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Contaminant transport modelling under random sources

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Abstract Contaminant transport modelling is characterized by severe uncertainty. The effects of this uncertainty are evident in the results of some post-audit studies, in which field conditions that have actually developed are compared with model predictions made years earlier. In general, studies of this type indicate that groundwater models have not enjoyed great success as predictive tools. While much discussion of model uncertainty has centred on spatial heterogeneity, it is possible that many of the failures have occurred primarily because the sources, which were eventually imposed in the field, differed from those represented in the simulations. This is because deterministic prediction of future conditions is often inaccurate due to the random nature of contaminant sources, in terms of their timing, locations, and magnitude. In this study, we develop a stochastic framework for accommodating random contaminant sources in conventional, deterministic transport models such as MT3D. We first classify the contaminant sources into two types: those occurring continuously with a deterministic component and random variations, and those occurring randomly at instantaneous discrete-time intervals. For the first type, the governing partial differential equation (PDE) is replaced by a stochastic PDE. The random variations are modelled by Brownian motion and the solution obtained by using Ito's integration technique. For the second type, Markovian analysis is used for discrete-time contamination events. Both approaches utilize a deterministic transport model to generate source response functions. The response functions are then integrated to yield probabilistic descriptions of contaminant transport, from which key statistical properties such as mean and variance can be drawn.

INTRODUCTION

Contaminant transport modelling is an essential component of any risk assessment and risk management pertinent to groundwater quality. However, it is recognised that contaminant transport modelling is associated with severe uncertainty. The effects of this uncertainty are evident in the results of some post-audit studies (e.g. Konikow, 1986; Anderson & Woessner, 1992), in which field conditions that have actually developed are compared with model predictions made years earlier. In general, studies of this type indicate that groundwater models have not enjoyed great success as predictive tools (e.g. Konikow & Bredehoeft, 1992). While much discussion of modelling uncertainty has centred on spatial heterogeneity in aquifer properties (e.g. Dagan, 1989; Gelhar, 1994; Dagan & Neuman, 1997), it is possible that many of the failures have occurred primarily because the sources which were eventually imposed in the field differed from those represented in the simulations. This is because deterministic prediction of future conditions is often inaccurate, due to the random nature of contaminant sources in terms of their timing, locations and magnitude.

In the absence of more effective methods to deal with uncertain sources, the Monte Carlo approach is generally used to make multiple predictive runs, each of which is based on one realization of the random function representing the contaminant source (Zheng & Bennett, 1995). While the approach is of general applicability, its utility in groundwater modelling and remediation assessment is limited by the intensive computational requirements. Analytical and numerical solutions that directly incorporate the random sources provide a more effective means for propagating the source uncertainties and for addressing these uncertainties in remediation designs.

In this study, we develop a stochastic framework for accommodating random contaminant sources in conventional, deterministic transport models such as MT3DMS (Zheng & Wang, 1998). We first classify the contaminant sources into two types: those occurring continuously with a deterministic component and random variations, and those occurring randomly at instantaneous discrete-time intervals. For the first type, the governing partial differential equation (PDE) is replaced by a stochastic PDE. The random variations are modelled by Brownian motion and the solution obtained by using Ito's integration technique. For the second type, Markovian analysis is used for discrete-time contamination events. Both approaches utilize a deterministic transport model to generate source response functions. The response functions are then integrated to yield probabilistic descriptions of contaminant transport from which key statistical properties such as mean and variance are drawn.

CHARACTERIZATION OF RANDOM SOURCES

Continuous-time random contaminant sources

A continuous-time random source, $C_s(t)$, may be expressed as Gaussian white noise (Gn):

$$C_s(t) = c_s(t) + \sigma n(t) \tag{1}$$

where $c_s(t)$ is a deterministic function of time t representing the mean, σ represents the standard deviation, and $n(t)$ is a random variable following a standard normal distribution, or the Gaussian white noise.

Strictly speaking, any sample path of Gn $\{n(t), t \geq 0\}$ is uncorrelated and nowhere continuous. Thus, the white noise is only an idealised mathematical model. A more appropriate model for a continuous random source is Brownian motion (Bm) (or Wiener process):

$$C_s(t) = c_s(t) + \sigma W(t) \tag{2}$$

where the Brownian motion $W(t)$ is defined as the integral of a Gn, $W(t) = \int_0^t n(s)\mathrm{d}s$.

Figure 1 shows a realization of a random source modelled as a Bm. One important property of Brownian motion is that, at any time, it follows a normal distribution, which is completely determined by the mean and variance/covariance of the under-

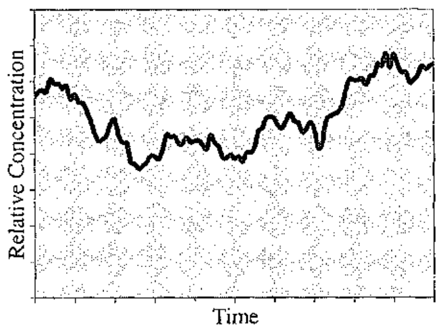

Fig. 1 A realization of continuous-time contaminant source.

lying process. Since linear operation on random variables with normal distributions still has a normal distribution, the computation is significantly simplified. The linear operations include linear combination of a number of variables, differentiation, and integration.

Discrete-time random contaminant sources

When the contaminant is released into the aquifer instantaneously at discrete-time points, the resulting concentration field does not have a continuous-time Gaussian process, which makes the problem much more complex to analyse. The total cumulated contaminant released into the aquifer is the sum of a random number of incidents, $\sum_{i=1}^{N(t)} C_{si}$, where $N(t)$ is the number of contamination events that occurred during the time interval [0, t], and C_{si} is the random amount of the contaminant released into the aquifer each time. Figure 2 illustrates a realization of the random, discrete-time contamination events. These random events consist of two random sequences: the timing $\{t_1, t_2 .. t_n\}$ and the magnitude $\{C_{s1}, C_{s2} ..., C_{sn}\}$.

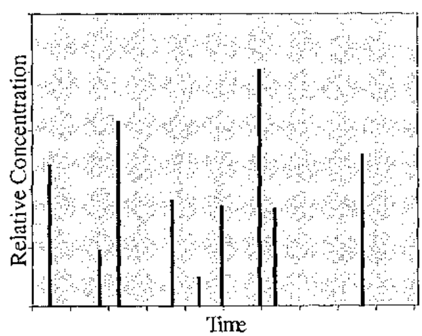

Fig. 2 A realization of discrete-time contaminant source.

In general, a random contamination event can occur at any time point. Furthermore, these events may not be dependent on one another. Under these assumptions of stationary and independent increments, the number of events $N(t)$ can be characterized by a Poisson process. That is, the probability of n contamination events occurring by time t has a Poisson distribution given by:

$$\Pr\{N(t)=n\}=\frac{(\lambda t)^n}{n!}\mathrm{e}^{-\lambda t}, \quad t\geq 0, n=0,1,2,... \tag{3}$$

where λ [T^{-1}] is the frequency of contamination events expressed in terms of the number of contamination events per unit of time. For example, if a study site is contaminated, on the average, five times per year (each contaminant event is assumed to be instantaneous), then λ = 5 year^{-1}. In addition, the two sequences of timing $\{t_1, t_2 ..., t_n\}$ and magnitude of releases $\{C_{s1}, C_{s2} ..., C_{sn}\}$ are considered independent so that the total amount of contaminant mass is a compound Poisson process. Using Markovian analysis, we can find statistical properties of the resulting solution. After the timing sequence is defined, the magnitude of the source can be described by a probability distribution function (PDF). Some commonly used PDFs are negative exponential, constant, uniform, and normal.

INCORPORATION OF RANDOM SOURCES INTO TRANSPORT MODELS

Ito's stochastic differential equations for continuous-time sources

Denote by L the linear operator in the transport governing equation as:

$$L=\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial}{\partial x_j}\right)-\frac{\partial}{\partial x_i}(v_i)-\beta \tag{4}$$

where D_{ij} is the dispersion coefficient tensor, v_i the linear velocity of the groundwater flow, and β the first-order reaction rate. We can then rewrite the transport governing equation as a stochastic differential equation (SDE):

$$\mathrm{d}C=L(C)\mathrm{d}t+\left(q_s C_s/\theta\right)\mathrm{d}t \tag{5}$$

where q_s is the sink/source flux, θ the aquifer porosity and C_s the random solute source concentration. C_s may be modelled as a Gaussian white noise or Brownian motion as shown in equations (1) and (2).

The SDE involving Gaussian white noise is referred to as Ito's stochastic differential equation. Thus, the SDE defined in equation (5) can be solved by using Ito's integration. Because of the linearity of equation (4), the resulting spatial-varying time-dependent solution will also have a normal distribution that enables us to compute the mean, standard deviation, covariance, and other statistical properties of the concentration field.

In a contaminant transport model with a deterministic source $C_s(t)$, the concentration $C(x,t)$ can be generally expressed as an integral of the source function $C_s(t)$ and a response function r (Bear, 1972; Wexler, 1986):

$$C(x,t)=\int_0^t C_s(\tau)r(x,t-\tau)\,\mathrm{d}\tau \tag{6}$$

where r is the (impulse) response function; x is one-, two-, or three-dimensional coordinates. The response function r is the solution of the concentration field due to an instantaneous solute source that occurs at time zero and has unit magnitude. The integral form can be interpreted as the limit of the sum of the products of the source at time τ and its response function from time τ to t:

$$C(x,t) = \int_0^t R(x,t-\tau)\mathrm{d}C_s(\tau) \tag{7}$$

where $R(t) = \int_0^t r(s)\mathrm{d}s$ is the (step) response function to a constant, continuous source of unit magnitude at $t = 0$. Equation (7) is in the form of Reimann-Stieltjes integrals.

For the contaminant source following a Brownian motion, we can substitute equation (2) into (7) to obtain the general solution:

$$C(x,t) = \int_0^t c_s(\tau)R(x,t-\tau)\mathrm{d}\tau + \int_0^t \sigma(\tau)R(x,t-\tau)\,\mathrm{d}W(\tau) \tag{8}$$

with the mean, variance, and covariance functions given below:

$$E[C(x,t)] = \int_0^t c_s(\tau)R(x,t-\tau)\,\mathrm{d}\tau \tag{9}$$

$$\mathrm{Var}[C(x,t)] = \int_0^t \sigma^2(\tau)R^2(x,t-\tau)\,\mathrm{d}\tau \tag{10}$$

$$\mathrm{Cov}[C(x_1,t_1),C(x_2,t_2)] = \int_0^t \sigma^2(\tau)R(x_1,t-\tau)R(x_2,t-\tau)\,\mathrm{d}\tau, \quad t = \min(t_1,t_2) \tag{11}$$

Markovian analysis of discrete-time sources

When the contamination events occur only at random instantaneous times and each time a random amount of contaminant mass is brought into the aquifer, the resulting process is not a Gaussian process. Markovian analysis provides a useful, efficient tool for such discrete-event dynamic systems (Ho & Cao, 1991). Under general assumptions, the contaminant level at time t can be written as:

$$C(x,t) = \sum_{i=1}^{N(t)} C_{si}r(x,t-\tau_i) \tag{12}$$

This so-called filtered Poisson process has many elegant results that have been known for years (e.g. Parzen, 1962). The methods used in analysing Poisson-related processes are integral transform methods such as Laplace transforms (LT). For a given distribution of the magnitude C_s, the LT of $C(x,t)$ can be derived following a similar procedure outlined in Parzen (1962, p. 146):

$$\mathrm{LT}\{C(x,t)\} = \exp\left\{\lambda\int_0^t E\left[\mathrm{e}^{-sC_s r(x,\tau)} - 1\right]\mathrm{d}\tau\right\} \tag{13}$$

The mean, variance/covariance functions, and other statistical measurements are available from the above LT after algebraic computation. For example:

$$E[C(x,t)] = \lambda E(C_s)\int_0^t r(x,\tau)\,\mathrm{d}\tau \qquad (14)$$

$$Var[C(x,t)] = \lambda E(C_s^2)\int_0^t r^2(x,\tau)\,\mathrm{d}\tau \qquad (15)$$

AN ILLUSTRATIVE EXAMPLE

To illustrate the approaches discussed above, consider two-dimensional advective-dispersive transport in a uniform flow field of infinite extent. The seepage velocity is 5 m day^{-1} and longitudinal and transverse dispersion coefficients are 5 and 1 m^2 day^{-1}, respectively. The Bm random source has a mean concentration of 1 ppm and a standard deviation of 0.2. The source injection flow rate is 12.5 m^3 day^{-1} m^{-3} and the aquifer porosity is 0.25. One realization of the random source and calculated concentrations at a receptor 50 m downgradient of the source are shown as the solid line and open circles, respectively, in Fig. 3. It can be seen that the calculated concentrations are less variable than the source function due to dispersion. The mean and standard deviation of the concentration solution are also shown in Fig. 3 as cross-patterned and dashed lines. Note that the uncertainty of the solution in terms of the standard deviation grows with time. For this simple problem, the response function is available analytically. For more complex problems involving spatial heterogeneity, a numerical simulator is needed to obtain the response function.

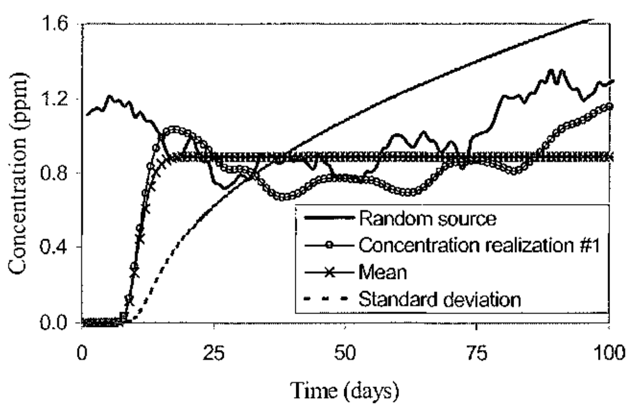

Fig. 3 Mean, standard deviation and one realization of calculated concentrations at a receptor 50 m downgradient of the random source.

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