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Towards a Nonperturbation Transport Theory in Hetereogeneous Aquifers[1]

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A large body of existing theories of flow and contaminant transport in aquifers ignore the presence of recharge, eliminate the boundary conditions, neglect transient conditions in groundwater flow, conceive hydraulic gradients as linear, and require parameter variability to be stationary and Gaussian. The most outstanding and difficult to justify assumption is the subjective "small" size of the stochastic terms (i.e., small perturbation methods), which usually is forced by considering the logarithm of the hydraulic conductivity. Several problems in flow and contaminant subsurface hydrology, such as the enhanced dispersion parameters with plume size or time after injection, remain to be observed in the light of a stochastic theory that allows a more realistic consideration of physical and hydrologic properties. In this article, an attempt is made to reformulate a contaminant transport equation (the variable dispersion equation, VDE) with transport parameters in terms of regional hydrologic and aquifer hydraulic properties, such as recharge rate, spatially random transmissivity, hydraulic gradient, aquifer thickness, and soil porosity. Subsequently, a general analytic procedure, the method of decomposition, is used to derive a solution to the VDE. This procedure does not require small perturbation, logarithmic transformations, or specific probability law assumptions. Comparison tests with existing theoretical and field results are given. The tests illustrate the enhanced dispersion and shifting concentration effects produced by the variable dispersion equation. Finally a generalization of the method to nonstationary dispersion in three-dimensional domains is proposed.

KEY WORDS: subsurface contaminant transport, groundwater pollution, mathematical analysis.

INTRODUCTION

Recent theoretical and field studies have demonstrated that the movement of inert solutes in aquifers is governed by a dispersion equation whose dispersion coefficient is a function of the spatial coordinates or travel time and that only under ideal circumstances, usually at the laboratory scale, the classical form of the convection dispersion equation (CDE) with constant coefficients is adequate for describing contaminant transport (Fried, 1975; Sudicky, 1986; Dagan, 1984).

In the search for the definition of transport equations which adequately

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represent the evolving nature of the dispersion parameters at large scale, stochastic analyses have played an important role. By conceiving the hydraulic conductivity as a random parameter, transport equations, and solutions have been derived (i.e., Bakr and others, 1978; Dagan, 1984; Gelhar and Axness, 1983; Neuman, Winter, and Neuman, 1987; Rubin, 1991). Unfortunately, a good portion of these studies rely on the small perturbation method of solution of random equations, which restricts its applicability to small variances in the random parameters. A variety of restrictive assumptions have been imposed in order to make a solution possible, and not necessary to reflect physical conditions. As a result, dispersion models ignore the presence of recharge, eliminate the boundary conditions, neglect transient conditions in groundwater flow, conceive hydraulic gradients as linear, and require parameter variability to be stationary and Gaussian. The most outstanding and difficult to justify assumption is the subjective "small" size of the stochastic terms, which usually is forced by considering the logarithm of the hydraulic conductivity. These assumptions may indicate that the problem being solved is no longer a proper representation of the physical problem whose solution is desired. For a summary and a critical review of stochastic methods to derive transport equations the reader is referred to Cushman (1984, 1987) and Sposito and Jury (1986). Other 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 Bhattacharya, 1986; Barry and Sposito, 1989; Yates, 1990).

Recently Serrano (1992a) attempted to incorporate aquifer physical variables in the definition of the functional form of dispersion parameters. A new equation of dispersion in a one-dimensional homogeneous aquifer with spatially dependent parameters given as functions of natural recharge rate from rainfall, aquifer transmissivity, head hydraulic gradient, aquifer thickness, and aquifer soil porosity was derived (the variable dispersion equation, VDE). In this article, aquifer heterogeneity is considered, as measured by the stochastic spatial variability in the transmissivity in a two-dimensional aquifer. A comparison of the relative impact of hydrologic-hydraulic variables, as opposed to aquifer heterogeneity, on the magnitude of the dispersion coefficient, and verification with other theoretical and field studies is included. Although the problem of spatially variable dispersion is related to the scale dependency of dispersion parameters in heterogeneous aquifers, a rigorous discussion is not presented on the topic (see Cushman, 1984).

A hypothetical phreatic aquifer at the regional scale is considered (Dagan, 1986) with the usual assumptions of planar dimensions larger than its thickness, formation properties of interest averaged for the depth and regarded as functions of the horizontal dimensions only, and Dupuit assumptions of shallow flow. A differential equation governing the flow in this aquifer with the given properties is written and solved for the expected groundwater pore velocity. Subsequently the solute transport dispersion coefficient is written in terms of the given hydrologic and hydraulic properties, and the corresponding dispersion equation is derived. Subsequently, a decomposition series solution for the expected concentration is built based on the characteristics of a particular analytical solution. Comparison tests of the solution to the expected VDE with the classical CDE and the Dagan's solution (Dagan, 1984) as applied to the Borden site experiment (Mackay and others, 1986) are given. Finally a generalization to three-dimensional solute transport subject to nonstationarity in the parameters is introduced.

Important features of the present work include the incorporation of hydrologic physical parameters and aquifer boundary conditions in the form of the dispersion coefficients, the consideration of the "raw" hydraulic conductivity in the flow equation, rather than its logarithm, and the implementation of the method of decomposition in the solution of the groundwater flow and groundwater transport equations.

The method of decomposition (Adomian, 1986, 1991, 1994) has evolved to become a systematic tool to obtain analytical solutions of ordinary, partial, integrodifferential, or delay differential, deterministic or stochastic, linear or nonlinear, equations. Among the many features of the method are its simplicity of implementation, flexibility, and a systematic approach to problem solving. The most important feature, however, is that there is no need to change the physical problem, or to linearize it, in order to obtain a solution. This represents an inviting scheme to reformulate many problems in subsurface hydrology. In groundwater hydrology, the method of decomposition has been used to analyze transient groundwater flow subject to random transmissivity (Serrano and Unny, 1987), to obtain a general solution of the random dispersion equation (Serrano, 1988), and to develop semianalytical solution of flow and transport equations subject to erratic variability in the velocity field (Serrano, 1992b). Recently some analytical solutions of the nonlinear groundwater flow equation (Serrano, 1995a) were presented. New refinements in the decomposition method (Adomian, 1991, 1994) were used to derive and solve transport equations with spatially variable dispersion parameters and compared with corresponding exact solutions (Serrano and Adomian, 1995).

THE VELOCITY FIELD IN A HETEROGENEOUS AQUIFER UNDER RECHARGE

In this section, the form of the groundwater velocity in a heterogeneous, long (as compared with its thickness), hypothetical unconfined aquifer exhibiting mild slopes and under steady recharge from rainfall is investigated. The governing flow equation with Dupuit assumptions is (Bear, 1979)

$$\frac{\partial}{\partial x}\left(T(x, y)\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T(x, y)\frac{\partial h}{\partial y}\right) = -I, \qquad 0 < x < \infty, -\infty < y < \infty \tag{1}$$

where $h(x, y)$ is the hydraulic head (m) above a specified datum; $T(x, y)$ is the aquifer transmissivity (m^2/month); x, y are the planar Cartesian coordinates (m); and I is the mean monthly recharge rate (m/month).

In this study our attention is focused on an aquifer with a regional groundwater flow direction coinciding with x and negligible net velocity in the y direction (i.e., "the Dagan aquifer"). In such a aquifer, the regional hydraulic gradients operate in the x direction mainly 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, whereas a relatively small increase in the transverse one. To gain insight into the effect of recharge and aquifer hydrology on the dispersion process, the problem is simplified by assuming that the transverse dispersion coefficient is not spatially dependent, and that the transmissivity field has a stationary correlation structure. In another section of this paper, a generalization to nonstationary velocity fields in three-dimensional domains is attempted. Thus, the transmissivity is represented as $T = \overline{T} + T'$, where $\overline{T} = E\{T\}$, $E\{\ \}$ is 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 is the transmissivity variance parameter ($(m^2/\text{month})^2$), and ρ is a correlation decay parameter (m^{-1}).

Without loss of generality, a knowledge of the boundary conditions at a point in the aquifer is assumed, $h(0, 0) = h_0$, $\partial h/\partial x(0, 0) = h_0'$, and $\partial h/\partial y\ (0, 0) = 0$. Selecting dimensionless spatial coordinate $\chi = x/L$, where L is a typical length (m), the longitudinal groundwater flow equation becomes

$$\frac{\partial^2 h}{\partial \chi^2} = -\frac{IL^2}{\overline{T}} - \frac{T'}{\overline{T}}\frac{\partial^2 h}{\partial \chi^2} - \frac{1}{\overline{T}}\frac{\partial T'}{\partial \chi}\frac{\partial h}{\partial \chi}, \qquad 0 < \chi < \infty \tag{2}$$

The boundary conditions on Equation (2) are $h(0) = h_0$, $\partial h/\partial \chi\ (0) = Lh_0'$.

The solution to Equation (2) may be expressed as $h = V + W$, where V satisfies

$$\frac{\partial^2 V}{\partial \chi^2} = -\frac{IL^2}{\overline{T}},\ V(0) = h_0, \qquad \frac{\partial V}{\partial \chi} = Lh_0' \tag{3}$$

and W satisfies

$$\frac{\partial^2 W}{\partial \chi^2} = f(\chi) = -\frac{T'}{\overline{T}}\frac{\partial^2 W}{\partial \chi^2} - \frac{1}{\overline{T}}\frac{\partial T'}{\partial \chi}\frac{\partial W}{\partial \chi} \tag{4}$$

The solution to Equation (3) is simply

$$V(\chi) = h_0 + Lh'_{0\chi} - \frac{IL^2\chi^2}{2\bar{T}} \tag{5}$$

The solution to Equation (4) may be expressed as

$$W(\chi) = \int_0^\infty G(\chi, \xi) f(\xi) d\xi \tag{6}$$

Because the Green's function associated with Equation (4) is $G(\chi, \xi) = U(\chi - \xi)(\chi - \xi)$, where $U(\ )$ is the unit step function, then the potential distribution in the aquifer is given by

$$h(\chi) = V(\chi) - \frac{1}{\bar{T}} \int_0^\chi (\chi - \xi) R(\xi) h(\xi) d\xi \tag{7}$$

where the random operator R is given by

$$R(\xi)h(\xi) = \left[T'(\xi) \frac{\partial^2}{\partial \xi^2} + \frac{\partial T'(\xi)}{\partial \xi} \frac{\partial}{\partial \xi} \right] h(\xi) \tag{8}$$

A decomposition series (Serrano, 1988) of (7) will yield the series $h(\chi) = \nu_1 + \nu_2 + \nu_3 + \ldots$, where

$$\nu_1(\chi) = V(\chi) \tag{9}$$

and any subsequent term

$$\nu_i(\chi) = -\frac{1}{\bar{T}} \int_0^\chi (\chi - \xi) R(\xi) \nu_{i-1}(\xi) d\xi, \qquad i > 1 \tag{10}$$

Numerical tests on the convergence rate of the series indicated that with moderately large realizations of the transmissivity of about 50% above or below an average of 1000.0 m^2/month, two terms in the series will generate a relative error of about 0.25%. For more rigorous tests on the convergence rate of decomposition series solutions to transport equations subject to large-variance parameters the reader is referred to Serrano (1992b). For a rigorous mathematical treatment of the convergence problem of decomposition series, the reader is referred to Gabet (1992, 1993, 1994), Abbaoui and Cherruault (1994), Cherruault (1989), and Cherruault, Saccomardi, and Some (1992).

With two terms in the series Equation (7) reduces to

$$\begin{aligned} h(\chi) = h_0 + Lh'_0\chi - \frac{IL^2\chi^2}{2\bar{T}} + \frac{IL^2}{\bar{T}^2} \int_0^\chi (\chi - \xi) \left[T'(\xi) + \xi \frac{\partial T'(\xi)}{\partial \xi} \right] d\xi \\ - \frac{Lh'_0}{\bar{T}} \int_0^\chi (\chi - \xi) \frac{\partial T'(\xi)}{\partial \xi} d\xi \end{aligned} \tag{11}$$

The total discharge in the χ direction per unit width is given by

$$q(\chi) = -(\overline{T} + T'(\chi)) \frac{\partial h}{\partial \chi}$$

Differentiating Equation (11), using Leibnitz's rule for differentiation of integrals, and substituting into the expression, the specific discharge could be written as $q(\chi) = \overline{q}(\chi) + q'(\chi)$, where

$$\overline{q}(\chi) = -Lh_0'\overline{T} + IL^2 r\chi + \frac{Lh_0'\sigma_T^2}{\overline{T}}(1 - e^{-\rho\chi}) \tag{12}$$

$$q'(\chi) = \left[\frac{IL^2\chi}{\overline{T}} - Lh_0'\right] T'(\chi) - \frac{IL^2}{\overline{T}} \int_0^\chi \left[T'(\xi) + \xi \frac{\partial T'(\xi)}{\partial \xi}\right] d\xi$$
$$+ Lh_0' \int_0^\chi \frac{\partial T'(\xi)}{\partial \xi} d\xi \tag{13}$$

$r = 1 - C_v^2$, $C_v = \sigma_T/\overline{T}$, the coefficient of variability of the transmissivity. Substituting χ by x/L in (12), and dividing by L, one finds the specific discharge, integrated for the depth, in terms of scalar distance:

$$E\{q(x)\} = \overline{q}(x) = -h_0'\overline{T} + Irx + \frac{h_0'\sigma_T^2}{\overline{T}}(1 - e^{-\rho x/L}) \tag{14}$$

Finally, the seepage velocity is given as $u(x) = \overline{u}(x) + u'(x)$, with $\overline{u}(x) = \overline{q}(x)/(nh_0)$, $u'(x) = q'(x)/(nh_0)$ and n the mean aquifer porosity.

Equation (14) indicates that the groundwater velocity varies with distance, with the recharge intensity, and with the degree of variability and correlation of the transmissivity. A few numerical tests further suggest that the aquifer geohydrologic variables play a more important role in determining the magnitude and evolution of the mean velocity field than the statistical variability and spatial correlation in the transmissivity. For example, Figure 1 shows the spatial distribution of the seepage velocity of an aquifer with the following properties: $h_0 = 10.0$ m, $L = 100.0$ m, $h_0' = -0.001$, $n = 0.3$, $I = 0.01$ m/month (10.0 mm/month), and $\overline{T} = 100.0$ m^2/month. Large variations in the correlation decay parameter, ρ, seem to have little effect on the velocity distribution, which would support an assumption neglecting the third term in Equation (14). The magnitude of the coefficient of variability of the transmissivity is relatively more important, but the recharge rate, the hydraulic gradient the porosity and the mean transmissivity seem to be the determinant elements of the magnitude and distribution of the mean seepage velocity. An interesting result is that a higher degree of variability in the transmissivity, as expressed by higher values in C_v, tend to

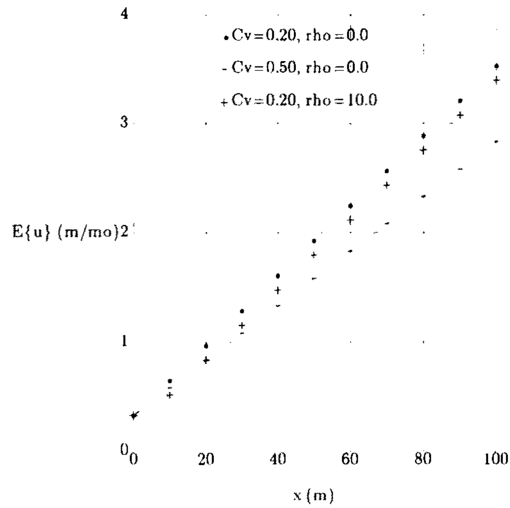

Figure 1. Expected seepage velocity with distance.

decrease the overall value of the mean seepage velocity, which suggests that groundwater velocities in heterogeneous aquifers are controlled by the sections with the lower, rather than the higher, transmissivities. However, these results need to be field verified.

THE DISPERSION EQUATION IN A HETEROGENEOUS AQUIFER

In this section we derive the form of the two-dimensional solute dispersion equation in the same hypothetical aquifer studied in the previous section. Assuming that the fundamental physical principles of convection, mechanical dispersion, and molecular diffusion hold, the general dispersion equation is (Bear, 1979)

$$\frac{\partial nC}{\partial t} - \nabla(D \cdot \nabla C) + \nabla \cdot (uC) = 0 \tag{15}$$

where C represents solute concentration (mg/l); t is the same coordinate (months); D is the dispersion tensor (m^2/month); u is the velocity vector (m/month); ∇ is the gradient operator. In a two-dimensional aquifer with Dupuit assumptions, regional groundwater velocity coinciding with x, principal dispersion components (longitudinal and transverse respectively) coinciding with x and y, and the dispersion coefficients expressed as functions of the variable field velocity, $\alpha_l u$ and $\alpha_t u$ (advection-dominated transport), where α_l and α_t are the longitudinal and transverse dispersivities respectively, Equation (15) becomes

$$\frac{\partial C}{\partial t} - \alpha_l u \frac{\partial^2 C}{\partial x^2} + \left(u - \alpha_l \frac{\partial u}{\partial x}\right) \frac{\partial C}{\partial x} + \frac{\partial u}{\partial x} C - \alpha_t u \frac{\partial^2 C}{\partial y^2} = 0,$$

$$-\infty < x < \infty, \ -\infty < y < \infty, \ 0 < t \tag{16}$$

Assuming no net velocity in the y direction, this is the two-dimensional version of the VDE in a heterogeneous aquifer. It reiterates the dependence of the dispersion coefficient on distance in an aquifer with nonuniform velocity. In this situation, the dispersion coefficient does not seem to reach an asymptotic value, and physically it will continue to grow to the end of the recharge zone. Equation (16) is subject to $C(\pm\infty, \pm\infty, t) = 0$, $C(x, y, 0) = C_i\delta(x)\delta(y)$, where C_i is a constant and $\delta(\ )$ is the Dirac's delta function (an "instantaneous spill" at $t = 0$). Substituting the deterministic and random components of u into Equation (16) and placing the random terms on the right side we obtain

$$\frac{\partial C}{\partial t} - \alpha_l \bar{u} \frac{\partial^2 C}{\partial x^2} + \left(\bar{u} - \alpha_l \frac{\partial \bar{u}}{\partial x}\right) \frac{\partial C}{\partial x} + \frac{\partial \bar{u}}{\partial x} C - \alpha_t \bar{u} \frac{\partial C}{\partial y^2} = Q(x, y)C \tag{17}$$

where the operator Q is given by

$$Q(x, y)C = \left|\alpha_l u' \frac{\partial^2}{\partial x^2} - \left(u' - \alpha_l \frac{\partial u'}{\partial x}\right) \frac{\partial}{\partial x} - \frac{\partial u'}{\partial x} + \alpha_t u' \frac{\partial^2}{\partial y^2}\right| C \tag{18}$$

The solution to Equation (17) can be written as

$$C(x, y, t) = C_i G(x, 0; y, 0; t, 0) + \int_0^t \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(x, x'; y, y'; t, t')Q(x', y', t') \cdot C(x', y', t')dt'dx'dy', \tag{19}$$

where $G(x, x'; y, y'; t, t')$ is the Green's function associated with Equation (17). A decomposition series solution to this equation may be expressed as (Serrano, 1988, 1992b).

$$C = g_1 + g_2 = \cdots \tag{20}$$

with

$$g_1(x, y, t) = C_i G(x, 0; y, 0; t, 0) \tag{21}$$

and in general

$$g_i(x, y, t) = \int_0^t \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(x, x'; y, y'; t, t') \cdot Q(x', y', t')g_{i-1}(x', y', t')dt'dx'dy' \tag{22}$$

Truncating the series at $i = 2$, which is a level acceptable in most previous applications, and taking expectations on Equation (19), thus the mean concentration is $E\{C(x, y, t)\} = \overline{C} = g_1$, which implies that the mean concentration satisfies Equation (17) with the right side set to zero. Substituting for the terms containing $\overline{u}$ and its derivatives, using Equation (14) after neglecting its third term, into Equation (17) we obtain the differential equation satisfying the mean concentration:

$$\frac{\partial \overline{C}}{\partial t} - \frac{\alpha_l}{nh_0}(Irx - h_0'\overline{T})\frac{\partial^2 \overline{C}}{\partial x^2} + \frac{1}{nh_0}(Irx - h_0'\overline{T} - \alpha_l rI)\frac{\partial \overline{C}}{\partial x}$$

$$+ \frac{Ir}{nh_0}\overline{C} - \frac{\alpha_t}{nh_0}(Irx - h_0'\overline{T})\frac{\partial^2 \overline{C}}{\partial y^2} = 0 \tag{23}$$

Now selecting a dimensionless time coordinate $\tau = It/nh_0$; dimensionless spatial coordinates $\chi = x/L$, $\eta = y/L$, and $\xi = r\chi + b$; dimensionless dispersivities $a = \alpha_l/L$ and $\beta = \alpha_t/L$; and the dimensionless velocity at the origin $b = -h_0'\overline{T}/LI$, the dimensionless form of Equation (23) is

$$\frac{\partial \overline{C}}{\partial \tau} - ar^2\xi\frac{\partial^2 \overline{C}}{\partial \xi^2} + r(\xi - ra)\frac{\partial \overline{C}}{\partial \xi} + r\overline{C} - \beta\xi\frac{\partial^2 \overline{C}}{\partial \eta^2} = 0,$$

$$-\infty < \xi < \infty,\ -\infty < \eta < \infty,\ 0 < \tau$$

$$\overline{C}(\pm\infty, \eta, \tau) = \overline{C}(\xi, \pm\infty, \tau) = 0;\ \overline{C}(\xi, \eta, 0) = \delta(\xi - b)\delta(\eta) \tag{24}$$

This is the two-dimensional version of the dimensionless VDE derived by Serrano (1992a).

SOLUTION TO THE VARIABLE DISPERSION EQUATION

An exact solution of Equation (24) may be approached initially via defining the Fourier transform of the mean concentration as

$$F\{\overline{C}\} = c(\xi, \lambda, \tau) = \int_{-\infty}^{\infty} e^{j\lambda\eta}\overline{C}(\xi, \eta, \tau)d\eta, \qquad j = \sqrt{-1} \tag{25}$$

which reduces Equation (24) to

$$\frac{\partial c}{\partial \tau} - ar^2\xi\frac{\partial^2 c}{\partial \xi^2} + r(\xi - ra)\frac{\partial c}{\partial \xi} + (r + \lambda^2\beta\xi)c = 0$$

$$c(\pm\infty, \lambda, \tau) = 0, \qquad c(\xi, \lambda, 0) = \delta(\xi - b) \tag{26}$$

Now define the Laplace transform as

$$\mathcal{L}\{c(\xi, \lambda, \tau)\} = C'(\xi, \lambda, s) = \int_0^{\infty} e^{-s\tau}c(\xi, \lambda, \tau)d\tau \tag{27}$$

which reduces Equation (26) to

$$ar^2\xi \frac{\partial^2 C'}{\partial \xi^2} - r(\xi - ra)\frac{\partial C'}{\tau\xi} - (\lambda^2\beta\xi + r + s)C' = -\delta(\xi - b)$$

$$C'(\pm\infty, \lambda, s) = 0 \tag{28}$$

After solving this equation and inverting the Laplace transform (Serrano, 1992a),

$$C'(\xi, \lambda, \tau) = \frac{\exp\left|\left(1 - \frac{ar}{2}ar\right)(\xi - b)\right| \exp\left\{-\left|ar^2\left(1 - \frac{ar}{2}ar\right)^2 + \lambda^2\beta + r\right|\tau\right\}}{\sqrt{(4\pi ar^2\tau^3}} \cdot \int_{\infty}^{\xi - b} \left(\frac{\xi - b - 2\rho}{\rho}\right) \exp\left\{-\left|\frac{(\xi - b + 2\rho)^2}{4ar^2\tau} - \rho\right|\right\} d\rho \tag{29}$$

Inverting Equation (29) will yield the desired solution for the mean concentration, which may be expressed as

$$\overline{C}(\xi, \eta, \tau) = C_i \Psi(\xi, \tau), \Phi(\eta, \tau) \tag{30}$$

$$\Psi(\xi, \tau) = \frac{\exp\left|\left(1 - \frac{ar}{2}ar\right)(\xi - b)\right| \exp\left\{-\left|ar^2\left(1 - \frac{ar}{2}ar\right)^2 + r\right|\tau\right\}}{\sqrt{4\pi ar^2\tau^3}} \cdot \int_{-\infty}^{\xi - b} \left(\frac{\xi - b + 2\rho)}{\rho}\right) \exp\left\{-\left|\frac{(\xi - b + 2\rho)^2}{4ar^2\tau} - \rho\right|\right\} d\rho \tag{31}$$

$$\Phi(\eta, \tau) = \frac{1}{\sqrt{4\pi\beta\tau}} \exp\left(-\frac{\eta^2}{4\beta\tau}\right) \tag{32}$$

Serrano (1992a) used the one-dimensional deterministic version of this solution to investigate the relative effect of recharge rate, transmissivity, hydraulic gradient, aquifer thickness, and soil porosity on contaminant distribution in an aquifer. However, it has been determined that this solution exists and is stable for only a few values of the parameter a, which limits its applicability to only a few theoretical results. An alternative decomposition series solution to the VDE will offer flexibility with respect to the selection of the parameters while providing the convenience of a successive computational scheme. From Equation (30) and Equation (31) we may see that, in terms of χ and τ, Ψ satisfies

$$\frac{\partial \Psi}{\partial \tau} - ab\frac{\partial^2 \Psi}{\partial \chi^2} + b\frac{\partial \Psi}{\partial \chi} = O(\chi, \tau)\Psi \tag{33}$$

where the operator O is given by

$$O(\chi, \tau)\Psi = r\left[a\chi\frac{\partial^2}{\partial \chi^2} - (\chi - a)\frac{\partial}{\partial \chi} - 1\right]\Psi \tag{34}$$

Formally, the solution to Equation (33) is

$$\Psi(\chi, \tau) = G(\chi, 0; \tau, 0) + \int_0^\tau \int_{-\infty}^{\infty} G(\chi, \chi'; \tau, \tau')O(\chi', \tau')\Psi(\chi', \tau')d\chi' d\tau' \tag{35}$$

where G in this situation is the well known Green's function of the CDE,

$$G(\chi, \chi'; \tau, \tau') = \frac{1}{\sqrt{4\pi ab(\tau - \tau')}}\exp\left(-\frac{[\chi - \chi' - b(\tau - \tau')]^2}{4ab(\tau - \tau')}\right) \tag{36}$$

Now a decomposition series solution for Equation (35) is constructed, one which uses the CDE as an initial iteration and its well-behaved kernel for subsequent iterations (Serrano, 1992b): $\Psi = \psi_1 + \psi_2 + \cdots$, where

$$\psi_1(\chi, \tau) = G(\chi, 0; \tau, 0) \tag{37}$$

$$\psi_i(\chi, \tau) = \int_0^\tau \int_{-\infty}^{\infty} G(\chi, \chi'; \tau, \tau')O(\chi', \tau')\psi_{i-1}(\chi', \tau')d\chi' d\tau' \tag{38}$$

A theorem with proof delineating the convergence conditions of a decomposition series similar to the given one was presented by Serrano (1992b). The most critical criterion would require that $r(\chi_{max} - a)\tau_{max}/2 < 1$, where χ_{max} and τ_{max} are the maximum dimensionless distance and dimensionless time in the simulations, respectively. This condition is satisfied easily in the verification tests, as seen in the next section. With two terms in the series (initial numerical tests indicated that additional terms contributed less than 10% to the solution), the integrand in Equation (38) is analytical and the solution to the VDE, in summary, reduces to

$$\overline{C}(\chi, \eta, \tau) = C_i\Psi(\chi, \tau) \cdot \Phi(\eta, \tau) \tag{39}$$

$$\Psi(\chi, \tau) = G(\chi, 0; \tau, 0) + r\int_0^\tau \int_{-\infty}^{\infty} G(\chi, \chi'; \tau, \tau')f(\chi', \tau')d\chi' d\tau' \tag{40}$$

$$f(\chi', \tau') = \frac{\exp\left(-\frac{(x' - b\tau')^2}{4ab\tau'}\right)}{\sqrt{4\pi ab\tau^3}}$$

$$\cdot \left\{ \frac{a\chi'^2(\chi' - b\tau')^2}{(2ab\tau')^2} - \frac{a\chi'^2 + (\chi' - b\tau')(3a\chi' - \chi'^2)}{2ab\tau'} - (2\chi' - a) \right\} \tag{41}$$

$$\Phi(\eta, \tau) = \frac{1}{\sqrt{4\pi\beta(1 - b)\tau}} \exp\left(-\frac{\eta^2}{4\beta(1 + b)\tau}\right) \tag{42}$$

and G is given by Equation (36).

VERIFICATION WITH OTHER THEORTICAL AND FIELD RESULTS

In this section a preliminary comparison of the VDE alternative solution is given. Equations (39) through (42), with the two-dimensional CDE and the two-dimensional Dagan's model as applied to the Borden site experiment. The classical deterministic CDE under constant dispersion coefficient and constant pore velocity resulting from neglecting recharge results from (16) as

$$\frac{\partial C}{\partial t} - \alpha_l u \frac{\partial^2 C}{\partial x^2} + u \frac{\partial C}{\partial x} - \alpha_t u \frac{\partial^2 C}{\partial y^2} = 0,$$

$$-\infty < x < \infty, \ -\infty < y < \infty, \ 0 < t \tag{43}$$

subject to

$$C(\pm\infty, y, t) = 0, \ C(x\ y, 0) = C_i\delta(x)\delta(y) \tag{44}$$

Defining the velocity according to Equation (14) with $I = \sigma_T = 0$, expressing Equation (43) in dimensionless form and solving,

$$C(\chi, \eta, \tau) = C_i \frac{1}{\sqrt{4\pi ab\tau}} \exp\left(-\frac{(\chi - b\tau)^2}{4ab\tau}\right) \frac{1}{\sqrt{4\pi\beta b\tau}} \exp\left(-\frac{\eta^2}{4\beta b\tau}\right) \tag{45}$$

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

$$\frac{\partial \overline{C}}{\partial t} - D_1(t) \frac{\partial^2 \overline{C}}{\partial x^2} + u \frac{\partial \overline{C}}{\partial x} - D_2(t) \frac{\partial^2 \overline{C}}{\partial y^2} = 0,$$

$$-\infty < x < \infty, \ -\infty < y < \infty, \ 0 < t \tag{46}$$

subject to Equation (44). The longitudinal dispersion coefficient is defined as

$$D_1(t) = 0.74ul_Y\sigma_Y^2\left\{1 - 1 \cdot \frac{5}{\gamma} - \frac{3e^{-\gamma}}{\gamma^2} + \frac{3}{\gamma^3}(1 - e^{-\gamma})\right\} + D_{dl} \quad (47)$$

where l_Y and σ_Y^2 are the correlation length and variance of the log hydraulic conductivity, respectively; $\gamma = ut/l_Y$; D_{dl} is the longitudinal pore scale dispersion coefficient. The transverse dispersion coefficient is defined as

$$D_2(t) = \frac{0.74ul_Y\sigma_Y^2}{2\gamma}\left\{1 - \frac{6}{\gamma^2} + 2e^{-\gamma}\left|1 + \frac{3}{\gamma} + \frac{3}{\gamma^2}\right|\right\} + D_{d2} \quad (48)$$

where D_{d2} is the transverse pore scale dispersion coefficient.

The solution to (46) has been derived by Barry and Sposito (1989) as

$$\overline{C}(x, y, t) = C_i \frac{1}{\sqrt{4\pi\phi_1}} \exp\left(-\frac{(x - ut)^2}{4\phi_1}\right) \frac{1}{\sqrt{4\pi\phi_2}} \exp\left(-\frac{y^2}{4\phi_2}\right) \quad (49)$$

where

$$\phi_i(\tau) = \int_0^t D_i(t')dt', \qquad i = 1, 2 \quad (50)$$

The results of the Borden site experiment have been documented extensively in the literature (Mackay and others, 1986). Our attention is focused on the implementation of the two-dimensional Dagan's model to vertically averaged bromide and chloride concentrations at the Borden site reported by Barry, Coves, and Sposito (1988). Incomplete sampling of the solute plume during the early sampling sessions, as well as assumptions made with respect to the data analysis produced an important degree of uncertainty in the specification of the initial conditions of the model (Barry, Coves, and Sposito, 1988). In order to assure identical initial conditions that are not affected by measurement uncertainty or by the particular integration procedure used, it was decided to approximate the initial condition for the three models, the CDE, the Dagan's, and the VDE, as a delta function. Knowing that this assumption will make it difficult to assess the results with respect to the field data, the main features of peak concentration, peak location, and overall plume evolution will be observed.

The parameter values for the Borden aquifer are: $\alpha_l = 0.011$ m; $\alpha_t = 0.0033$ m; $\sigma_Y^2 = 0.24$; $l_Y = 2.8$ m; $\overline{u} = 0.091$ m/day; $D_{d1} = 0.001$ m^2/day; $D_{d2} = 0.0003$ m^2/day; $h_0' = 6.0$ m; $n = 0.33$; the mean hydraulic conductivity $\overline{K} = 6.18$ m/day; $h_0' = 0.0056$; $\overline{T} = \overline{K}h_0 = 1112.4$ m^2/month; for a lognormal distribution, the variance of the hydraulic conductivity is $\sigma_K^2 = \overline{K}^2(e^{\sigma_Y^2} - 1) =$

10.36 $(m^2/day)^2$, or σ_K = 3.22 m^2/day; the transmissivity standard deviation is $\sigma_T = \sigma_K h_0$ = 19.39 m^2/day = 579.34 m^2/month; the coefficient of variability for the hydraulic conductivity or the transmissivity, $C_v = \sigma_T/\overline{T}$ = 0.52; if we set L = 1, then $a = \alpha_l/L$ = 0.011, $\beta = \alpha_t/L$ = 0.0033; with a moderate recharge value of I = 0.01 m/month for southwestern Ontario obtained from water balance studies (Serrano, Whiteley, and Irwin, 1985), we have $b = -h_0\overline{T}/LI$ = 622.94; setting values of t in months, corresponding values of $\tau = It/nh_0$ can be obtained.

Simulations were done using three models to calculate concentration distributions at times corresponding to the measurement schedule after tracer injection at the Borden site (Mackay and others, 1986). A realistic value of resident initial concentration at the time of injection, C_i, may be deduced from the vertically integrated surfaces fitted to measured data one day after injection (Barry, Coves, and Sposito, 1988). For the situation of Bromide, 3.87 kg of solute were injected. Knowing that the tracer occupied about 25 m^2 of surface area, an integrating depth of 6.0 m, and an average porosity of 0.33, the initial resident concentration is approximately 78.2 mg/l.

A comparison with measured results (in particular with those of Barry, Coves, and Sposito (1988), which depict the plume evolution) suggests that the three models approximate well the location of the peak concentration at any time. Figure 2 shows the simulated Bromide breakthrough curve along the x axis (assumed as coinciding with the regional groundwater flow direction) at

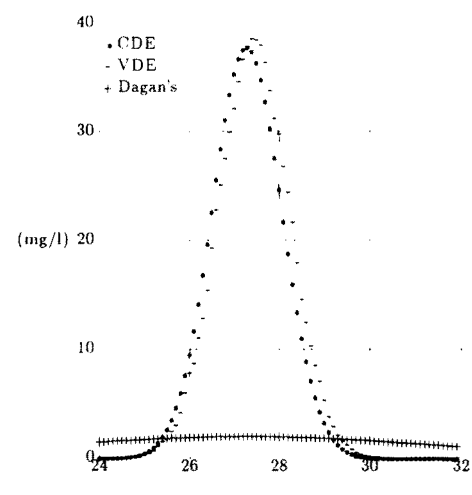

Figure 2. Comparison between CDE, VDE, and Dagan's model as applied to Borden site.

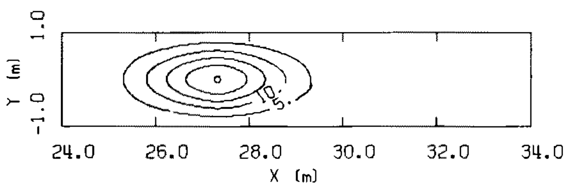

Figure 3. Bromide concentration contours (mg/l) according to VDE.

t = 260 days Figure 3 shows the simulated Bromide areal distribution using the VDE at the same time, and Figure 4 the corresponding areal distribution using the Dagan's model.

The models exhibit inherent differences worth noting. The VDE and the CDE in this example seem to predict well the peak concentration magnitude, but exhibit substantially lower spatial contaminant dispersion, whereas the Dagan's model predicts a lower peak concentration magnitude, but a large spatial contaminant dispersion. Because of the increasing value of the dispersion coefficient with distance, the VDE produces a shifted plume with somewhat greater spatial dispersion than that of the CDE. This discrepancy will increase as the travel distance increases [see Serrano (1992a), Fig. 2 for an observation of this effect with the exact dimensionless VDE]. The Dagan's model-generated plume increases in dispersion with travel time with a dispersion coefficient reaching an asymptotic value. A possible explanation for the discrepancy between the Dagan model and the VDE lies in the differences in the mathematical procedure employed. The Dagan model assumes a Gaussian probability distribution for $\log(K)$, whereas the present work does not assume a particular probability law and considers the statistical properties of the actual transmissivity; also the Dagan model uses the small perturbation method of solution of the differential

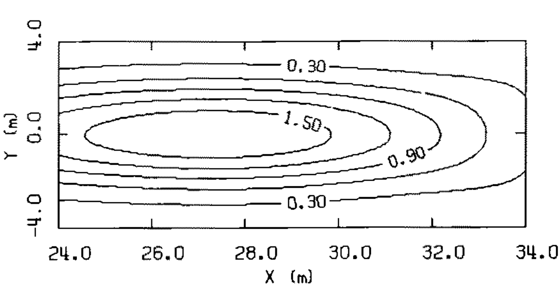

Figure 4. Bromide concentration contours (mg/l) according to Dagan's model.

equations, whereas the present work uses the method of decomposition and does not impose a restriction on the size of the random terms.

The Dagan's model seems to be sensitive to hydraulic conductivity variability. A moderate coefficient of variability, $C_r = 0.2$ for the "raw" hydraulic conductivity will cause a reduction of about 50% in peak concentration and a corresponding enhanced spatial dispersion with respect to the CDE. As $C_r \to 0$ ($\sigma_Y^2 \to 0$), the Dagan's model coincides with the CDE. The VDE produces an opposite effect with respect to variability in the transmissivity. Although being substantially less sensitive to C_r, the VDE produces a plume with a decreasing shifting and enhanced dispersion effect as C_r increases. As $C_r \to 1.0$, the VDE coincides with the CDE. However, as $C_r \to 0.0$, the discrepancy between the CDE and the VDE is maximum. An objective physical explanation of this inverse effect with respect to statistical transmissivity variability is given in the section on "The Velocity Field . . ." (i.e., Fig. 1), where it was determined that the greater the value of C_r the less the mean groundwater velocity.

GENERALIZATION TO THREE-DIMENSIONAL NONSTATIONARY DISPERSION

The theoretical development in the previous sections assumed a stationary exponential correlation structure in the transmissivity, and a two-dimensional dispersion in essentially a one-dimensional flow field. The transverse dispersion was considered independent of spatial coordinates. An improvement of this scenario added spatial dependency in the transverse dispersion, and studied the effect of chemical spills originated in the unsaturated zone on the resulting nonpoint source and nonsymmetric plume in the saturated zone (Serrano, 1995b). An additional improvement considered a two-dimensional transmissivity correlation structure (Serrano, 1995a).

Recent refinements in the decomposition method (Adomian, 1991, 1994) suggest that a generalization of this approach to three-dimensional domains subject to more realistic nonstationary velocity fields is possible. Consider for example the three-dimensional solute continuity equation in a large domain. For simplicity let us neglect the Fickian dispersion caused by local heterogeneities:

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(u_x C) + \frac{\partial}{\partial y}(u_y C) + \frac{\partial}{\partial z}(u_z C) = 0, \qquad C(x, y, z, t) \in \Gamma,\ 0 < t$$

$$C = 0, \qquad C \in \partial\Gamma$$

$$C(x, y\, z, 0) = f(x, y, z) \tag{51}$$

where f represents the known initial contaminant distribution; and u_x, u_y, u_z are the three-dimensional nonstationary transient velocity components whose statistical properties are functions of the known statistical properties of the hydraulic conductivity, the aquifer boundary conditions and the recharge rate. The new decomposition procedure would rewrite (51) as

$$L_t C + \frac{\partial}{\partial x}(u_x C) + \frac{\partial}{\partial y}(u_y C) + \frac{\partial}{\partial z}(u_z C) = 0 \tag{52}$$

where $L_t = \partial/\partial t$, and its inverse, L_t^{-1} is the definite integral from 0 to t. Operating with the inverse, the solution to (52) is

$$C = -L_t^{-1}\frac{\partial}{\partial x}(u_x C) - L_t^{-1}\frac{\partial}{\partial y}(u_y C) - L_t^{-1}\frac{\partial}{\partial z}(u_z C) \tag{53}$$

C in the right side of (52) may be expressed as the series

$$C = C_0 + C_1 + C_2 + \cdots \tag{54}$$

or after taking expectations

$$\overline{C} = \overline{C}_0 + \overline{C}_1 + \overline{C}_2 + \cdots \tag{55}$$

where C, $\overline{C}_0$, $\overline{C}_1$, $\overline{C}_2$, . . . are $E\{C\}$, $E\{C_0\}$, $E\{C_1\}$, $E\{C_2\}$, . . . respectively. The first term in the decomposition series is:

$$C_0 = \overline{C}_0 = f \tag{56}$$

Thus, the first term in the series is the initial condition. Similarly

$$C_1 = -L_t^{-1}\frac{\partial}{\partial x}(u_x C_0) - L_t^{-1}\frac{\partial}{\partial y}(u_y C_0) - L_t^{-1}\frac{\partial}{\partial z}(u_z C_0)$$

$$C_1 = -L_t^{-1}\frac{\partial u_x}{\partial x} f - L_t^{-1} u_x \frac{\partial f}{\partial x} - L_t^{-1}\frac{\partial u_y}{\partial y} f - L_t^{-1} u_y \frac{\partial f}{\partial y}$$
$$- L_t^{-1}\frac{\partial u_z}{\partial z} f - L_t^{-1} u_z \frac{\partial f}{\partial z}$$

$$\overline{C}_1 = -L_t^{-1}\frac{\partial \overline{u}_x}{\partial x} f - L_t^{-1} \overline{u}_x \frac{\partial f}{\partial x} - L_t^{-1}\frac{\partial \overline{u}_y}{\partial y} f - L_t^{-1} \overline{u}_y \frac{\partial f}{\partial y}$$
$$- L_t^{-1}\frac{\partial \overline{u}_z}{\partial z} f - L_t^{-1} \overline{u}_z \frac{\partial f}{\partial z} \tag{57}$$

Thus the second term in the series is based on the previously computed first term and on the known first moment of the velocity. In general, any term could be computed as

$$C_i = -L_t^{-1}\frac{\partial}{\partial x}(u_x C_{i-1}) - L_t^{-1}\frac{\partial}{\partial y}(u_y C_{i-1}) - L_t^{-1}\frac{\partial}{\partial z}(u_z C_{i-1}), \qquad i \geq 1 \tag{58}$$

that is the ith order term is based on the $(i - 1)$th order term, and the expected ith order term is based on the ith order, or lower order, moment of the random input terms, but not higher order (i.e., hierarchy methods). This is an important feature that allows the modeler to compute decomposition terms up to the corresponding known order of the random terms in the differential equation without having to neglect unknown higher order moments. If the field in question is Gaussian, then an infinite set of terms (an exact solution) in principle could be determined. Without information on the particular probability law of the velocity field, which is the usual situation, we may approximate a solution to the transport differential equation if information on the lower order moments of the random functions is available. For instance, if information up to the second-order moment in the input quantities is available, the expected mean term in the series is from (57),

$$
\begin{aligned}
\overline{C}_2 = L_t^{-1} L_t^{-1} \Bigg\{ & 2 \frac{\partial \overline{u_x u_x}}{\partial x} \frac{\partial f}{\partial x} + \frac{\partial^2 \overline{u_x u_x}}{\partial x^2} f + \overline{u_x u_x} \frac{\partial f}{\partial x} + \frac{\partial^2 \overline{u_x u_y}}{\partial x \partial y} f \\
& + \frac{\partial \overline{u_x u_y}}{\partial y} \frac{\partial f}{\partial x} + \frac{\partial \overline{u_x u_y}}{\partial x} \frac{\partial f}{\partial y} + \overline{u_x u_y} \frac{\partial^2 f}{\partial x \partial y} + \frac{\partial^2 \overline{u_x u_z}}{\partial x \partial z} f \\
& + \frac{\partial \overline{u_x u_z}}{\partial z} \frac{\partial f}{\partial x} + \frac{\partial \overline{u_x u_z}}{\partial x} \frac{\partial f}{\partial z} + \overline{u_x u_z} \frac{\partial^2 f}{\partial x \partial z} \frac{\partial^2 \overline{u_x u_y}}{\partial x \partial y} f \\
& + \frac{\partial \overline{u_x u_y}}{\partial x} \frac{\partial f}{\partial y} + \frac{\partial \overline{u_x u_y}}{\partial y} \frac{\partial f}{\partial x} + \overline{u_x u_y} \frac{\partial^2 f}{\partial x \partial y} + \frac{\partial^2 \overline{u_y u_y}}{\partial y^2} f \\
& + 2 \frac{\partial \overline{u_y u_y}}{\partial y} \frac{\partial f}{\partial y} + \overline{u_y u_y} \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 \overline{u_y u_z}}{\partial y \partial z} f + \frac{\partial \overline{u_y u_z}}{\partial z} \frac{\partial f}{\partial y} \\
& + \frac{\partial \overline{u_y u_z}}{\partial y} \frac{\partial f}{\partial z} + \overline{u_y u_z} \frac{\partial^2 f}{\partial y \partial z} + \frac{\partial^2 \overline{u_x u_z}}{\partial x \partial z} f + \frac{\partial \overline{u_x u_z}}{\partial x} \frac{\partial f}{\partial z} \\
& + \frac{\partial \overline{u_x u_z}}{\partial z} \frac{\partial f}{\partial x} + \overline{u_x u_z} \frac{\partial^2 f}{\partial x \partial z} + \frac{\partial^2 \overline{u_y u_z}}{\partial y \partial z} f + \frac{\partial \overline{u_y u_z}}{\partial y} \frac{\partial f}{\partial z} \\
& + \frac{\partial \overline{u_y u_z}}{\partial z} \frac{\partial f}{\partial y} + \overline{u_y u_z} \frac{\partial^2 f}{\partial y \partial z} + \frac{\partial^2 \overline{u_z u_z}}{\partial z^2} f + 2 \frac{\partial \overline{u_z u_z}}{\partial z} \frac{\partial f}{\partial z} + \overline{u_z u_z} \frac{\partial^2 f}{\partial z^2} \Bigg\} \qquad (59)
\end{aligned}
$$

where $\overline{u_i u_j}$ represents the (cross) correlation function $E\{u_i u_j\}$. Equation (59) indicates that the expected third term in the decomposition series requires up to the second-order moment of the velocity field, but not higher than two. All of the terms in (52) are computable and analytic if the velocity correlation functions (i.e., if the transmissivity correlation), and the initial conditions are analytic. This represents a promising procedure to study dispersion in heterogeneous aquifers subject to varied forms nonstationary velocity fields. Current research is focusing on the definition of the general form of hydraulic conductivity and velocity fields using the concept of fractal geometry (i.e., Paredes and Elorza, 1992; Wheatcraft and Tyler, 1988).

CONCLUSIONS

An investigation into the characteristics of the dispersion equation in heterogeneous aquifers subject to recharge and nonuniform velocity was conducted. The method of decomposition, which does not require small perturbation assumptions, logarithmic transformations, or specific probability laws, was employed. The results indicated that aquifer regional hydrogeologic variables such as mean transmissivity, hydraulic gradient, mean porosity, aquifer thickness, and recharge rate from rainfall generate a variable with distance mean groundwater velocity, which in turn produces a variable with distance dispersion coefficient. Aquifer heterogeneity, as represented by the statistical spatial variability of the transmissivity, seems to play a less important role in the magnitude and spatial variability of the dispersion coefficient. Greater transmissivity variances seem to produce relatively lower values of mean groundwater velocity, in contrast to what is accepted currently, which implies that the mean velocity in a long, thin, aquifer is controlled by the lower realizations, rather than the higher values, and that mean dispersion in a homogeneous aquifer is greater than in a heterogeneous one with the same mean transmissivity. An equation such as the VDE which includes the functional dependency of the regional variables on the dispersion coefficient seems to partially explain the spatial evolution of the dispersion coefficient and offers a promising concentration forecasting tool for practical applications.

A preliminary field comparison between the VDE, the CDE, and the two-dimensional Dagan's model emphasized the shifting and enhanced dispersion effects of the VDE resulting from a variable velocity field. These effects are maximum if the statistical variability in the transmissivity is minimum (deterministic), as opposed to the Dagan's model which is sensitive to statistical variability in the hydraulic conductivity and produces a greater plume dispersion with greater statistical variability. The dispersion coefficient modeled by the VDE increases with distance to the point where recharge ends, whereas the one modeled by the Dagan's model increases with travel time to an asymptotic value.

Extensions of the analysis to nonstationary dispersion in three-dimensional domains seem promising. Future research should be devoted to the definition of specific forms of conductivity and velocity fields, the transient analysis of regional recharge and its effect on the time and space variability of the dispersion coefficient.

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