aquifer porous media. For the purpose of the present illustration, assume that other sources of uncertainty can be neglected, or are very small in magnitude with respect to the reaction term uncertainty. The modelling equation is equation (1) with the uncertain term appearing as a spatially random forcing function \( g(x,\omega) = \omega(x) \), a constant source at the origin \( k = C_0 \), and with initial condition \( C(x, 0) = 0 \). We assume that the deterministic trend in the reactive term has already been removed and that we may represent the purely random component of this term as a White Gaussian Noise process in space and smooth in time \( \omega(x) = dB(x)/\Delta t \) with the properties given by equation (21) with the independent variable \( x \) instead of \( t \). It is clear that the actual properties of the uncertain term will have to be obtained after an analysis of field concentration measurements along \( x \) and an appropriate ergodic assumption.

The solution to the differential equation in this case is given by equation (14), where \( C_j \) is given by equation (19) and \( C_1 \) is obtained from equations (3) and (15) as

\[
C_1(x, t, \omega) = \int_0^\infty \left( \frac{1}{4\pi D(t-\tau)^{3/2}} \left\{ \exp \left[ -\frac{(x-u(t-\tau)-s)^2}{4D(t-\tau)} \right] - \exp \left[ -\frac{(x-u(t-\tau)+s)^2}{4D(t-\tau)} \right] \right\} \right) w(s, \omega) ds d\tau
\]

Integrating with respect to \( \xi \) and solving the product of exponentials, we obtain two spatial integrals which may be manipulated into integrals of exponentials of second degree polynomials whose solutions are exact\textsuperscript{33}. Thus
equation (29) becomes

$$\sigma_c^2 = q \int_0^t \int_0^1 \frac{1}{(4?^2 d m_1)^{1/2}} \times \left\{ \exp\left( \frac{m_3^2 - 4m_1m_3}{4m_1} \right) \text{erfc}\left( \frac{m_3}{(4m_1)^{1/2}} \right) \right. $$

$$- \exp\left( \frac{g_2^2 - 4m_1m_3}{4m_1} \right) \text{erfc}\left( \frac{g_2}{(4m_1)^{1/2}} \right) $$

$$- \exp\left( \frac{h_2^2 - 4m_1m_3}{4m_1} \right) \text{erfc}\left( \frac{h_2}{(4m_1)^{1/2}} \right) $$

$$+ \exp\left( \frac{p_2^2 - 4m_1m_3}{4m_1} \right) \text{erfc}\left( \frac{p_2}{(4m_1)^{1/2}} \right) \right\} \, dp \, d\tau \quad (30)$$

where

$$a = x - u(t - \tau), \quad b = 4D(t - \tau),$$
$$c = x - u(t - \rho), \quad d = 4D(t - \rho),$$
$$m_1 = \frac{b + d}{bd}, \quad m_2 = \frac{-2cb - 2da}{bd}, \quad m_3 = \frac{da^2 + bc^2}{bd},$$
$$g_2 = \frac{2bc - 2da}{bd}, \quad h_2 = \frac{2da - 2bc}{bd},$$
$$p_2 = \frac{2ad + 2bc}{bd},$$

Equations (14), (22), (26) and (30) were 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 equation (26) 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 equation (26) 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 3.1. Fig. 2 shows an example of the simulations carried out at $t=15$ days. The variation of either the mean, a sample function and the standard deviation of the concentration around the mean with respect to distance is represented. The same parameter values used in the previous application were inserted in the equations, except that the variance parameter was chosen as $q=0.1$. The mean values coincide with the deterministic solution.

The results demonstrate the expected direct increase in the dispersion of the concentration around the mean with distance. This phenomenon has been noted in the hydrologic literature and it is interesting to observe that a model like this one may explain the stochastic nature of a set of field data whose erratic nature accounts for the reactive features of the main contaminant. However the most important result here indicates a direct increase in the statistical dispersion of the concentration around the mean with time. Although intuitively we should not expect time stochasticity because we are dealing with a disturbing space stochastic process, the results suggest that by disturbing the advective-dispersive equation with a spatial stochastic process, the output concentration function will be a space-time stochastic process. This may be easily observed by studying the form of equation (25). We may add that this phenomenon has not been mentioned in previous work related to the spatial

![Fig. 2. Stochastic concentration in space at t=15 days](image-url)
stochasticity of the dispersion process and that assumptions ignoring the time stochasticity of the system are probably not appropriate. We may conclude that the problem of space-time stochasticity is a most interesting one and that much future research should be devoted to the analysis and implications of space-time stochasticity on the predictability of the concentration function. In particular, measurement efforts should be devoted to the identification of the random processes involved.

3.3 Investigating pollution variability near a source

Let us now consider the groundwater pollution problem of section 2 when the highest degree of uncertainty comes from the time variability of the concentration of the source at the origin and other uncertain terms are comparatively small. Assume that in this extremely practical case there is a high degree of uncertainty associated with the history of deposition of solid or liquid wastes in the pond, and that the objective of the modelling tasks is to predict the variability of the concentration near the pond. That is, some monitoring wells have been constructed a short distance from the pond and we wish to develop a model which would predict the random nature of the concentration at the wells. This will allow us to forecast the concentration values and to design and test remedial measures if appropriate. Assume that the average concentration in the pond tends to be a constant \( C_0 \) but there is a totally unpredictable component \( w(t, \omega) \) derived from the illegal nature of the waste-dump site.

For the purpose of the illustration, assume that field measurements have demonstrated that the function \( w \) is described by a White Gaussian Noise process in time with the properties described by equation (21). The governing differential equation is equation (1) subject to a boundary source \( k(t) = C_0 + w(t) \) and with the forcing function, the parameters and initial condition equal to zero. From equations (14), (18) and (19), the general solution of the differential equation is given by

\[
C(x, t) = \Phi(x, t) + \frac{x}{4\pi D^{1/2}} \int_0^t \exp \left[ -\frac{(x-u(t-\tau))^2}{4D(t-\tau)} \right] \frac{w(\tau, \omega)}{(t-\tau)^{3/2}} d\tau
\]

(31)

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

\[
\sigma_c^2 = \frac{q^2}{4\pi D} \int_0^t \frac{1}{(t-\tau)^3} \exp \left[ -\frac{(x-u(\tau))^2}{2D(t-\tau)} \right] d\tau
\]

(32)

As in the previous sections, equations (31) and (32) were used in the generation of sample functions, the calculation of the mean and the standard deviation of the concentration with respect to time. The sample function was calculated by generating a sample of \( w \) as a limiting random walk function for an interval of one day and solving equation (31). The integrals were solved numerically and the singularities were treated by using the Gauss-Legendre quadrature method.

Fig. 3 shows the stochastic evolution of the concentration with respect to time for \( x=0.5 \) m. The mean concentration at the pond was assumed \( C_0 = 1.0 \) mg/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

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Fig. 3. Stochastic concentration with time at \( X=0.5 \) m

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boundary decreases as the distance from the boundary increases for a zero-mean stationary process. This of course depends on the type and variance of the disturbing process, but in general the concentration variance approaches to zero beyond several meters of distance from the boundary and the process is then governed by the mean source concentration. This may indicate qualitatively that the effect of stochasticity of the boundaries is relatively less important than the effect of distributed-source stochasticity on the overall stochasticity of the concentration function.

3.4 Modelling large-scale groundwater pollution uncertainty

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

\[
\frac{\partial C}{\partial t} - D_1 \frac{\partial^2 C}{\partial x^2} - D_2 \frac{\partial^2 C}{\partial y^2} - D_3 \frac{\partial^2 C}{\partial z^2} + u \frac{\partial C}{\partial x} = \frac{d\beta(t)}{dt}
\]

(33)

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

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

where \(C(x, y, z, t, \omega) \equiv H^1(\mathbb{R}^3)\) is the stochastic process representing the concentration of a principal contaminant in the fluid (mg/lit); \(D_1\) is the longitudinal dispersion coefficient in the x direction (m²/day); \(D_2\) is the lateral dispersion coefficient in the y and z direction (m²/day); \(u\) is the average pore velocity in the x direction; \(x, y, z\) are the three-dimensional cartesian coordinates; \(C_0\) is a constant point source at the origin; and \(d\beta(t)/dt = w\)

represents a White Gaussian Noise process in time disturbing the system and with the properties given by equation (21).

We assume that the solution to this equation may be written as equation (14), with \(x\) representing the three-dimensional coordinate system. The operator \(A\), such that

\[AC_1 = \left(-D_1 \frac{\partial^2}{\partial x^2} - D_2 \frac{\partial^2}{\partial y^2} - D_3 \frac{\partial^2}{\partial z^2} + u \frac{\partial}{\partial x}\right)C_1\]

generates a strongly continuous semigroup given by

\[
J(x, y, z) = \frac{1}{8(\pi D_1 D_2 D_3)^{1/2}} \times \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp \left[ -\frac{1}{4t} \left( \frac{(x-u(t-t))^2}{D_1} \right) \right]
\]

\[
+ \frac{(y-y')^2}{D_2} + \frac{(z-z')^2}{D_3} \right] f(x', y', z') \, dx' \, dy' \, dz'
\]

(34)

This is easy to see by analogy with equation (15). Thus according to equations (3), the solution for the random component \(C_1\) is

\[
C_1 = \int_0^t \frac{w(t)}{8(\pi D_1 D_2 D_3)^{1/2}} \times \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp \left[ -\frac{1}{4(t-t)} \left( \frac{(x-u(t-t)-x')^2}{D_1} \right) \right]
\]

\[
+ \frac{(y-y')^2}{D_2} + \frac{(z-z')^2}{D_3} \right] \, dx' \, dy' \, dz' \, dt
\]

(35)

The space integrals have exact solutions. Thus

\[
C_1 = \int_0^t \left[ 1 + \text{erf} \left( \frac{x-u(t-t)}{(4D_1(t-t))^{1/2}} \right) \right] \left[ 1 + \text{erf} \left( \frac{y}{(4D_2(t-t))^{1/2}} \right) \right]
\]

\[
\times \left[ 1 + \text{erf} \left( \frac{z}{(4D_3(t-t))^{1/2}} \right) \right] w(t) \, dt
\]

(36)

where \(\text{erf}(\cdot)\) denotes the ‘error function’ such that \(\text{erf}(z) = 1 - \text{erf}(z)\). Similarly the solution for the deterministic component \(C_2\) in equation (14) is deduced from equations (3) and (34) as

\[
C_2 = \int_0^t \frac{C_0}{8(\pi D_1 D_2 D_3)^{1/2}} \times \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp \left[ -\frac{1}{4(t-t)} \left( \frac{(x-u(t-t)-x')^2}{D_1} \right) \right]
\]

\[
+ \frac{(y-y')^2}{D_2} + \frac{(z-z')^2}{D_3} \right] \delta(x') \delta(y') \delta(z') \, dx' \, dy' \, dz' \, dt
\]

(37)

or

\[
C_2 = C_0 \int_0^t \frac{1}{8(\pi D_1 D_2 D_3)^{1/2}} \times \exp \left[ -\frac{1}{4D(t-t)} \left( \frac{(x-u(t-t))^2}{D_1} + \frac{y^2}{D_2} + \frac{z^2}{D_3} \right) \right] \, dt
\]

(38)

This integral has an exact solution. Thus

\[
C_2 = \Phi = C_0 \frac{1}{8\pi D_1 R} \exp \left( \frac{uR}{2D_1} \right)
\]

\[
\times \left\{ \exp \left( \frac{uR}{2D_1} \right) \left[ 1 - \text{erf} \left( \frac{u(t-t)}{(4D_1(t-t))^{1/2}} \right) \right] \right\}
\]

\[
+ \exp \left( \frac{-uR}{2D_1} \right) \left[ 1 + \text{erf} \left( \frac{u(t-t)}{(4D_1(t-t))^{1/2}} \right) \right] \right\}
\]

(39)

where

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

After equation (4), the mean concentration function is given by equation (22). Let us set

\[E_x(t) = \left\{ 1 + \text{erf} \left( \frac{x-u(t-t)}{4D_1(t-t)^{1/2}} \right) \right\}
\]

(40)
\[ E_r(t) = \left\{ 1 + \operatorname{erf} \left[ \frac{y}{\sqrt{4D_2(t-t)^{1/2}}} \right] \right\} \quad (41) \]

and
\[ E_\alpha(t) = \left\{ 1 + \operatorname{erf} \left[ \frac{z}{\sqrt{4D_2(t-t)^{1/2}}} \right] \right\} \quad (42) \]

After equations (6) and (21), we calculate the variance function by using equations (14), (22) and (40) through (42)
\[ E[(C-\Phi)^2] = \sigma^2 \]
\[ = q \int_0^\infty \int_0^\infty \delta(t-\tau)E_r(t)E_\alpha(\tau)E_r(\tau)E_\alpha(\tau)E_r(\tau)E_\alpha(\tau) d\xi d\tau \quad (43) \]

or
\[ \sigma^2 = q \int_0^\infty E_r^2(t)E_\alpha^2(\tau)E_r(\tau)E_\alpha(\tau) d\tau \quad (44) \]

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

3.5 Modelling groundwater pollution subject to evolving heterogeneities

In this section we consider the groundwater pollution problem of section 2 when the modeller has identified the parameters as the most important source of uncertainty and other sources of uncertainty are negligible. To illustrate the theory presented in section 2 concerning the case of stochastic parameters, we consider here the contaminant transport equation subject to time-stochastic dispersion coefficient. As stated in section 1, much of the emphasis on parameter stochasticity in the hydrologic literature has been confined to the problem of small spatial stochasticity in the hydraulic conductivity and the dispersion coefficient. The results of the present research demonstrates that it may not be appropriate to ignore the inherent temporal dynamic behaviour of the system. Therefore we introduce in this section a new solution to the mass transport equation in aquifers which acknowledges the dispersion coefficient as a fluctuating environmental parameter. This time-random fluctuations are due to the uncertainty generated by the complex dispersion process and the natural evolution of the system. The following development may also be applied to a spatially-random dispersion coefficient and velocity field, but we choose to analyse an untreated temporal stochasticity for cases when the spatial stochasticity could be neglected. The following solution also has the same advantages exhibited by all semigroup solutions, that is, it is not restricted to small variance in the parameter and that any stochastic process in \( L_2(\Omega) \) could be used.

In this case the modelling equation is
\[
\frac{\partial C}{\partial t} - (D(t) + D'(t, \omega)) \frac{\partial^2 C}{\partial x^2} + u \frac{\partial C}{\partial x} = 0, \quad 0 \leq x \leq \infty, \quad t > 0
\]
\[ C(x, 0) = 0; \quad C(0, t) = C_0; \quad C(\infty, t) = 0 \quad (45) \]

where \( D(t) \) is a deterministic trend in the dispersion coefficient; \( D'(t, \omega) \) is a stochastic process disturbing \( D \).

For this example, let us assume that \( D(t) = D \) is a constant and that \( D'(t, \omega) = w(t, \omega) \) is a White Gaussian Noise process in time with the properties given by equation (21).

Following the procedure described in section 2, we write equation (45) as
\[
\frac{\partial C}{\partial t} - D \frac{\partial^2 C}{\partial x^2} + u \frac{\partial C}{\partial x} = D' \frac{\partial^2 C}{\partial x^2} \quad (46)
\]

The solution of this equation is given by equation (10) and (14) as
\[
C = \Phi(x, t) + \int_0^\infty \frac{1}{4\pi D(t-t)^{1/2}}
\times \left\{ \exp \left[ -\frac{(x-u(t-t)-s)^2}{4D(t-t)} \right] - \exp \left[ -\frac{(x-u(t-t)+s)^2}{4D(t-t)} \right] \right\} D' \frac{\partial^2 C}{\partial x^2} ds dt \quad (47)
\]

where the semigroup in equation (10) is given by equation (15); \( D' \) is spatially independent of \( C \); and \( \Phi(x, t) \) is given by equation (19).

Next we define \( C = C_1 + C_2 + C_3 + \ldots \), and
\[
W(t, s) = \exp \left[ -\frac{(x-u(t-t)-s)^2}{4D(t-t)} \right] - \exp \left[ -\frac{(x-u(t-t)+s)^2}{4D(t-t)} \right] \quad (48)
\]

Equation (47) becomes
\[
C = \Phi(x, t) + \int_0^\infty \frac{D(t)}{4\pi D(t-t)^{1/2}}
\times \left\{ \int_0^\infty W(t, s) \frac{\partial^2 \Phi(t, s)}{\partial s^2} ds dt \right\} \quad (49)
\]

The calculation of the series can be carried on to a desired accuracy. This is a computational problem in which the number of terms will vary according to the variance of the stochastic processes involved and the desired accuracy. Let us truncate, for now, at the first term in the series and assume it to be equal to the first solution, that is, \( C_1 = \Phi \).

Thus we re-write equation (49) as
\[
C = \Phi + \int_0^\infty \frac{D(t)}{4\pi D(t-t)^{1/2}} \left\{ \int_0^\infty W(t, s) \frac{\partial^2 \Phi(t, s)}{\partial s^2} ds dt \right\} \quad (50)
\]

Integrating by parts twice with respect to \( s \) and calculating the second derivative of \( W \), it is easy to show
that equation (50) becomes

\[ C(x, t, \omega) = \Phi(x, t) + \int_0^t \ddot{D}(\tau) \frac{D'(\tau)}{4\pi D(t-\tau)^{1/2}} \gamma(\tau) d\tau + \int_0^t \int_0^\infty \Phi(s, \tau) \psi(s, \tau) ds d\tau \tag{51} \]

where

\[ \gamma(\tau) = x - u(t-\tau) \exp \left[ -\frac{(x-u(t-\tau))^2}{4D(t-\tau)} \right] \tag{52} \]

\[ \psi(\tau, s) = \frac{1}{2D(t-\tau)} \left\{ \exp \left[ -\frac{(x-u(t-\tau)-s)^2}{4D(t-\tau)} \right] \right. \\
\left. \times \left[ 1 + \frac{(x-u(t-\tau)-s)^2}{2D(t-\tau)} \right] + \exp \left[ -\frac{(x-u(t-\tau)+s)^2}{4D(t-\tau)} \right] \right\} \tag{53} \]

From this expression we can generate sample functions. The mean value of the concentration is obtained by taking expectations on both sides of equation (51) and using equation (21):

\[ E[C(x, t)] = \Phi(x, t) \tag{54} \]

In order to calculate the concentration variance we use equations (13), (21) and (51). After some algebraic manipulation we obtain

\[ E[(C - \Phi)^2] = \sigma_c^2 \]

\[ = q \int_0^\infty \frac{\gamma^2(\tau)}{4\pi D(t-\tau)^2} d\tau + 2q \int_0^\infty \int_0^\infty \psi(s, \tau) \Phi(s, \tau) ds d\tau \frac{\rho^2}{4\pi D(t-\tau)^2} d\rho \tag{55} \]

Higher order moments can be obtained in a similar manner.

Equations (19) and (51) through (55) were programmed in the micro-computer in order to obtain several numerical examples of the stochastic properties of the concentration. An average pore velocity \( u = 0.2 \) m/day, a mean dispersion coefficient \( D = 0.1 \) m\(^2\)/day, a concentration at the origin \( C_0 = 1.0 \) m\( \text{gr} \)/lit, and a variance parameter \( q = 0.1 \) were assumed. The integrals were numerically evaluated using 24 points Gauss-Legendre quadrature, which gives very accurate values for singular integrals. It was found that the space integrals converge very rapidly. Fig. 4 is a digital plotter output of the program for a point in space \( x = 6.0 \) m from the origin. It is interesting to note that as the observation distance increases the sample functions become smoother. The mean concentration coincides with the deterministic solution, whereas the sample concentration oscillates above and below the mean concentration with increasing distance from the mean as time increases. The exact measurement of the dispersion around the mean is given by the standard deviation function, which shows a direct monotonic increasing magnitude with time. Thus the results indicate a Brownian type of behaviour of the

![Graph](image)

**Fig. 4.** Stochastic concentration with time at \( X = 6.0 \) m

concentration with a continuously increasing variance value, as one might have expected. Thus we may conclude that a model such as the one presented in this section may explain the stochastic nature of the concentration in an aquifer.

4. CONCLUSIONS

A new methodology to model the time and space evolution of a contaminant in a system of aquifers was presented. The method is capable of handling the case when certain components of the model, such as the geohydrologic information, the boundary conditions, the magnitude and variability of the sources or physical parameters or a combination of the above are uncertain and defined in stochastic terms. The method is based on applications of modern mathematics to the solution of the resulting stochastic transport equations. It was found that this new methodology presents considerable advantages over the existing modelling methods. Thus the theory satisfies a more general modelling need by providing, if desired, a systematic global concentration information on the sample functions, the mean, the variance, correlation functions or higher-order moments based on a similar information of any "size", anywhere, of the input functions. This more realistic statistical representation of the concentration distribution is a valuable tool in designing and testing preventive or remedial alternatives by engineers and planners.

Several individual applications were shown in order to illustrate the methodology when the different cases of uncertainty appear in groundwater pollution problems. The method could be used to solve more difficult problems of groundwater pollution modelling subject to complex distributed sources.

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