

Contaminant Transport Models Under Random Sources

by P. Patrick Wang¹ and Chunmiao Zheng²

Abstract

While the discussion of model uncertainty has centered on spatial heterogeneity, it is possible that ground water models have not enjoyed much success as predictive tools often because the sources that 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, location, and magnitude. This paper presents a stochastic framework for accommodating random contaminant sources in conventional, deterministic advection-dispersion transport models. The contaminant sources are first classified 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 modeled by Gaussian noise or Brownian motion, and the solution is obtained by using Ito's integration technique. For the second type, Markovian analysis is used for discrete-time contamination events. Both approaches use a deterministic transport model to generate response functions at any observation location and time. The response functions are then integrated to yield probabilistic description of contaminant transport, from which key statistical properties such as mean, standard deviation, and confidence interval can be drawn.

Introduction

Contaminant transport modeling is an essential component of any risk assessment and risk management pertinent to ground water quality. However, it is recognized that contaminant transport modeling is associated with large uncertainty. The effects of this uncertainty are evident in the results of some postaudit studies (e.g., Konikow 1986; Anderson and 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 ground water models have not enjoyed great success as predictive tools (e.g., Konikow and Bredehoeft 1992; Oreskes et al. 1994; Zheng and Bennett 2002). While much discussion of modeling uncertainty has centered on spatial heterogeneity in aquifer

properties (e.g., Dagan 1989; Gelhar 1994; Zhang and Neuman 1995; Dagan and Neuman 1997; Zhang 2002; Rubin 2003), it is possible that many of the failures have occurred primarily because the sources that were eventually imposed in the field differed from those represented in the simulations (de Marsily et al. 1992). This is because deterministic prediction of future conditions is often impossible, due to the random nature of contaminant sources, in terms of timing, location, and magnitude. Clearly, for contaminant transport modeling to become a more reliable and useful tool in long-term, risk-based assessment of ground water quality, it is imperative that sound theoretical frameworks and practical tools be developed to deal with random contaminant sources in a systematic and rigorous manner.

Research on the uncertainty of contaminant sources has not received adequate attention in the literature. Most of the earlier published work in this area addressed the effects of spatially random recharge or leakage on hydraulic head and flow distributions (e.g., Rubin and Dagan 1987; Hantush and Mariño 1994a, 1994b). In recent years, interests in random source-related problems have increased (e.g., Cinlar and Kao 1991; Skaggs and Kabala 1994, 1995; Ramaswami and Small 1994; Snodgrass and

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Received December 29, 2003; accepted August 26, 2004.

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Kitanidis 1997; Neupauer and Wilson 2001, 2002). Cinlar and Kao (1991) studied random flows of particles in a random field. Particles enter the field at random times and places. Each particle is carried by the flow for some random amount of time and then leaves the field. Skaggs and Kabala (1994, 1995) investigated the problem of identifying the history of contaminant releases in the past. More recently, Snodgrass and Kitanidis (1997) used a geostatistical approach to identify the contaminant source. The past contamination event was treated as an unknown time-dependent function. From the data obtained at the observation wells, the unknown function was estimated using the least squares and other more sophisticated methods. Neupauer and Wilson (2001, 2002) presented a backward probabilistic model that can provide information about the former location of contamination in a nonuniform, transient flow field.

A random source may be in the form of random timing, random location, and random amount of mass loading. Ramaswami and Small (1994) assumed that the aquifer of interest had a random number of contaminant sources. They investigated the spatial variation in the concentration of a nonreactive solute, resulting from the random variation in the spatial location and discharge rate associated with the source areas in the subsurface medium. In their study, the number of contaminant sources in the aquifer was assumed to be a random variable following a Poisson distribution. Each contaminant source was randomly located in the space with a continuous, constant injection rate. Analytical solutions were given for the mean, variance, and covariance of steady-state concentration in a homogeneous aquifer.

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 (e.g., Zheng and Bennett 2002). While the approach is of general applicability, its utility in ground water modeling and remediation assessment is limited by the intensive computational requirements. Analytical and numerical solutions that directly incorporate random sources provide a more effective means for propagating the source uncertainties and for addressing these uncertainties in contaminant transport modeling and remediation assessment.

The primary goal of this paper is to develop a stochastic approach for dealing with random contaminant sources. To accomplish it, we will first categorize the random sources into two types: those occurring continuously with a deterministic component and random variations and those occurring randomly at instantaneous, discrete-time instances. For the continuous source, the random source is assumed to have a deterministic term plus a noise term. The noise part is modeled as a Gaussian white noise (Gn) or a Brownian motion (Bm). For the discrete-time random source, a stochastic approach referred to as the discrete-event dynamic systems (DEDS) (Ho and Cao 1991) will be employed.

In the subsequent discussions, we will first define the contaminant transport model used in this study and introduce the concepts of Bm and DEDS. Next, we discuss

how to incorporate the random sources into the contaminant transport model. Finally, we use simple examples to illustrate the concepts and techniques presented in the paper. More detailed mathematical derivations are provided in the appendices for interested readers.

Stochastic Transport Models with Random Sources

Contaminant Transport Model

The partial differential equation (PDE) for transport of a conservative contaminant in a saturated medium can be expressed as (Zheng and Bennett 2002):

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_i} (v_i C) + \frac{q_s}{\theta} C_s \quad (1)$$

where C is the concentration of the contaminant, D_{ij} the dispersion coefficient tensor, v_i the linear velocity of ground water flow, θ the effective porosity, q_s the sink/source flow rate, and C_s the concentration of the sink/source flux.

Equation 1, along with a set of initial and boundary conditions, forms the mathematical model of contaminant transport. When those conditions and the aquifer properties are known, the solution of the concentration distribution can be uniquely determined either analytically for simple cases or numerically for general cases. When the source term C_s is a time-dependent random process, however, the aforementioned PDE becomes a stochastic PDE and its solution has to be in the form of either probability cumulative distribution function (CDF) or probability density function (PDF). To focus on the random contamination sources, we assume that the dispersion coefficient, flow velocity, and other aquifer properties are deterministic variables and can be completely defined. The random contaminant sources are characterized by the timing, the magnitude, and the location of the contamination events that will be discussed subsequently.

From the CDF (or PDF) of the solution of Equation 1, important statistical quantities such as the mean, standard deviation, and covariance are obtained so that we are able to quantify contaminant transport under uncertainty. A typical question that can be answered from the solution would be the following: At any time in the future, what is the chance that a region Ω of interest in the aquifer will be contaminated? Or specifically, what is the probability that the contaminant concentration is below the standard level c_0 set by a regulator? This may be expressed mathematically as

$$F(x, c_0, t) = \Pr \{ C(x, t) \leq c_0 \}, x \in \Omega \quad (2)$$

The function F describes the contaminant level at any time t and location x . In remediation design, we may be interested in how to determine the injection/extraction rates so that a desired confidence interval, say at the 90% significant level, is achieved for the long run:

$$\lim_{t \rightarrow \infty} \Pr \{ C(x, t) \leq c_0 \} = 90\%, x \in \Omega \quad (3)$$

Both analytical and numerical solutions can be derived for the transport model as expressed in Equation 1 subject to random sources. Analytical solutions provide valuable insights into transport behavior and are useful as screening tools. This paper focuses on analytical solutions under simple aquifer conditions. For a general three-dimensional aquifer, the transport solutions can be obtained numerically in conjunction with a general transport simulator such as MT3DMS (Zheng and Wang, 1999).

Characterization of Random Sources

A contaminant source may contain three random components: timing, amount, and location. The timing is when a contamination event occurs; the amount is how much contaminant mass is released into the aquifer when it occurs; the location is where the incident happens. In this work, only the timing and magnitude of the contaminant source term are treated as random variables. The source location is either known or can be identified through an inverse modeling procedure (e.g., Neupauer and Wilson 2001, 2002). We also assume that the probabilistic distributions of the random contaminant releases are known or at least the means and variances can be estimated. For example, the normal distribution is often a robust assumption for the magnitude of contaminant releases. The number of random contamination events is usually assumed to follow a Poisson distribution, which is a reasonable assumption when the contamination sources are mutually independent.

The random contamination events and sources can be further characterized by two types and analyzed by different approaches depending upon the nature of the applications. The first type assumes that the contaminant source is persistently present. Such a continuous random source will be modeled by Bm, and its solution is sought by using Ito's stochastic integration techniques. The other type assumes that the contaminant events occur only at discrete-time instants and last for short periods of time. The underlying stochastic processes are no longer Gaussian. Markovian processes can then be employed (e.g., Ali Khan and Gain 1968). A combination of these two is that contamination events occur at random time instants and last for random amounts of time.

Continuous-Time Random Contaminant Source

The most frequently used model is the Gn. In this case, the continuous-time random source is written as

$$C_s = c_s(t) + \sigma n(t) \quad (4)$$

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, the Gaussian noise. These noises are independent of one another. Figure 1a illustrates a realization of the random source following a Gn with a constant mean $c_s(t) = 1$ ppm and a standard deviation $\sigma = 0.2$ ppm.

Strictly speaking, any sample path of Gn $\{n(t), t \geq 0\}$ is uncorrelated and nowhere continuous. Thus, the white noise is just an idealized mathematical model. In practice, the sample paths are dependent. Thus, a

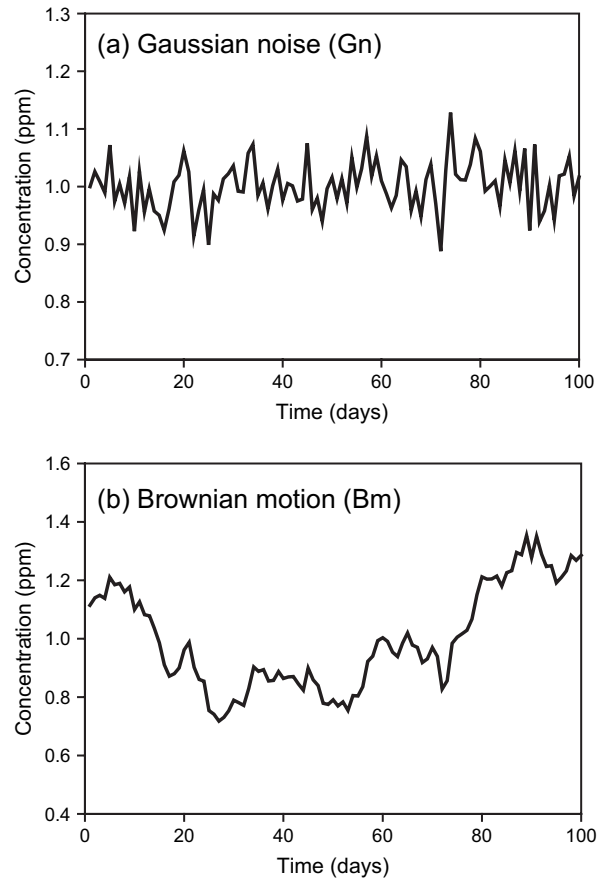


Figure 1. Illustration of a continuous-time contaminant source modeled as (a) Gaussian noise (Gn) and (b) Brownian motion (Bm). The source has a mean concentration of 1 ppm and a standard deviation of 0.2 ppm.

continuous random source can be modeled as a Bm (or Wiener process), which is often written in a differential form as

$$dC_s(t) = c_s(t)dt + \sigma dW \quad (5)$$

with $C_s(0) = c_{s0}$, $W(0) = 0$. Here, the Bm $W(t)$ is defined as the integral of a Gn

$$W(t) = \int_0^t n(s)ds \quad (6)$$

Alternatively, the differential form is $dW = n(t)dt$.

Figure 1b gives a realization of the random source modeled as a Bm with the same parameters as in Figure 1a, i.e., constant mean $c_{s0} = 1$ ppm; $c_s(t) = 0$, for $t > 0$; and standard deviation $\sigma = 0.2$ ppm. Both sample paths use the same random number sequence for comparison purposes. One can clearly see that the sample path of Bm is much smoother than that of Gn.

One important property of Bm is that, at any time, it follows a normal distribution, which is completely determined by the mean and variance/covariance of the underlying process. Since a linear operation on random variables with normal distributions still yields 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 does not have a continuous-time Gaussian process, which makes the problem much more complex to analyze. The total amount of cumulative contaminant released into the aquifer is the sum of a random number of incidents:

$$\sum_{i=1}^{N(t)} C_{si} \quad (7)$$

where $N(t)$ is the number of contaminant releases that occurred during the time interval $[0, t]$ and C_{si} is the random amount of contaminant each time released into the aquifer. Figure 2 illustrates a realization of the random, discrete-time contamination events. These random events consist of two random sequences: the timings $\{t_1, t_2, \dots, t_n\}$ and the magnitudes $\{C_{s1}, C_{s2}, \dots, C_{sn}\}$.

Generally speaking, a random contamination event has the same probability of occurrence at any point in time. Also, these events are independent from each other. Under these assumptions of stationary and independent increments, the number of events $N(t)$ can be characterized by the Poisson process. That is, the probability that n contamination events occurred by time t has a Poisson distribution given by

$$\Pr\{N(t) = n\} = \frac{(\lambda t)^n}{n!} e^{-\lambda t}, t \geq 0, n = 0, 1, 2, \dots \quad (8)$$

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 the study site is contaminated, on the average, five times per year (each contamination event is assumed to be instantaneous), then $\lambda = 5/\text{year}$. In addition, those two sequences of timing and magnitude of releases are independent so that the total amount of contaminant mass given in Equation 7 is a compound

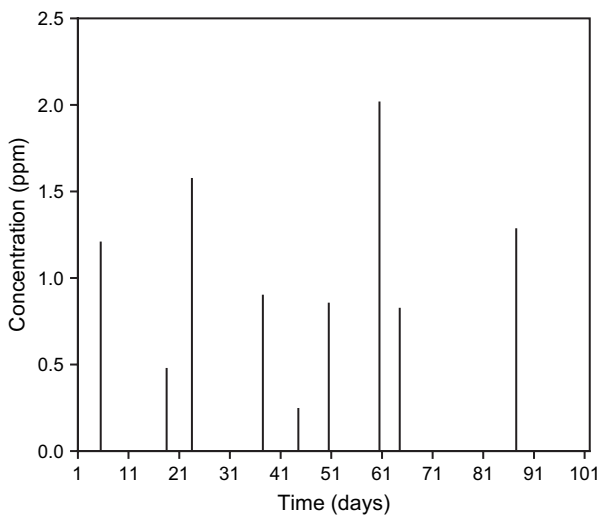


Figure 2. An illustration of a discrete-time contaminant source with random timing and magnitude. The source has a mean of 1 ppm and a standard deviation of 0.5441 ppm. The frequency of occurrence is 0.1/d.

Poisson process. Using Markovian analysis, we can find statistical properties of solution C .

Although Bm and Poisson process have completely different distributions, they share many properties. First, both have the property of independent increments; the changes, or increments, between two disjoint time intervals are two independent random variables. Second, both possess the property of stationary increments; they have no preference between time intervals. In other words, they are homogeneous in time domain. Third, both are Markov processes with the important memory-less property. The Poisson process has been widely used in mathematical modeling because it simplifies the mathematical derivation and computational implementation as shown in the following discussion.

After defining the timing sequence, let us now describe the probability distribution of the source magnitude. Once a contamination event occurs, a random amount of contaminant mass is released into the aquifer. Let Z denote the random amount of contaminant mass released into the aquifer in a random contamination incident, and $B(z)$ and $b(z)$ the CDF and PDF of Z , respectively, i.e., $B(z) = \Pr\{Z \leq z\}$ and $b(z) = dB(z)/dz$. Some commonly used CDFs are negative exponential, constant, uniform, and normal as shown subsequently:

1. Negative exponential distribution

$$B(z) = 1 - e^{-\mu z}, z \geq 0 \quad (9)$$

The mean is $E(Z) = 1/\mu$ and variance $\text{Var}(Z) = 1/\mu^2$.

2. Constant distribution

$$B(z) = 1, z \geq z_0 \\ = 0, \text{ otherwise} \quad (10)$$

The mean is z_0 and variance 0.

3. Uniform distribution

$$B(z) = 0, z < a \\ = \frac{z-a}{b-a}, a \leq z \leq b \\ = 1, z > b \quad (11)$$

The mean is $E(Z) = (a + b)/2$ and variance $\text{Var}(Z) = (b-a)^2/12$.

4. Normal distribution

$$B(z) = \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^z e^{-\frac{(y-\mu)^2}{2\sigma^2}} dy \quad (12)$$

The mean is $E(Z) = \mu$ and variance $\text{Var}(Z) = \sigma^2$.

Incorporation of Random Sources in Transport Models

Ito's Stochastic Differential Equations

For a random source with white noise, the problem is modeled using Ito's stochastic differential equation. Although the PDE in Equation 1 is a spatial-varying, time-dependent function, essentially it is a linear function of the concentration C . Denoting by L the linear operator in Equation 1 as

$$L = \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial}{\partial x_j} \right) - \frac{\partial}{\partial x_i} v_i \quad (13)$$

we can then rewrite the PDE as a stochastic differential equation (SDE) as

$$dC = L(C)dt + \frac{q_s}{\theta} dC_s \quad (14)$$

where the random solute source C_s may be modeled as a Gn or Bm as discussed previously.

The SDE involving Gn is referred to as Ito's stochastic differential equation. Thus, the SDE defined in Equation 14 is under the Ito's sense and thus can be solved by using Ito's integration (Soong 1973). For some special cases where the SDE is reducible (Gard 1988), analytical solutions exist. Because of the linearity of Equation 13, 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 1992; Park and Zhan 2001)

$$C(x,t) = \int_0^t C_s(\tau) r(x,t-\tau) d\tau \quad (15a)$$

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 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 . The aforementioned solution form can be written in a number of equivalent statements after substitution of integral variables and simple algebraic manipulation as derived in Appendix A:

$$C(x,t) = \int_0^t C_s(t-\tau) r(x,\tau) d\tau \quad (15b)$$

$$C(x,t) = \int_0^t C_s(t-\tau) d_\tau R(x,\tau) \quad (15c)$$

$$C(x,t) = C_s(0)R(t) + \int_0^t R(x,t-\tau) dC_s(\tau) \quad (15d)$$

where $R(x,t) = \int_0^t r(x,s) ds$ is the (step) response function to a constant, continuous source of unit magnitude at time zero. Equations 15c and 15d are in the form of Riemann-Stieltjes integrals.

For a Gn contaminant source, the solution form of the SDE can be obtained after substituting Equation 5 into Equation 15a and using the fact that $dW = ndt$

$$C(x,t) = \int_0^t c_s(\tau) r(x,t-\tau) d\tau + \int_0^t \sigma(\tau) r(x,t-\tau) dW(\tau) \quad (16)$$

Note that both mean c_s and standard deviation σ are explicitly expressed as time-dependent functions. The

first integral in the solution gives the deterministic portion (or the mean of the solution), and the second term is an Ito's stochastic integral representing the variation of the solution. Analytical response function r can be obtained for simple aquifers that will be discussed in the next section; numerical solution probably is the only choice for complex situations. From the general solution form in Equation 16, we can compute the mean, variance, and covariance function of concentrations at two different locations and time points as given in integral forms (see Appendix A for derivation):

$$E[C(x,t)] = \int_0^t c_s(\tau) r(x,t-\tau) d\tau \quad (17)$$

$$\text{Var}[C(x,t)] = \int_0^t \sigma^2(\tau) r^2(x,t-\tau) d\tau \quad (18)$$

$$\text{Cov}[C(x_1,t_1), C(x_2,t_2)] = \int_0^{t=\min(t_1,t_2)} \sigma^2(\tau) r(x_1,t_1-\tau) r(x_2,t_2-\tau) d\tau, \quad (19)$$

For the contaminant source following a Bm, we use the solution form Equation 15d:

$$C(x,t) = c_{s0} R(x,t) + \int_0^t c_s(\tau) R(x,t-\tau) d\tau + \int_0^t \sigma(\tau) R(x,t-\tau) dW(\tau) \quad (20)$$

Now the mean, variance, and covariance functions can be computed in a similar manner:

$$E[C(x,t)] = \int_0^t c_s(\tau) R(x,t-\tau) d\tau \quad (21)$$

$$\text{Var}[C(x,t)] = \int_0^t \sigma^2(\tau) R^2(x,t-\tau) d\tau \quad (22)$$

$$\text{Cov}[C(x_1,t_1), C(x_2,t_2)] = \int_0^{t=\min(t_1,t_2)} \sigma^2(\tau) R(x_1,t_1-\tau) R(x_2,t_2-\tau) d\tau, \quad (23)$$

Markovian Analysis of Poisson Processes

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 DEDS. Under general assumptions, the contaminant level at time t can be written as a random sum of the response functions:

$$C(x,t) = \sum_{i=1}^{N(t)} C_{si} r(x,t-\tau_i) \quad (24)$$

This so-called filtered Poisson process has many elegant results (e.g., Parzen 1962; Ross 1996). The methods used in analyzing 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, page 146):

$$\text{LT}\{C(x,t)\} = \exp \left\{ \lambda \int_0^t E \left[e^{-sC_s r(x,\tau)} - 1 \right] d\tau \right\} \quad (25)$$

where λ has been defined for Equation 8.

The expectation inside the integral is taken on the random source C_s . The mean, variance/covariance functions, and other statistical measurements are available from the above LT after algebraic computation. For example, the mean and variance of $C(x,t)$ are, respectively, derived in integral forms that can be evaluated analytically or numerically:

$$E[C(x,t)] = \lambda E(C_s) \int_0^t r(x,\tau) d\tau \quad (26)$$

$$\text{Var}[C(x,t)] = \lambda E(C_s^2) \int_0^t r^2(x,\tau) d\tau \quad (27)$$

Note that the random variable C_s is not a time-dependent function. Thus, it is moved out of the integrals.

One can see that the response functions r and R play an important role in continuous-time, Gaussian processes and discrete-time, non-Gaussian processes. Once they are known, the statistical properties of the process can be calculated, from which the confidence intervals mentioned previously can be estimated for risk-based assessment.

Illustrative Examples

One-Dimensional Case

Consider solute transport in a one-dimensional semi-infinite aquifer with a constant flow velocity and dispersion coefficient. The governing PDE is given by

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} \quad (28)$$

The initial condition is given as follows

$$C(x,0) = 0, \quad x \geq 0 \quad (29)$$

and the boundary conditions are

$$qC - \theta D \frac{\partial C}{\partial x} = q_s C_s, \quad x = 0 \quad (30)$$

$$C(\infty, t) = 0$$

where q_s and C_s are the fluid inflow rate and concentration of a Bm random source specified as a third-type boundary condition at the origin. The (step) response function R has a closed form given by Wexler (1992):

$$R(x,t) = \frac{1}{2} \text{erfc} \left[\frac{x-vt}{2\sqrt{Dt}} \right] + \sqrt{\frac{v^2 t}{\pi D}} \exp \left[-\frac{(x-vt)^2}{4Dt} \right] - \frac{1}{2} \left(1 + \frac{vx + v^2 t}{D} \right) \exp \left(\frac{vx}{D} \right) \text{erfc} \left[\frac{x+vt}{2\sqrt{Dt}} \right] \quad (31)$$

where $\text{erfc}()$ represents the complimentary error function defined as

$$\text{erfc}(x) = 1 - \frac{2}{\sqrt{\pi}} \int_0^x \exp(-y^2) dy \quad (32)$$

The mean of the Bm random source C_s is 1 ppm and the standard deviation is 0.2 ppm as shown in Figure 1b. The flow velocity and dispersion coefficient are 0.5 m/d and 0.5 m²/d, respectively. The concentrations at two observation points located 5 and 10 m from the source are integrated from the response and source functions. Figure 3 shows the breakthrough curves at the two observation points as compared with the source function. Note that both the source and breakthrough curves at the observation points represent one realization of a probabilistic distribution. While the breakthrough curves at both observation points exhibit significant variations as a reflection of the Bm source, it can be seen that closer to the source, the more variable is the concentration distribution. This is expected as the dispersion acts to dampen the concentration variation.

To show the effect of flow velocity on the uncertainty of calculated concentrations, the standard deviation of calculated concentrations at an observation point located 10 m from the source is plotted in Figure 4 as a function of flow velocity under different observation times. This set of results is based on the same Bm random source as shown in Figure 1b. The uncertainty associated with the random source is propagated from the source location to the observation point. The concentration standard deviation at the observation point is dictated by the uncertainty at the random source, but it is also controlled by the flow velocity. Figure 4 shows that the larger the flow velocity is, the more uncertainty at the source is propagated to the observation point. Furthermore, a higher amount of uncertainty is propagated as time goes on.

Figure 5 shows the effect of dispersion coefficient on the uncertainty of calculated concentrations at the same

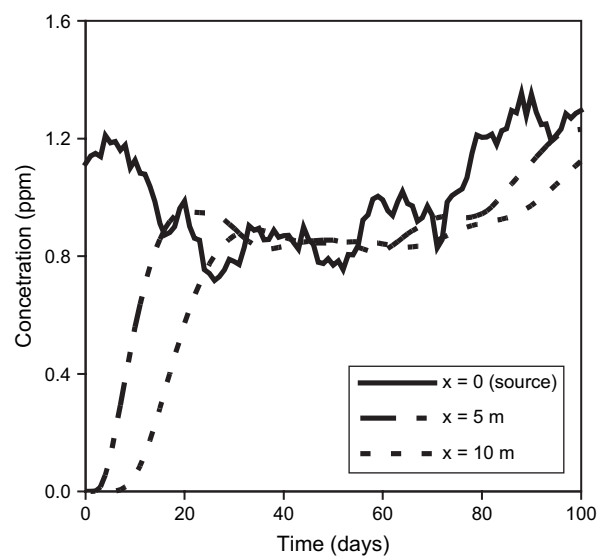


Figure 3. A random source realization and the resulting concentration breakthrough curves at two observation points 5 and 10 m from the source in a one-dimensional aquifer. Aquifer properties are given in the text. The random source follows a Bm as shown in Figure 1b.

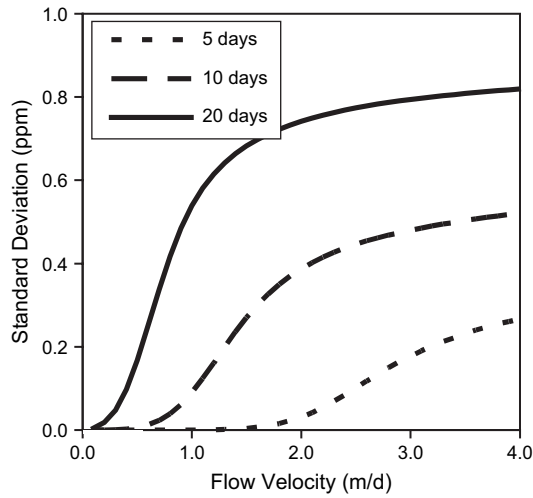


Figure 4. Standard deviation of calculated concentrations as a function of flow velocity for a Bm source at an observation point 10 m from the source. Other parameters are identical to those given for Figure 3.

location point. The flow velocity is fixed at 0.5 m/d, while all other parameters are identical to those shown in Figure 4. Similar to the effect of flow velocity, the standard deviation of calculated concentrations also increases with the dispersion coefficient, but the rate of change appears slower. This indicates that the uncertainty propagation is more sensitive to the flow velocity (advection) than dispersion coefficient (dispersion) for this test example at the selected observation times.

Two-Dimensional Case

Continuous-Time Random Source

The governing PDE for transport in a two-dimensional aquifer of infinite areal extent with a constant flow

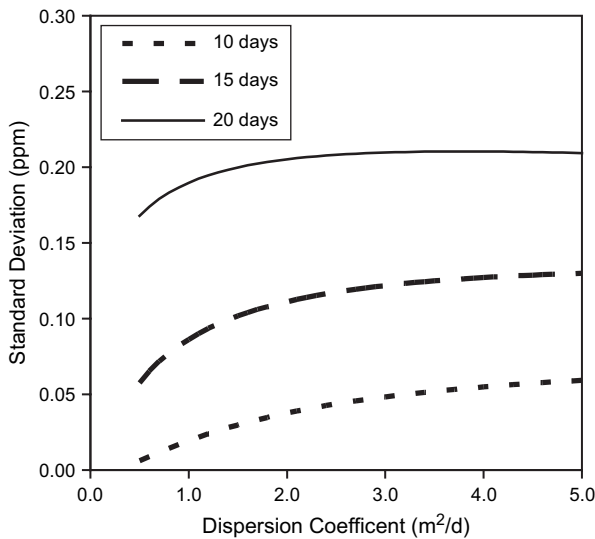


Figure 5. Standard deviation of calculated concentrations as a function of dispersion coefficient for a Bm source at an observation point 10 m from the source. Other parameters are identical to those given for Figure 3.

velocity and uniform dispersion coefficients is of the form:

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} - v \frac{\partial C}{\partial x} + \frac{q_s}{\theta} C_s \quad (33)$$

with the following initial and boundary conditions:

$$\begin{aligned} C(x, y, 0) &= 0 \\ \lim_{x, y \rightarrow \pm\infty} C(x, y, t) &= 0 \\ \lim_{x \rightarrow \pm\infty} \frac{\partial C}{\partial x}(x, y, t) &= 0 \\ \lim_{y \rightarrow \pm\infty} \frac{\partial C}{\partial y}(x, y, t) &= 0 \end{aligned} \quad (34)$$

where D_x and D_y are the longitudinal and transverse components of the dispersion coefficient. The flow velocity vector is assumed to align with the x axis.

The analytical solution to the problem as given in Equations 33 and 34 is available in Wexler (1992). The aquifer parameters used in this example are $D_x = 5 \text{ m}^2/\text{d}$, $D_y = 1 \text{ m}^2/\text{d}$, $v = 5 \text{ m/d}$, $q_s = 12.5 \text{ m}^3/\text{d}/\text{m}^3$, and $\theta = 0.25$. The analytical solution constitutes the response function required for integration with the source function to obtain the concentrations at any observation point and time.

Figure 6 shows the random source and two concentration breakthrough curves at 50 and 100 m directly downstream from the source along the x axis. The same Bm random source shown in Figure 1b is used in this example. It is clear that the farther away from the source, the less variation in the calculated concentrations, similar to the one-dimensional example shown in Figure 3. Note that both the source and resulting breakthrough curves shown in Figure 6 represent one realization of a probabilistic distribution.

Figure 7 shows the mean and upper and lower limits of the 90% confidence interval for the concentrations calculated at 50 m from the same Bm source. For

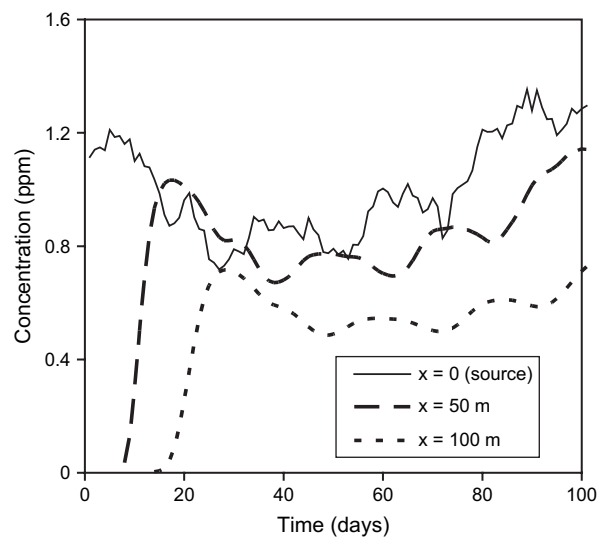


Figure 6. Concentration breakthrough curves at two observation points 50 and 100 m directly downstream from a Bm random source in a two-dimensional aquifer. Aquifer properties are given in the text. The Bm random source is the same as shown in Figure 1b.

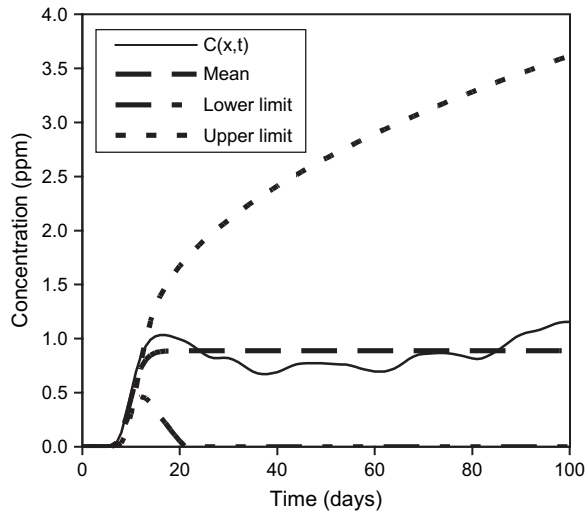


Figure 7. Calculated concentrations along with the mean and 90% confidence interval limits at an observation point 50 m directly downstream from a Bm point source in a two-dimensional aquifer. Other parameters are identical to those given for Figure 6.

comparison, the one realization of the concentration distribution at 50 m shown in Figure 6 is repeated in Figure 7. It is noteworthy that the upper limit of the 90% confident interval continues to increase with time, suggesting that the Bm source introduces more and more uncertainties into the transport solution.

Figure 8 shows the standard deviation of calculated concentrations at 50 m from the same Bm source as a function of flow velocity under different observation times. Again, the concentration standard deviation at the observation point is affected by the flow velocity that transports the uncertainty from the source location to the observation point. The dependency of the concentration

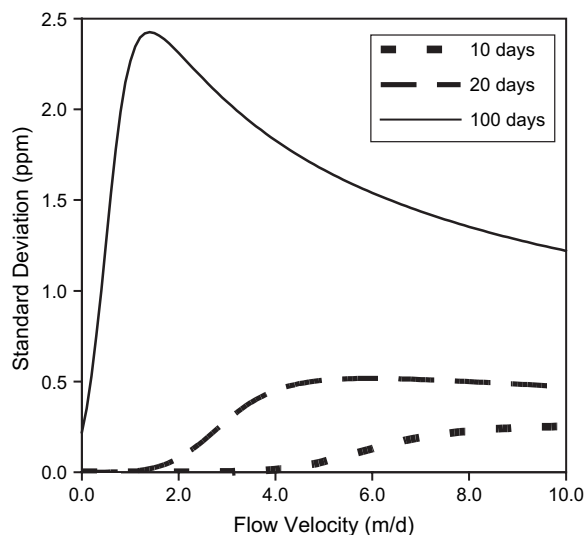


Figure 8. Standard deviation of calculated concentrations as a function of flow velocity for a Bm point source at an observation point 50 m directly downstream from the source. Other parameters are identical to those given for Figure 6.

standard deviation on flow velocity is quite different at different observation times. At a late time, the standard deviation reaches a peak at a specific velocity and then decreases with increasing velocities, while this phenomenon is not seen at earlier observation times. This suggests that the uncertainty at an observation point is the confluence of multiple factors, including the stochastic process at the random source, the timing and location of observation, and the transport process in the aquifer.

Figure 9 shows the standard deviation vs. the longitudinal dispersion coefficient D_x while the transverse dispersion coefficient is kept the same at $1 \text{ m}^2/\text{d}$. Again, the observation point is set at 50 m from the source. The standard deviation increases with the longitudinal dispersion coefficient at early times. However, at later times, the trend is reversed, with the standard deviation decreasing as the dispersion coefficient increases. This is primarily due to the stochastic nature of the random Bm source. It again demonstrates the complex nature of uncertainty at an observation point in response to a random Bm source. Thus, no general conclusions can be drawn from this and previous test problems regarding the dependency of the concentration uncertainty at an arbitrary observation location on any specific factors.

Discrete-Time Random Source

For this example, the discrete-time random source shown previously in Figure 2 is used. The source has a mean of 1 ppm and a standard deviation of 0.5441 ppm. The frequency of random events is 0.1/d. That is, on the average, one random contamination event occurs during a 10-d period. Except for the different source, all other parameters remain unchanged from those used in the aforementioned continuous-time case.

Figure 10 shows the concentration distribution for a high-velocity scenario ($v = 5 \text{ m/d}$), and Figure 11 shows

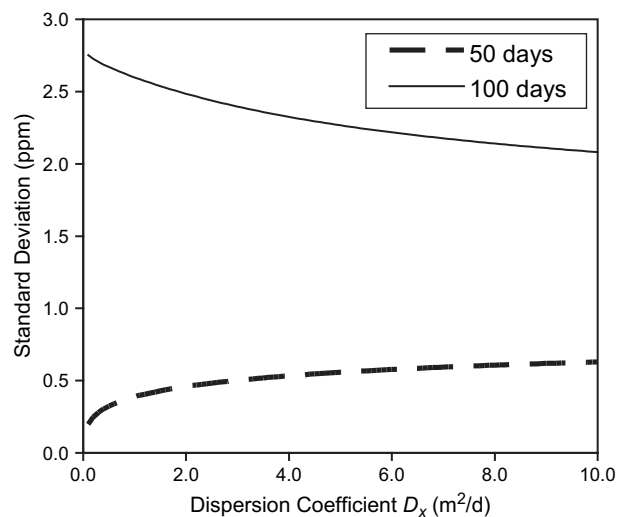


Figure 9. Standard deviation of calculated concentrations as a function of longitudinal dispersion coefficient for a Bm point source at an observation point 50 m directly downstream from the source. Other parameters are identical to those given for Figure 6.

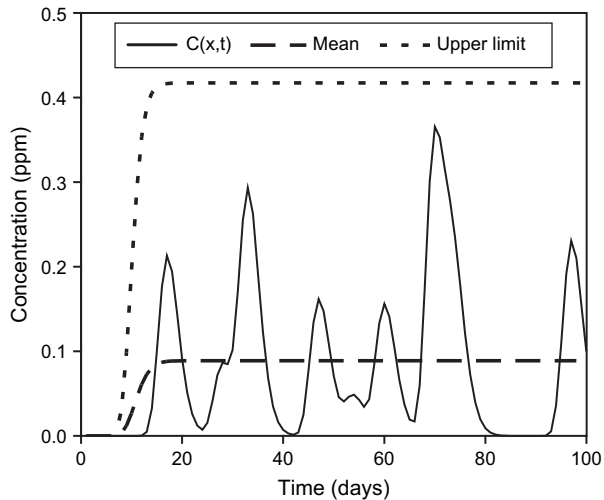


Figure 10. Calculated concentrations along with the mean and upper limit of 90% confidence interval at an observation point 50 m directly downstream from the source under a high-flow velocity scenario ($v = 5$ m/d). The discrete-time random source is the same as shown in Figure 2. Other parameters are identical to those given for Figure 6.

the concentration distribution for a low-velocity scenario ($v = 1$ m/d). The observation location is at 50 m directly downstream from the source. Although we can calculate the variance of the concentration at any location and time, the resulting probability distribution does not follow a normal distribution any more. Therefore, the upper limits of the 90% confidence interval given in Figures 10 and 11 are only an approximation. The lower limits are zero, which are along the x axes of the figures. For the high-velocity scenario, the discrete nature of the source is well maintained as advection dominates over dispersion. For the low-velocity scenario, the concentration distribution is much smoother as the discrete source dissipates more

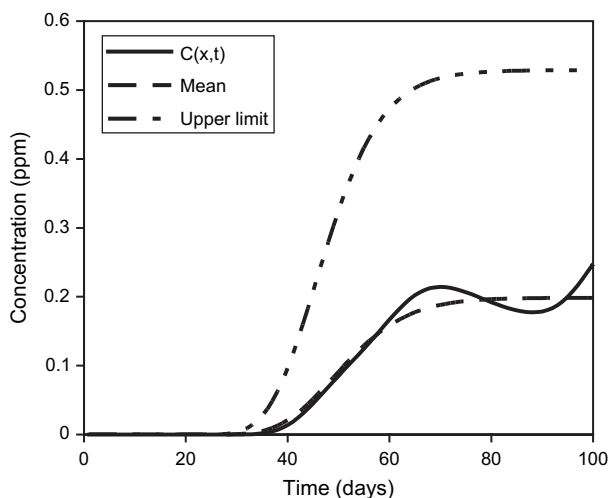


Figure 11. Calculated concentrations along with the mean and upper limit of 90% confidence interval at an observation point 50 m directly downstream from the source under a low-flow velocity scenario ($v = 1$ m/d). Other parameters are identical to those given for Figure 10.

significantly and as the role of dispersion becomes more important.

Summary and Conclusions

A major uncertainty in contaminant transport modeling arises from the randomness of contaminant sources. The randomness is characterized by the random time at which a contamination event may occur and the random amount of contaminant that may be released into the aquifer. Research on the uncertainty of contaminant sources has not received adequate attention in the literature. This paper addresses the effects of random sources on contaminant transport.

This paper presents a stochastic framework for accommodating random contaminant sources in conventional, deterministic advection-dispersion transport models. The contaminant sources are first classified 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 PDE is replaced by a stochastic PDE. The random variations are modeled by Gaussian noise or Bm, and the solution is obtained by using Ito's integration technique. For the second type, Markovian analysis is used for discrete-time contamination events. Both approaches use a deterministic transport model to generate source response functions. The response functions are then integrated to yield probabilistic description of contaminant transport, from which key statistical properties such as mean and variance can be drawn.

Three examples in one- and two-dimensional aquifers are presented to illustrate the concepts discussed in this paper. These examples involve both continuous-time and discrete-time random sources. The concentrations at any observation point and time in response to any realization of the random source can be computed along with the mean and associated uncertainty (standard deviation) of the probabilistic concentration distribution. For the simplicity of presentation, only simple examples are used so that analytical solutions are available for the response functions that are required for integration with the random source functions to obtain the concentration distributions at any observation point and time. For more complex problems, a numerical simulator such as MT3DMS (Zheng and Wang 1999) can be applied to obtain the response function under general field conditions.

The stochastic approach developed in this study will help us understand and predict contaminant transport under random contaminant sources. From a theoretical point of view, Ito's stochastic differential equation is introduced as a means of accounting for random sources in transport modeling. For non-Gaussian contaminant sources, Markovian analysis is introduced to handle discrete-time random events. From a practical point of view, the stochastic models of contaminant sources can be integrated with and implemented on the basis of conventional advection-dispersion models so that practical tools can be developed for risk-based assessment and remediation of ground water-related environmental problems.

Acknowledgments

The funding for this work was provided in part by a grant from the U.S. EPA (EPA grant number R823136). We are grateful to Roseanna Neupauer, Sean McKenna, and an anonymous reviewer, whose constructive comments have led to the improvement of this paper.

Appendix A. Derivation of Equations 15 through 19

To obtain Equation 15b, we simply make substitution $z = t - \tau$, $dz = -d\tau$:

$$\begin{aligned} C(x, t) &= - \int_t^0 C_s(t-z)r(x, z)dz \\ &= \int_0^t C_s(t-\tau)r(x, \tau)d\tau \end{aligned} \quad (A1)$$

For Equation 15c, we introduce a new variable

$$R(x, t) = \int_0^t r(x, s)ds \quad (A2)$$

Then, we have $dR = rdt$ that gives us Equation 15c. Equation 15d can be obtained from Equation 15c by first integrating by parts:

$$\begin{aligned} C(x, t) &= \int_0^t C_s(t-\tau)dR(x, \tau) \\ &= C_s(0)R(x, t) - C_s(t)R(x, 0) - \int_0^t R(x, \tau)d\tau C_s(t-\tau) \end{aligned}$$

Note that $R(x, 0) = 0$. Changing the integral variable will yield Equation 15d.

To derive the mean and variance in Equations 17 through 18, we use the properties of Bm

$$E(dW) = 0 \quad (A3a)$$

$$\text{Var}(dW) = dt \quad (A3b)$$

Exchanging the order of expectation and integral gives us Equations 17 and 18

$$\begin{aligned} E[C(x, t)] &= E \left[\int_0^t C_s(\tau)r(x, t-\tau)d\tau \right] \\ &= \int_0^t E[C_s(\tau)]r(x, t-\tau)d\tau = \int_0^t c_s(\tau)r(x, t-\tau)d\tau \end{aligned} \quad (A4)$$

$$\begin{aligned} \text{Var}[C(x, t)] &= \int_0^t \text{Var}[\sigma(\tau)r(x, t-\tau)dW] \\ &= \int_0^t \sigma^2(\tau)r^2(x, t-\tau)d\tau \end{aligned} \quad (A5)$$

Finally, to determine the covariance, we use the fact that $E[dW(\tau_1)dW(\tau_2)] = d\tau_1$, $\tau_1 = \tau_2$; 0 otherwise. For the case $t_1 \leq t_2$, we have

$$\begin{aligned} &\text{Cov}[C(x_1, t_1), C(x_2, t_2)] \\ &= \int_0^{t_1} \int_0^{t_2} \text{Cov}[C_s(\tau_1)r(x_1, t_1 - \tau_1), C_s(\tau_2)r(x_2, t_2 - \tau_2)]d\tau_1d\tau_2 \\ &= \int_0^{t_1} \sigma^2(\tau)r(x_1, t_1 - \tau)r(x_2, t_2 - \tau)d\tau \end{aligned} \quad (A6)$$

For the case $t_1 > t_2$, we simply replace t_1 by t_2 . A similar derivation can be found in Soong (1973).

Appendix B. Derivation of Equations 26 and 27

It is known that the mean value of a random variable X can be obtained from its LT by differentiating with respect to the Laplace variable and then evaluating the derivative at zero, i.e.,

$$\begin{aligned} E(X) &= -\frac{d}{ds}[\text{LT}(s)]_{s=0} \\ E(X^2) &= -\frac{d^2}{ds^2}[\text{LT}(s)]_{s=0} \end{aligned} \quad (B1)$$

and in general the k th moment of the random variable can be obtained by

$$E(X^k) = (-1)^k \frac{d^k}{ds^k}[\text{LT}(s)]_{s=0} \quad (B2)$$

In our problem, the first (partial) derivative is obtained by applying chain rule

$$\begin{aligned} E[C(t, x)] &= -\exp \left\{ \lambda \int_0^t E \left[e^{-sC_s r(x, \tau)} - 1 \right] d\tau \right\}_{s=0} \\ &\times \frac{\partial}{\partial s} \left[\lambda \int_0^t E \left[e^{-sC_s r(x, \tau)} - 1 \right] d\tau \right]_{s=0} \\ &= - \left[\lambda \int_0^t E \left[e^{-sC_s r(x, \tau)} (-C_s r(x, \tau)) \right] d\tau \right]_{s=0} \\ &= \lambda \int_0^t E[C_s r(x, \tau)]d\tau = \lambda E(C_s) \int_0^t r(x, \tau)d\tau \end{aligned} \quad (B3)$$

Similarly, the variance can be obtained from the second moment.

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