

NON-FICKIAN TRANSPORT IN HETEROGENEOUS SATURATED POROUS MEDIA

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ABSTRACT: Existing theories of flow and contaminant transport in aquifers are either based on Monte Carlo simulations or small perturbation solutions of the governing stochastic partial differential equations, which limit the applications to cases of small variances in the physical parameters. In most cases the "smallness" is a subjective statement from the modeler or is forced by considering the logarithm of the random quantities. This article constitutes a preliminary attempt to reanalyze the problem of flow and contaminant transport in a hypothetical heterogeneous aquifer without the usual assumptions of small perturbation, logarithmic transformation, a specific probability law, and disregard for the underlying hydrologic problem. Statistical properties of the pore velocity are derived from the inherent ground water flow problem; a non-Fickian dispersion equation is derived by assuming two scales, a small and a large one; and a solution of the dispersion equation is obtained. A general analytic procedure, the decomposition method is used in the solution of the flow and dispersion equations. Finally, some comparisons with existing results are presented.

INTRODUCTION

Recent theoretical and field studies have demonstrated that the movement of inert solutes in aquifers is governed by a dispersion equation whose dispersion coefficients are functions of the spatial coordinate or travel time, and that only under ideal circumstances, i.e., usually at the laboratory scale, the classical form of the convection dispersion equation with constant coefficients is adequate for describing contaminant transport (Fried 1975; Dagan 1984).

In the search for the definition of transport equations that adequately represent the evolving nature of the dispersion parameters at large scales, some researchers have conceived the variability of the dispersion parameters as deterministic evolving or periodic functions of space or time (Pickens and Grisak 1981; Gupta and Bhatthacharya 1986; Barry and Sposito 1989; Yates 1990). Recently Serrano (1992b, 1993) attempted to incorporate aquifer-physical variables in the definition of the functional form of dispersion parameters. An equation of dispersion in one- and two-dimensional homogeneous and heterogeneous aquifers with scale-dependent parameters given as functions of natural recharge rate from rainfall, aquifer transmissivity, head hydraulic gradient, aquifer thickness, and aquifer soil porosity were derived. It was found that aquifer recharge partially explains the scale dependency of aquifer parameters, even in homogeneous aquifers, and that its inclusion implies the solution of difficult equations with spatially variable coefficients.

Stochastic analyses have played an important role with a variety of studies that investigate the effect of field scale heterogeneities on the dispersion phenomenon. Researchers have focused on representations of the hydraulic conductivity tensor as realizations of a random field, and its influence on the ground water velocity variability and the dispersion parameters. For a summary and a critical review of stochastic methods to derive transport equations the reader is referred to Cushman (1987), and Sposito and Jury (1986). The major advantage of existing solution methods of stochastic transport equations is that they have permitted the development of some fundamental understanding of the phenomenon of mass trans-

port in aquifers. The major disadvantage is that most of them have been built based on excessive restrictions and assumptions created for the purpose of making the mathematics of the problem tractable and the solution of the equations possible, and not necessarily to reflect physical conditions. Except for the Monte Carlo simulation approaches, which are empirical and expensive, most of the existing stochastic theories of dispersion are based on the small perturbation assumption, whereby the stochastic terms in the differential equation are assumed to be small and thus the truncation of the series may be justified. However, the size of "small" is usually a subjective statement of the modeler since no mathematical criteria restricting the acceptable bounds in the variances is presented. It has become widely acceptable to force the "smallness" in the random quantities by considering its logarithm. Although some univariate lognormal distributions have been fitted to the hydraulic conductivity of some aquifers, the lognormality of this parameter is usually assumed to justify the small perturbation solution. These assumptions may mean that the problem being solved is no longer a proper representation of the physical problem whose solution is desired. Cristakos et al. (1993), Loaiciga and Mariño (1990), and Cushman (1993) have demonstrated that many of the assumptions of the small perturbation conception of ground water are restrictive. Oliver and Christakos (1995) showed that products of spatial derivatives of the conductivity and hydraulic gradients, usually present in perturbation expansions, are not negligible. Using an exact solution, they established the conditions under which such assumptions are correct.

This article constitutes a preliminary attempt to reanalyze the problem of flow and contaminant transport in a hypothetical heterogeneous aquifer without the usual assumptions of small perturbation, logarithmic transformation, a specific probability law, and disregard for the underlying hydrologic problem. It does not pretend to be the complete answer to the problem of dispersion in a general three-dimensional aquifer, but rather a fundamental basis for subsequent work in the field, and hopefully a stimulus to reexamine flow and transport problems in ground water under the light of general analytic techniques.

In the next sections, statistical measures of the pore velocity are derived in terms of the corresponding statistical measures of the transmissivity and determinant field measurable bulk hydrogeologic properties. Subsequently, a large-scale dispersion equation is derived based on the solute mass conservation and the random nature of the pore velocity. The Fickian approximation is avoided except as an initial term for the small scale problem, an assumption generally accepted. A solution of the dispersion equation in terms of the mean concentration

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distribution and expressions for the equivalent time-dependent dispersion parameters are given. Finally, a comparison with the classical theory, the Dagan model, and field tracer tests in the Borden aquifer is described with favorable results.

To observe the natural large variability effect of the transmissivity, the "raw" transmissivity, rather than its logarithm, is considered in the flow equation. For the same reasons, the decomposition method (Adomian 1994; Serrano 1988), rather than the small perturbation method, is used for the solutions of the flow and the dispersion equation. A specific measure to assure convergence of the series solution is given. This measure is based on a theorem with proof (Serrano 1992a). Assumptions on the underlying probability distribution of the transmissivity have been avoided and information on the mean and spatial correlation structure is used instead (stationarity assumed out of necessity). From the applied point of view, this is the only reasonable information obtained from field data banks. In this study, only two scales of dispersion are adopted: A small scale of the order of less than 10 m, where the classical convection dispersion equation and the Fickian approximation are assumed valid, and a large scale of the order of tens of m, where the dispersion mechanism is controlled by the aquifer heterogeneity.

VELOCITY FIELD IN HETEROGENEOUS AQUIFER

In this section we investigate the form of the ground water velocity in a heterogeneous, long (compared to its thickness), hypothetical unconfined aquifer exhibiting mild slopes and with the usual assumptions of planar dimensions much larger than its thickness; formation properties of interest averaged over the depth and regarded as functions of the horizontal dimensions only; and Dupuit assumptions of shallow flow (Dagan 1986). The governing flow equation is (Bear 1979)

$$\frac{\partial}{\partial x} \left[T(x, y) \frac{\partial h}{\partial x} \right] + \frac{\partial}{\partial y} \left[T(x, y) \frac{\partial h}{\partial y} \right] = 0, \quad 0 < x < \infty, -\infty < y < \infty \quad (1)$$

where $h(x, y)$ = hydraulic head (m) above a specified datum; $T(x, y)$ = aquifer transmissivity (m^2/month); and x, y = spatial Cartesian coordinates (m).

We focus our attention on an aquifer with a regional ground water flow direction coinciding with x and negligible net velocity in the y -direction. In such an aquifer, the regional hydraulic gradients operate mainly in the x -direction, causing a significantly greater variability in the longitudinal pore velocity than in the transverse pore velocity. As a result, the field scale longitudinal dispersion coefficients will be greater than those in the transverse direction. This is the reason why some field studies report a strong scale dependency in the longitudinal dispersion coefficient, while a relatively small increase in the transverse one. Therefore, in this study, we will assume that the transverse dispersion coefficient follows a small scale representation, and that the effect of the random variability in the transverse pore velocity on the random variability of the longitudinal pore velocity is negligible. Under preparation is an analysis of the full three-dimensional random velocity field.

We further represent the transmissivity as $T = \bar{T} + T'$, where $\bar{T} = E\{T\}$, $E\{\}$ = the expectation operator; the random field T' has the properties $E\{T'\} = 0$; $E\{T'(x_1, y_1)T'(x_2, y_2)\} = \sigma_T^2 e^{-\rho|x_1-x_2|} e^{-\rho|y_1-y_2|}$; σ_T^2 = transmissivity variance parameter [$(\text{m}^2/\text{month})^2$], and ρ = correlation decay parameter (m^{-1}). The preceding simplified representation of aquifer heterogeneity in the transmissivity attempts to be in line with current research in the stochastic analysis of ground water flow and contaminant transport, while reducing the mathematical complexity.

Without loss of generality, we assume knowledge of the

boundary conditions at a point in the aquifer, $h(0, 0) = h_0$; $(\partial h/\partial x)(0, 0) = h'_0$; and $(\partial h/\partial y)(0, 0) = 0$. The flow equation becomes

$$\frac{\partial^2 h}{\partial x^2} = -\frac{1}{\bar{T}} \frac{\partial T'}{\partial x} \frac{\partial h}{\partial x}, \quad 0 \leq x < \infty, \quad h(0) = h_0, \quad \frac{\partial h}{\partial x}(0) = h'_0 \quad (2)$$

The solution to this differential equation is

$$h(x) = h_0 + h'_0 x - \frac{1}{\bar{T}} \int_0^x G(x; \xi) \frac{\partial T'(\xi)}{\partial \xi} \frac{\partial h}{\partial \xi} d\xi \quad (3)$$

where $G(x; \xi)$ = Green's function associated with (2). It is given by (Serrano 1992b)

$$G(x; \xi) = U(x, \xi)(x - \xi) \quad (4)$$

where $U(\cdot)$ = unit step function. Substituting (4) into (3)

$$h(x) = h_0 + h'_0 x - \frac{1}{\bar{T}} \int_0^x (x - \xi) \frac{\partial T'(\xi)}{\partial \xi} \frac{\partial h}{\partial \xi} d\xi \quad (5)$$

A decomposition series of (5) could be built as (Serrano 1992a) $h(x) = h_0 + h_1 + h_2 + \dots$, where h_0 = head with respect to the bottom of the aquifer at the origin

$$h_1(x) = h'_0 x \quad (6)$$

$$h_2(x) = -\frac{1}{\bar{T}} \int_0^x (x - \xi) \frac{\partial T'(\xi)}{\partial \xi} \frac{\partial h_1(\xi)}{\partial \xi} d\xi \quad (7)$$

and in general

$$h_i(x) = -\frac{1}{\bar{T}} \int_0^x (x - \xi) \frac{\partial T'(\xi)}{\partial \xi} \frac{\partial h_{i-1}(\xi)}{\partial \xi} d\xi \quad (8)$$

The convergence of the series of (5) requires that $\max[T'(x)] < 1$ for the sample functions, where $\max(\cdot)$ = maximum operator, and that $C_v = \sigma_T/\bar{T} < 1$ for the expected heads, where C_v = coefficient of variability of the transmissivity (Serrano 1992a). Unless the transmissivity is assumed to follow a Gaussian random field, its third moment is usually unknown. Usually, however, only the first two moments are available from field measurements conducted with reasonable detail, and therefore it is only possible to calculate the first three terms in the decomposition series. It is known that this represents an accurate scheme for most practical applications (Serrano and Unny 1987).

Substituting (6) and (7) into (5) and differentiating with respect to x , one obtains the hydraulic gradient in the direction of the regional ground water flow

$$\frac{\partial h}{\partial x} \approx \frac{\partial}{\partial x} (h_0 + h_1 + h_2) = h'_0 - \frac{h'_0}{\bar{T}} \frac{\partial}{\partial x} \left[x \int_0^x \frac{\partial T'(\xi)}{\partial \xi} d\xi \right] + \frac{h'_0}{\bar{T}} \frac{\partial}{\partial x} \left[\int_0^x \xi \frac{\partial T'(\xi)}{\partial \xi} d\xi \right] \quad (9)$$

Applying Leibnitz rule for differentiation under integrals and solving

$$\frac{\partial h}{\partial x} = h'_0 - \frac{h'_0}{\bar{T}} \int_0^x \frac{\partial T'(\xi)}{\partial \xi} d\xi \quad (10)$$

The large-scale component of the pore velocity, u_x , averaged over the vertical, may be estimated as $u_x(x) = -(T/nh_0)(\partial h/\partial x)$. On using (10)

$$u_x(x) = -\frac{h_0}{nh_0} \left[\bar{T} + T' - \int_0^x \frac{\partial T'(\xi)}{\partial \xi} d\xi - \frac{1}{\bar{T}} \int_0^x T'(x) \frac{\partial T'(\xi)}{\partial \xi} d\xi \right] \quad (11)$$

We remark that this is the large scale component of the pore velocity, that is, the one controlled by the random variability

in the transmissivity at the large scales. Taking expectations on both sides of (11) we obtain the mean pore velocity, \bar{u}_x

$$\bar{u}_x = E\{u_x(x)\} = -\frac{h'_0}{nh_0} \left[\bar{T} - \frac{\sigma_T^2}{\bar{T}} (1 - e^{-\rho x}) \right] \quad (12)$$

This is the same expression obtained by Serrano (1993) when the recharge rate is set to zero. It was noted there that the relative magnitude of the second term in the right side of (12) is small as compared to that of the first. In other words, the effect of the correlation decay parameter of the transmissivity on the average pore velocity is small as compared to that of the aquifer regional hydraulic gradient in the absence of recharge. With this approximation

$$\bar{u}_x \approx -(h'_0 \bar{T} / nh_0) \quad (13)$$

Similarly, from (11) the random component of the pore velocity is

$$u'_x(x) = u_x - \bar{u}_x = -\frac{h'_0}{nh_0} \left[T' - \int_0^x \frac{\partial T'(\xi)}{\partial \xi} d\xi \right] \quad (14)$$

The right side of this equation illustrates the concept of two scales of motion: One small scale operating at short distances, and one of increasing importance as the distance from the source increases (the integral term). From (14) the two point correlation function of the pore velocity, R_{uu} , at locations x_1 and x_2 may be derived. Substituting for the assumed exponentially decaying form of the transmissivity correlation function, differentiating under the integrals, calculating the correlation of the derivatives, and solving, one obtains

$$E\{u'_x(x_1)u'_x(x_2)\} = R_{uu} = \left(\frac{h'_0 \sigma_T}{nh_0} \right)^2 [(e^{-\rho x_2} + 2\rho x_1 - 2e^{-\rho(x_2-x_1)} + 2)], \quad (15)$$

$$x_1 \leq x_2$$

Finally, set $x_1 = x_2 = x$ to obtain the variance of the pore velocity, σ_u^2 , as

$$\sigma_u^2 = \left(\frac{h'_0 \sigma_T}{nh_0} \right)^2 (2\rho x + e^{-\rho x}) \quad (16)$$

This equation indicates that the variance of the pore velocity increases with distance. For large values of ρ the increase is linear with distance, whereas for small values of ρ the increase is nonlinear with distance. Eq. (16) further illustrates the concept of two scales of motion: A small scale controlled by the exponential term, and a large scale that grows with distance. In practice, however, it is found that natural aquifers exhibit large correlation lengths. Therefore $\rho \rightarrow 0$, and $\sigma_u^2 \rightarrow (h'_0 \sigma_T / nh_0)^2$, as expected.

SOLUTE DISPERSION IN HETEROGENEOUS AQUIFER

In this section we study the form of the dispersion equation in a two-dimensional unconfined aquifer with Dupuit assumptions subject to a random transmissivity. In the previous section we investigated the statistical properties of the pore velocity in such an aquifer and now the parameters of the dispersion equation are derived in terms of those properties. The solute mass continuity equation is (Bear 1979)

$$\frac{\partial C}{\partial t} + \frac{\partial(u_x C)}{\partial x} + \frac{\partial(u_y C)}{\partial y} = 0 \quad (17)$$

where C = solute concentration (mg/L); t = time coordinate (months); $u_x, u_y = x, y$ components of the pore velocity vector, respectively; and the rest of the terms as before.

From the observation that the dispersion parameters are functions of distance, and after the results in the preceding

section, particularly (11), (12), and (14), it is assumed in the present work that two mechanisms of dispersion are present: One primarily operating at the small scale where the dispersion is controlled by the variability in the pore size and the pore velocity at this scale; and one operating at large scale where the dispersion is controlled by the aquifer heterogeneity in the transmissivity at this scale. At the small scale level the effect of the second mechanism would be negligible, because of the small distances involved, while at the large scale level both mechanisms are present but the second is the dominant one, because of the large distances involved. Thus, we define the large scale pore velocity in the x -direction as $u_x(x) = \bar{u}_x + u'_{px} + u'_x$, where u'_{px} = random component of the small scale pore velocity, and u'_x = random component of the large scale pore velocity as before.

With the x coordinate coinciding with the (mean) regional ground water pore velocity, the mean y component, \bar{u}_y , of the pore velocity is zero. Thus the y (transverse) component of the pore velocity is defined as $u_y = u'_{py} + u'_y$, where u'_{py} = random component in the y -direction of the pore scale velocity; and u'_y = random component of the large scale pore velocity in the y -direction. For an infinite aquifer and an instantaneous point source (a spill) at the origin, (17) becomes

$$\frac{\partial C}{\partial t} + \frac{\partial(\bar{u}_x C)}{\partial x} + \frac{\partial(u'_{px} C)}{\partial x} + \frac{\partial(u'_x C)}{\partial x} + \frac{\partial(u'_{py} C)}{\partial y} + \frac{\partial(u'_y C)}{\partial y} = 0 \quad (18)$$

subject to

$$-\infty < x < \infty, -\infty < y < \infty, 0 < t, C(\pm\infty, y, t) = C(x, \pm\infty, t) = 0, \quad (19)$$

$$C(x, y, 0) = C_i \delta(x) \delta(y)$$

where C_i = magnitude of the initial mass; and $\delta(\cdot)$ = Dirac's delta function.

Adopting the Fickian approximation at the small scale, $u'_{px} C \approx -D_x(\partial C/\partial x)$ and $u'_{py} C \approx -D_y(\partial C/\partial y)$, where D_x and D_y = dispersion coefficients (m²/month) in x and y , respectively, defined as the product of a small-scale (laboratory) dispersivity times the mean longitudinal pore velocity. The large-scale concentration may be written as

$$C(x, y, t) = C_i X(x, t) \cdot Y(y, t) \quad (20)$$

where $X(x, t)$ satisfies

$$\frac{\partial X}{\partial t} + \bar{u}_x \frac{\partial X}{\partial x} = D_x \frac{\partial^2 X}{\partial x^2} - \frac{\partial(u'_x X)}{\partial x}, \quad X(\pm\infty, t) = 0, X(x, 0) = \delta(x), \quad (21)$$

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

and $Y(y, t)$ satisfies

$$\frac{\partial Y}{\partial t} - D_y \frac{\partial^2 Y}{\partial y^2} = -\frac{\partial(u'_y Y)}{\partial y}, \quad Y(\pm\infty, t) = 0, Y(y, 0) = \delta(y), \quad (22)$$

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

The solution to (21) may be expressed as the decomposition series (Serrano 1992a) $X = X_0 + X_1 + X_2 + \dots$, where the first term, X_0 , satisfies

$$\frac{\partial X_0}{\partial t} + \frac{\partial(\bar{u}_x X_0)}{\partial x} = D_x \frac{\partial^2 X_0}{\partial x^2}, \quad X_0(\pm\infty, t) = 0, X_0(x, 0) = \delta(x), \quad (23)$$

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

which indicates that the first approximation to a scale dependent solute dispersion is a convection dispersion equation with a constant small scale dispersion coefficient. Its solution is

$$X_0(x, t) = \frac{e^{-[(x-\bar{u}_x t)^2/4D_x t]}}{\sqrt{4\pi D_x t}} \quad (24)$$

Any subsequent term, X_i , in the expansion of (21) satisfies

$$\frac{\partial X_i}{\partial t} + \bar{u}_x \frac{\partial X_i}{\partial x} = -\frac{\partial(u'_x X_{i-1})}{\partial x}, \quad X_i(\pm\infty, t) = 0, X_i(x, 0) = 0, \\ -\infty < x < \infty, 0 < t, i \geq 1 \quad (25)$$

The Green's function of this differential equation, $G(x, t; x', t')$, satisfies

$$\frac{\partial G}{\partial t} + \bar{u}_x \frac{\partial G}{\partial x} = 0, \quad G(\pm\infty, t; x', t') = 0, G(x, 0; x', t') = \delta(x), \\ -\infty < x < \infty, 0 < t \quad (26)$$

Defining the Laplace transform of G as $\hat{G} = \int_0^\infty e^{-st} G dt$, (26) reduces to

$$d\hat{G}/dx + (s/\bar{u}_x)\hat{G} = \delta(x)/\bar{u}_x \quad (27)$$

Solving this equation and Laplace inverting, one obtains

$$G(x, t; x', t') = \delta\{(t - t') - [(x - x')/\bar{u}_x]\} \quad (28)$$

which represents the pure translation effect of continuity.

Now the solution of (25) may be expressed in terms of the Green's function as

$$X_1(x, t) = -\int_0^t \int_{-\infty}^\infty G(x, t; x', t') \frac{\partial}{\partial x'} [u'_x X_{i-1}(x', t')] dx' dt' \quad (29)$$

Using (24), (28), and (29), and solving the internal spatial integral, the second term in the series solution of (21) is

$$X_1(x, t) = -\int_0^t \frac{\partial}{\partial x} [u'_x(x - \bar{u}_x t + \bar{u}_x t') X_0(x - \bar{u}_x t)] dt' \quad (30)$$

Similarly, using (28), (29), and (30), the third term in the solution of (21) is

$$X_2(x, t) = \int_0^t \frac{\partial}{\partial x} \left[\frac{\partial X_0(x - \bar{u}_x t)}{\partial x} \right. \\ \left. \cdot \int_0^t u'_x(x - \bar{u}_x t + \bar{u}_x t') u'_x(x - \bar{u}_x t + \bar{u}_x \tau) d\tau - X_0(x - \bar{u}_x t) \right. \\ \left. \cdot \int_0^t u'_x(x - \bar{u}_x t + \bar{u}_x t') \frac{\partial u'_x(x - \bar{u}_x t + \bar{u}_x \tau)}{\partial x} d\tau \right] dt' \quad (31)$$

Higher-order elements in the series solution could be derived. However, the calculation of the expected value of such terms would require information on the moments of order greater than two, and as stated, this information is usually not available in most applications. Therefore the solution to (21) is approximated as $X(x, t) \approx X_0 + X_1 + X_2$, where the components X_0, X_1, X_2 are given by (24), (30), and (31), respectively. The solute concentration is then given by (20). On taking expectations on both sides of (20), the mean concentration is given by

$$E[C(x, y, t)] = \bar{C}(x, y, t) = C_x \bar{X}(x, t) \cdot \bar{Y}(y, t) \quad (32)$$

where $\bar{X}(x, t) = E\{X(x, t)\} = X_0 + \bar{X}_1 + \bar{X}_2$, with $E\{X_i\} = \bar{X}_i$, $i = 1, 2$. $\bar{Y}(y, t) = E\{Y(y, t)\}$ is obtained from solving (22) in a similar way. Since u'_x is a zero mean random process (see previous section), taking expectations on (30) yields $\bar{X}_1 = 0$. Taking expectations on (31) and using the pore velocity correlation function (15) derived in the previous section, with $x_1 = x - \bar{u}_x t + \bar{u}_x \tau$, $x_2 = x - \bar{u}_x t + \bar{u}_x t'$, one obtains, after some manipulation

$$\bar{X}_2(x, t) = \left[\frac{h'_0 \sigma_T}{nh_0} \right]^2 X_0 \left(Z e^{-\rho(x-\bar{u}_x t)} (W - \rho^2) + W \left\{ -\frac{2e^{-\rho \bar{u}_x t}}{\rho^2 \bar{u}_x^2} + \frac{\rho \bar{u}_x t^3}{3} \right. \right. \\ \left. \left. + t^2 [\rho(x - \bar{u}_x t) + 1] - \frac{2t}{\rho \bar{u}_x} + \frac{2}{\rho^2 \bar{u}_x^2} \right\} \right) \quad (33)$$

where

$$W = \left(\frac{x - \bar{u}_x t}{2D_x t} \right)^2 - \frac{1}{2D_x t}, \quad Z = \frac{1}{\rho \bar{u}_x} \left[\frac{1}{\rho \bar{u}_x} - e^{-\rho \bar{u}_x t} \left(t + \frac{1}{\rho \bar{u}_x} \right) \right] \quad (34)$$

Numerical tests on the form of $\bar{X}(x, t)$ indicated that the mean x component of the concentration spatial distribution is a Gaussian distribution with a time-dependent first moment with respect to the origin (the center of mass of the plume, $\mu = \bar{u}_x t$), and a time-dependent second moment with respect to the mean (the plume variance, ϕ_x). This longitudinal plume variance is given by $\phi_x = \int_{-\infty}^\infty (x - \mu)^2 \bar{X}(x, t) dx$. Substituting in this expression for \bar{X} [(24) and (33)], integrating term by term and using the moments properties of Gaussian distributions

$$\phi_x = 2D_x t + \left(\frac{h'_0 \sigma_T}{nh_0} \right)^2 \left[\frac{2}{3} \rho \bar{u}_x t^3 + 2t^2 - \frac{4t}{\rho \bar{u}_x} + \frac{4}{\rho^2 \bar{u}_x^2} - \frac{4e^{-\rho \bar{u}_x t}}{\rho^2 \bar{u}_x^2} \right. \\ \left. + 2Ze^{\rho^2 D_x t} (1 + 2\rho^2 D_x t) \right] \quad (35)$$

An analysis of convergence on the preceding decomposition series solution to (21) indicates that solution is strictly valid for $t < t_m$ (Serrano 1992a), where t_m = maximum simulation time given by $t_m = 1/(\rho x_m)$, where x_m = maximum longitudinal scale in the simulations. Using the shifting properties of Gaussian curves, the longitudinal plume variance is calculated as $k\phi_x(t_m)$, $k = t/t_m$. This restriction does not affect the transverse component.

After following a similar procedure as for the longitudinal part, it was found that large scale transverse dispersion has a range of values substantially lower than those in the longitudinal direction. The transverse plume variance is given by

$$\phi_y = 2D_y t + \rho^2 \left(\frac{h'_0 \sigma_T}{nh_0} \right)^2 D_y t^2 \quad (36)$$

In summary, the mean concentration distribution is given by

$$\bar{C}(x, y, t) = C_i \bar{C}_x(x, t) \bar{C}_y(y, t) \quad (37a)$$

$$\bar{C}_x(x, t) = e^{-[(x-\bar{u}_x t)^2/2k\phi_x(t_m)]} / \sqrt{2\pi k\phi_x(t_m)} \quad (37b)$$

$$\bar{C}_y(y, t) = Y(y, t) = e^{-[y^2/2k\phi_y(t_m)]} / \sqrt{2\pi k\phi_y(t_m)} \quad (38)$$

$$k = t/t_m, \quad t_m = 1/[\rho x_m (h'_0 \sigma_T / nh_0)^2] \quad (39)$$

and $\phi_x(t_m), \phi_y(t_m)$ = plume variances evaluated at $t = t_m$, (35) and (36), respectively.

VERIFICATION WITH EXISTING RESULTS

Field verification of ground water pollution models of chemical spills is a difficult problem due to the relative lack of reliable databases documenting environmental accidents; the subjective account of certain parameters, particularly the initial concentration and mass; and the inherent inaccuracies of certain measurement strategies. Most field databanks possess a degree of uncertainty comparable to that of the mathematical model after the adoption of many assumptions and approximations. Another problem relates to the verification of the moments of a stochastic model (i.e., the mean concentration, \bar{C}) with what appears to be a single realization (a sample function) of the concentration, C , taken in the field. Aware of these obstacles, an attempt of verification may be approached by comparing the simulation results with a controlled tracer experiment. Our objective would then be to observe if the mathematical model reproduces the enhanced dispersion observed in the field, and the general characteristics of the plume. Thus, in this section we study a preliminary comparison be-

tween the dispersion model developed in the previous section [(35)–(39)] with the two-dimensional convection dispersion equation and the two-dimensional Dagan model as applied to the Borden site experiment.

The classical deterministic convection dispersion equation with constant dispersion coefficients applied to the hypothetical aquifer is given by

$$\frac{\partial C}{\partial t} - D_x \frac{\partial^2 C}{\partial x^2} + \bar{u}_x \frac{\partial C}{\partial x} - D_y \frac{\partial^2 C}{\partial y^2} = 0, \quad -\infty < x < \infty, -\infty < y < \infty, 0 < t \quad (40a)$$

$$C(\pm\infty, y, t) = C(x, \pm\infty, t) = 0, \quad C(x, y, 0) = C_0 \delta(x) \delta(y) \quad (40b)$$

The solution to this differential equation is

$$C(x, y, t) = \frac{e^{-[(x-\bar{u}_x t)^2/4D_x]}}{\sqrt{4\pi D_x t}} \cdot \frac{e^{-(y^2/4D_y t)}}{\sqrt{4\pi D_y t}} \quad (41)$$

The two-dimensional version of the Dagan model (Dagan 1984, 1986) conceives a convection dispersion equation for the mean concentration with time-dependent dispersion coefficients:

$$\frac{\partial \bar{C}}{\partial t} - D_1(t) \frac{\partial^2 \bar{C}}{\partial x^2} + \bar{u}_x \frac{\partial \bar{C}}{\partial x} - D_2(t) \frac{\partial^2 \bar{C}}{\partial y^2} = 0, \quad -\infty < x < \infty, -\infty < y < \infty, 0 < t \quad (42)$$

subject to the same boundary and initial conditions imposed on (40). The longitudinal (x -direction) dispersion coefficient is defined as

$$D_1(t) = \frac{0.74 \bar{u}_x \sigma_y^2}{\rho} \left[1 - \frac{1.5}{\tau} - \frac{3e^{-\tau}}{\tau^2} + \frac{3}{\tau^3} (1 - e^{-\tau}) \right] + D_x \quad (43)$$

where σ_y^2 = variance of the log hydraulic conductivity; and $\tau = \rho \bar{u}_x t$. The transverse (y -direction) dispersion coefficient is defined as

$$D_2(t) = \frac{0.74 \rho \bar{u}_x \sigma_y^2}{2\tau} \left[1 - \frac{6}{\tau^2} + 2e^{-\tau} \left(1 + \frac{3}{\tau} + \frac{3}{\tau^2} \right) \right] + D_y \quad (44)$$

The solution to (42) was derived by Barry and Sposito (1989) as

$$\bar{C}(x, y, t) = \frac{e^{-[(x-\bar{u}_x t)^2/4\phi_1]}}{\sqrt{4\pi\phi_1}} \cdot \frac{e^{-(y^2/4\phi_2)}}{\sqrt{4\pi\phi_2}} \quad (45)$$

where $\phi_1(t) = \int_0^t D_1(t') dt'$, $\phi_2(t) = \int_0^t D_2(t') dt'$.

The results of the Borden site experiment have been extensively documented in the literature (Mackay et al. 1986). We focus our attention on the implementation of the two-dimensional Dagan model to vertically averaged bromide and chloride concentrations at the Borden site reported by Barry et al. (1988). The parameter values for the aquifer are: $\bar{u}_x = 2.73$ m/month, $\sigma_y^2 = 0.38$, $D_x = 0.03$ m²/month, $D_y = 0.009$ m²/month, $h_0 = 6.0$ m, $n = 0.33$; the mean transmissivity is (Serrano 1993) $T = 1,112.4$ m²/month; as calculated from the point hydraulic conductivity values. The transmissivity standard deviation is $\sigma_T = 579.34$ m²/month as deduced from the log conductivity variance σ_y^2 fitted to a log normal distribution. One should expect a lower value for the large scale "raw" transmissivity variance than that estimated from point log conductivity measures. However, the raw transmissivity variance is not available. If we use the value derived from the log conductivity variance, it would imply that the Borden site exhibits a coefficient of variability in the transmissivity of $C_v = \sigma_T/T = 0.52$, which is probably too large if we consider that the aquifer has been classified as mildly heterogeneous. The coefficient $\rho = 0.357$ m⁻¹ is interpreted as the inverse of the log

conductivity correlation length l_x in the Dagan model. For the Borden site $l_x = 2.8$ m. However, since the present model uses the raw transmissivity, it is logical to believe that the correlation length is substantially greater than the log conductivity-based value. However, such information is not available and a nominal value is adopted.

By analogy of our solution with (45), one may conclude that the mean concentration in the proposed model satisfies a convection dispersion equation with time dependent dispersion coefficients, in agreement with the Dagan's model. However, an application of both models to the Borden aquifer reveals that important differences between the two models exist. After observing that $\phi_1(t) = \phi_x/2$, differentiating (35) with respect to t , accounting for the restriction $t < t_m$, one obtains an expression for an effective time dependent dispersion coefficient, $\bar{D}(t)$. Fig. 1 illustrates a comparison between \bar{D} and D_1 as a function of time after the injection. The present model produces dispersion coefficient values that are substantially greater than those given by the Dagan model. This is due to the sensitivity of the present model to aquifer heterogeneity as measured by the variance in the transmissivity. Since we adopted the transmissivity variance calculated from the log conductivity variance fitted for the Borden tests, there is reason to believe that the raw transmissivity variance is smaller than that, and therefore the dispersion coefficient values are exaggerated. Also it is interesting to note that the present model does not exhibit an asymptotic value in the dispersion parameter; it will continue to grow with time. Possible reasons for the discrepancy are the fundamental differences in the mathematical procedures and the assumptions adopted by the two models. The Dagan model considers a flow equation subject to a log normal hydraulic conductivity distribution with a small variance, and it solves it using the small perturbation method. The present model does not restrict the conductivity field to a specific probability law or to a small variance, and it solves the equations using the decomposition method (i.e., the solution is analytic and the convergence, rather than the size of the random quantities, dictates the accuracy of the solution).

In an investigation on the effect of recharge on contaminant dispersion, Serrano (1992b, 1993) also concluded that, in the presence of recharge, the dispersion coefficient does not appear to have an asymptotic value, and its value would only be limited by the end of the recharge zone or the presence of a physical aquifer boundary. An independent confirmation on the nonexistence of an asymptotic value of the dispersion coefficient was given by Paredes and Elorza (1992). They de-

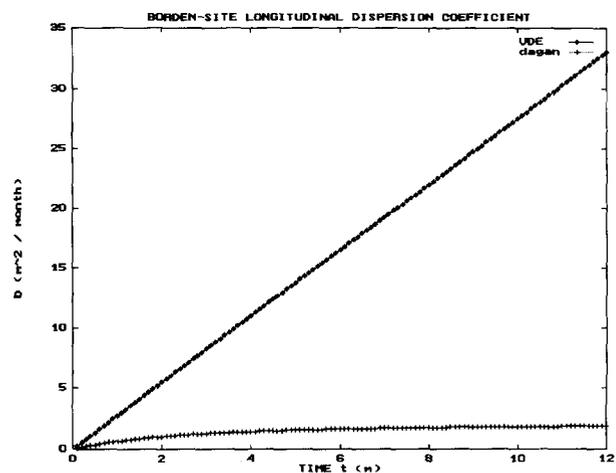


FIG. 1. Comparison between Present and Dagan Models Longitudinal Dispersion Coefficients As Applied to Borden Aquifer

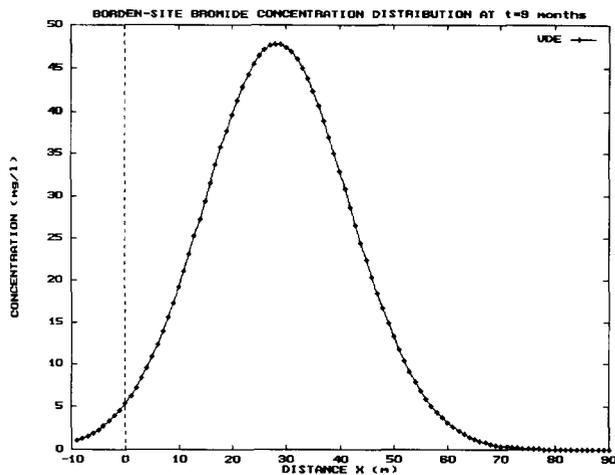


FIG. 2. Borden Site Bromide Concentration Distribution Nine Months after Injection

veloped a dispersion model determined by nonstationary random walk techniques, and the concept of fractal geometry.

To assess the effectiveness of the present model to reproduce the enhanced dispersion of a contaminant plume, longitudinal breakthrough curves of the proposed model were compared with the observed bromide concentration contours reported by Barry et al. (1988). In particular, breakthrough curves using (35)–(39) were generated at the same times displayed by the observed data in Figure 5 of Barry et al. (1988). A preliminary comparison indicated that the model appears to reproduce the main features of the measured plume: peak concentration magnitude, peak location, and approximate longitudinal contaminant range (spread). The spread appears to be overestimated by the present model. Again this is due to the exaggerated raw transmissivity variance calculated from the log conductivity variance estimated for the Borden site. We remark this is a preliminary comparison. Although the results are qualitatively encouraging, further analyses should be conducted with more detailed field tracer tests. Fig. 2 illustrates a longitudinal breakthrough curve of the mean bromide concentration versus distance nine months after the injection as calculated by the proposed model [the variable dispersion equation (VDE)]. In this case the convection dispersion equation breakthrough curve (not included) generates a substantially higher peak magnitude and a reduced plume variance, as compared to the VDE.

SUMMARY AND CONCLUSIONS

Several problems in flow and contaminant subsurface hydrology, such as the scale dependency of the dispersion parameters, remain to be observed in the light of a systematic theory that includes the possibility of using normal, and sometimes large, variances in the random parameters, or at least with a rigorous mathematical framework that allows the construction of convergence theorems objectively restricting the sizes of the variances in the uncertain parameters.

A preliminary analysis of the problem of flow and contaminant transport in a hypothetical aquifer without the assumptions of small perturbation, logarithmic transformations, and specific probability laws was conducted. Two scales of dispersion were assumed: a small scale of the order of less than 10 m, where the dispersion is controlled by the variability in the pore size and the pore velocity at this scale; and one large scale of the order of tens of m, where the dispersion is controlled by the aquifer heterogeneity in the transmissivity. At the small-scale level the effect of the second mechanism is negligible, because of the small distances involved, while at the large scale level both mechanisms are present but the sec-

ond is the dominant one, because of the large distance involved.

Comparison with theoretical models, such as the Dagan model and the classical convection dispersion equation, as applied to the Borden aquifer, indicated that the proposed model qualitatively reproduced the enhanced longitudinal dispersion reported in the literature. However, the present model gives dispersion values that continue to grow with time and does not exhibit an asymptotic value. Reasons for the discrepancy could be explained by the differences in the mathematical treatment, and in the assumptions between the classical and the present approaches. Although the results are qualitatively encouraging, further numerical analyses based on detailed tracer tests are needed.

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