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The Form of the Dispersion Equation Under Recharge and Variable Velocity, and Its Analytical Solution

SERGIO E. SERRANO

Department of Civil Engineering, University of Kentucky, Lexington

In this article an attempt is made to describe field scale solute transport parameters in terms of regional hydrologic and aquifer hydraulic properties, such as recharge rate, transmissivity, hydraulic gradient, aquifer thickness and soil porosity. Aquifers subject to natural recharge from rainfall exhibit groundwater velocities which vary with distance and with the recharge intensity. This in turn generates an evolving transport dispersion coefficient which increases with distance even in a homogeneous aquifer with constant dispersivity. The dispersion equation in an aquifer subject to recharge and variable groundwater velocity is one with coefficients given as variable functions of distance. A new stable analytical solution of this equation is presented along with numerical comparisons with the classical convection dispersion equation and sensitivity tests on the effect of hydrologic-hydraulic variables on the contaminant evolution. It was found that the recharge rate substantially affects the contaminant distribution and may partially explain the scale dependence of dispersion parameters. Transmissivity and hydraulic gradient values also determine the velocity distribution and therefore the rate of migration. It would appear that constant, laboratory scale, dispersivities may be sufficient for the modeling of field scale concentrations if an equation which accounts for the effects of hydrologic and hydraulic variables is used.

1. INTRODUCTION

It has become evident that the classical form of the convection dispersion equation (CDE) with constant coefficients is inadequate for describing field scale transport of inert solutes in aquifers. Fitted dispersion coefficients of the CDE are sometimes several orders of magnitude greater than those at the laboratory scale for the same porous media [e.g., *Fried*, 1975]. Field experiments, as well as many theoretical studies, have demonstrated that the dispersion coefficients are functions of time or travel distance [e.g., *Sudicky*, 1986; *Dagan*, 1984], and that new techniques must be developed in order to provide a representation of the concentration field with a clear predictive capability.

Many efforts have been devoted to perfect an understanding of the dispersion phenomena at large scales. Stochastic analyses have been major contributors in this area with a variety of studies investigating the effect of field scale heterogeneities on the dispersion phenomena. Researchers have focused on representations of the hydraulic conductivity tensor as realizations of a random field, and its influence on the groundwater 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]. Recent approaches have concentrated on the definition of the velocity field and the dispersion coefficient as time or spatial random functions [*Serrano*, 1988*a*, *b*; *Rubin*, 1990].

Alternatively, deterministic approaches that account for the scale dependence of dispersion parameters are beginning to appear. For instance, *Pickens and Grisak* [1981] developed a finite element model with a dispersivity parameter as a time function. *Gupta and Bhattacharya* [1986] presented an analysis for the case of periodic porous media. Even less abundant are the analytical solutions of scale dependent dispersion equations. *Barry and Sposito* [1989] introduced an analytical solution of a CDE with time dependent coefficients. Recently, *Yates* [1990] developed an analytical solution with a spatially dependent dispersivity. These encouraging results could be enhanced if the constants and functions involved in the arbitrary representations of the temporal or spatial transport parameters were given a physical interpretation.

The present article attempts to derive a new transport equation with scale dependent parameters given as functions of the regional hydrologic and aquifer hydraulic variables. Under the hypothesis that aquifer physical variables control not only the flow regime but also the concentration evolution and the scale dependence of the dispersion parameters, an effort is made to investigate the effect of some key aquifer properties on the functional form of transport dispersion parameters. The properties considered included natural recharge rate from rainfall, aquifer transmissivity, head hydraulic gradient, aquifer thickness, and aquifer soil porosity. Given the apparent absence of recharge rates in most groundwater dispersion studies and the importance, in principle, of this fundamental hydrologic input function in most regions of the globe, one should feel motivated to consider the effect of recharge from rainfall on dispersion. A hypothetical phreatic aquifer at the regional scale was considered [*Dagan*, 1986] 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. A differential equation governing the flow in this aquifer with the above properties was written and solved for the groundwater pore velocity (section 2). Subsequently, the solute transport dispersion coefficient was written in terms of the above hydrologic and hydraulic properties (section 3), and the corresponding dispersion equation was derived (section 4). Finally, a stable analytical solution of the dimensionless version of the dispersion equation was obtained by using a particular solution in combination with the

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Laplace transform (section 5), and comparison tests with the classical CDE as well as a numerical illustration of the effect of hydrologic and hydraulic properties on the concentration evolution were given (section 6).

2. The Groundwater Flow Velocity Under Steady Recharge

In the past, many studies of dispersion in aquifers have based their theoretical analyses on assumptions of the regional groundwater flow regime. Typical representations include a steady state velocity in the absence of recharge. In this section we intend to derive a simple expression of the groundwater flow velocity in a phreatic aquifer under steady recharge. This expression will in turn help in the definition of the solute dispersion coefficient in terms of measurable aquifer hydraulic parameters (such as the mean transmissivity, the boundary head and hydraulic gradient, the aquifer thickness, the soil porosity) and the regional hydrologic recharge regime. Initially, a homogeneous aquifer is considered, but as will be seen, the effect of recharge on the velocity distribution and the contaminant distribution may be as important as that of aquifer heterogeneity in the hydraulic conductivity.

Consider a long (as compared with its thickness) hypothetical unconfined alluvial aquifer exhibiting mild slopes. The governing flow equation with Dupuit assumptions is [*Bear*, 1979]

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

$$0\leq x<\infty,\ 0\leq y<\infty,$$

where $h(x, y)$ is the hydraulic head (m) above a specified datum; T is the aquifer transmissivity (m^2/month); x, y are the planar Cartesian coordinates (m); and I is the mean aquifer recharge rate from precipitation (m/month). Although in practice a potential constraint is present in the flow system at some distance, the assumption of a semi-infinite aquifer is adopted in order to minimize the number of parameters involved and to reflect the fact that a far-field boundary condition would have little effect on the solute distribution. For a homogeneous aquifer, a regional groundwater velocity coinciding with x and negligible net velocity in the y direction, the flow equation reduces to

$$h_{xx}=-\frac{I}{T}, \qquad (2)$$

where the notation $h_{xx} = \partial^2 h/\partial x^2$ convenient for partial differential equations has been adopted. The boundary conditions imposed on (2) will affect the form of the solution. A practical situation occurs when the observer is located at $x = 0$, a piezometer at that point reads a head value of h_0, and the hydraulic gradient is approximated with the aid of this and a nearby piezometer as equal to h'_0. Presumably $x = 0$ is the location of a hazardous waste spill and the hydrologist is investigating the flow and transport conditions at the origin. Thus the boundary conditions imposed on (2) are

$$h(0)=h_0 \qquad h_x(0)=h'_0. \qquad (3)$$

The solution of (2), subject to (3) is

$$h(x)=h_0+h'_0x-\frac{I}{2T}x^2. \qquad (4)$$

If the hydraulic gradient is negative in the x direction, (4) indicates that h decreases with x. The specific discharge, q, everywhere in the domain of the aquifer is given by

$$q=-Th_x=-Th'_0+Ix, \qquad (5)$$

which indicates that the groundwater velocity will increase linearly with distance at a rate given by the recharge rate I. Note also that the transmissivity, T, and the hydraulic gradient at the origin, h'_0, are scaling parameters having the property of uniformly changing the velocity in the entire aquifer.

3. The Form of the Dispersion Equation Under Recharge

In this section we intend to use the equation of variable velocity, (5), to derive corresponding expressions for the average pore velocity, the dispersion coefficient and ultimately the dispersion differential equation in the same hypothetical phreatic aquifer subject to regional recharge.

The average pore velocity is simply $u = q/n$, where n is the mean aquifer porosity. From (5), the variable pore velocity is

$$u=\frac{1}{n}(Ix-h'_0T). \qquad (6)$$

If we accept that the fundamental physical principles of convection, mechanical dispersion and molecular diffusion are indeed the governing processes of transport of inert solutes in porous media, then the longitudinal dispersion coefficient, D, is given as $D = \alpha q/n$, where α is the dispersivity (m), and the molecular diffusion has been neglected under the assumption that we have advection-dominated transport. Using (6),

$$D=\frac{\alpha}{n}(Ix-h'_0T). \qquad (7)$$

Equation (7) indicates that the dispersion coefficient increases linearly with distance at a rate given by the recharge rate, even in a homogeneous aquifer with a constant dispersivity. We remark that in the present case the growth of the dispersion coefficient is the result of increased flow velocities generated from the recharge to the aquifer and not the result of field heterogeneity at a scale larger than the pore scale. In addition, the dispersion coefficient does not appear to reach an asymptotic value and physically would only decrease at the end of the recharge zone. The CDE is given by [*Bear*, 1979]

$$\frac{\partial nC}{\partial t}-\nabla(n\mathbf{D}\cdot\nabla C)+\nabla\cdot(\mathbf{q}C)=0,$$

where C represents solute concentration (mg/L); t is the time coordinate (months); $\mathbf{D}$ is the dispersion tensor (m^2/month); $\mathbf{q}$ is the velocity vector (m/month); ∇ is the gradient operator; and the rest of the terms are as before. Under the above assumptions this equation reduces to

$$\frac{\partial C}{\partial t} - \nabla(\mathbf{D}\cdot\nabla C) + \frac{\mathbf{q}}{n}\cdot\nabla C + \frac{I}{n}C = 0. \qquad (8)$$

For a homogeneous isotropic one-dimensional medium, **D** and **q** reduce to their longitudinal component, D and q, respectively, and (8) reduces to

$$\frac{\partial C}{\partial t} - \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right) + u\frac{\partial C}{\partial x} + \frac{I}{n}C = 0. \qquad (9)$$

Since D and u are variable functions of x, (9) does not reduce to the classical CDE, but instead to one that we prefer to call variable dispersion equation (VDE). Substituting (6) and (7) into (9) one obtains

$$C_t - \frac{\alpha}{n}(Ix - h_0'T)C_{xx} + \frac{1}{n}(Ix - h_0'T - \alpha I)C_x + \frac{I}{n}C = 0$$

$$0 \le x < \infty,\ 0 \le t < \infty, \qquad (10)$$

where

$$C_t = \frac{\partial C}{\partial t} \qquad C_x = \frac{\partial C}{\partial x} \qquad C_{xx} = \frac{\partial^2 C}{\partial x^2}.$$

It is interesting to note that, except for the dispersivity, the parameters in (10) are conveniently defined in terms of measurable hydrologic and hydraulic variables.

4. Analytical Solution of the Variable Dispersion Equation

In this section an analytical solution of (10) is attempted. It is convenient to represent the differential equation in dimensionless form in order to simplify the algebra and to assure dynamical similitude between model and field prototype. Choosing a dimensionless time coordinate, $\tau = It/nh_0$, and a dimensionless spatial cordinate, $\eta = x/L$, where L is a typical distance, (10) reduces to

$$C_\tau - \frac{\alpha}{L}\left(\eta - \frac{h_0'T}{IL}\right)C_{\eta\eta} + \left(\eta - \frac{h_0'T}{IL} - \frac{\alpha}{L}\right)C_\eta + C = 0$$

$$0 \le \eta < \infty,\ 0 \le \tau \le \infty. \qquad (11)$$

Now set $a = \alpha/L$, the dimensionless dispersivity, $T^* = T/L$, $b = -h_0'T^*/I$, and $\xi = \eta + b$. Then (11) becomes

$$C_\tau - a\xi C_{\xi\xi} + (\xi - a)C_\xi + C = 0 \qquad (12)$$

$$b \le \xi < \infty,\ 0 \le \tau < \infty.$$

We are particularly interested in two cases of practical interest: the case of a constant source boundary condition, and the case of an instantaneous point source at the left boundary. Therefore the boundary and initial conditions imposed on (12) are

$$C(b, \tau) = C_0 \qquad C(\infty, \tau) = 0$$

$$C(\xi, 0) = C_i\delta(\xi - b), \qquad (13)$$

where C_0 is the concentration magnitude at the left boundary, C_i is the concentration magnitude at the time of the spill, and $\delta(\ )$ is the Dirac's delta function. Defining the Laplace transform of C as

$$l\{(C(\xi, \tau)\} = \hat{C}(\xi) = \int_0^\infty e^{-s\tau}C(\xi, \tau)\, d\tau,$$

then the transformed (13) can be written as

$$a\xi\hat{C}_{\xi\xi} - (\xi - a)\hat{C}_\xi - (s+1)\hat{C} = -C_i,\ \delta(\xi - b). \qquad (14)$$

$$\hat{C}(b) = C_0/s \qquad \hat{C}(\infty) = 0. \qquad (15)$$

The solution of (14) is facilitated if one knows a particular solution. When $\xi > b$, a particular solution of the form $e^{m\xi}$, for m constant, exists if

$$a\xi m^2 - (\xi - a)m - (s+1) = 0. \qquad (16)$$

Using the formula for the solution of a quadratic algebraic equation, (16) implies that

$$m = \frac{(1-a) \pm [(1-a)^2 + 4a(s+1)]^{1/2}}{2a}. \qquad (17)$$

We can then express a solution of (14) as one of the form $\hat{C} = e^{m\xi}v$, where v is a function of ξ. Substituting into (14) and simplifying one obtains an ordinary differential equation for v:

$$v_{\xi\xi} + \left[2m - \frac{\xi - a}{a\xi}\right]v_\xi = 0. \qquad (18)$$

This equation may be reduced to a first-order ordinary differential equation by defining $p = v_\xi$. Thus

$$p_\xi + \left[2m - \frac{\xi - a}{a\xi}\right]p = 0, \qquad (19)$$

with a solution

$$p = c_1 \exp\left(-m\xi + \frac{\xi}{a} - \ln\xi\right) = c_1\frac{\exp\{[(1/a) - 2m]\xi\}}{\xi}, \qquad (20)$$

for c_1 an arbitrary constant. On integrating,

$$v = c_1\int \frac{\exp\{[(1/a) - 2m]\xi\}}{\xi}\, d\xi + c_2, \qquad (21)$$

for c_2 an arbitrary constant. The solution of (14) is

$$\hat{C}(\xi) = e^{m\xi}v = c_1 e^{m\xi}\int_0^\xi \frac{\exp\{[(1/a) - 2m]\rho\}}{\rho}\, d\rho + c_2 e^{m\xi}. \qquad (22)$$

Particular solutions for the two cases of interest are as follows.

Case 1: Constant Source Boundary Condition

Using (15), $c_1 = 0$, and $c_2 = C_0e^{-mb}/s$. Substituting into (22),

$$\hat{C}(\xi) = \frac{C_0}{s}e^{m(\xi - b)}. \qquad (23)$$

Substituting (17) with the negative sign option, the only bounded one, and taking the inverse Laplace transform, (23) becomes

$$C(\xi, \tau) = l^{-1}\{\hat{C}(\xi)\} = C_0 \exp\left[\left(\frac{1-a}{2a}\right)(\xi - b)\right] \cdot l^{-1}\left\{\frac{\exp\left\{-\frac{(\xi-b)}{a^{1/2}}\left[a\left(\frac{1-a}{2a}\right)^2 + 1 + s\right]^{1/2}\right\}}{s}\right\}. \tag{24}$$

This equation can be easily inverted with the aid of standard tables and using the properties of Laplace transform. Equation (24) reduces to

$$C(\xi, \tau) = C_0 \exp\left[\left(\frac{1-a}{2a}\right)(\xi - b)\right] \int_0^\tau \frac{(\xi - b)}{(4\pi a u^3)^{1/2}} \cdot \exp\left\{-\left[\frac{(\xi-b)^2}{4au} + \left(a\left(\frac{1-a}{2a}\right)^2 + 1\right)u\right]\right\} du. \tag{25}$$

It is easy to show that this equation reduces to

$$C(\xi, \tau) = \frac{C_0}{2} \exp\left[\left(\frac{1-a}{2a}\right)(\xi - b)\right] \cdot \left\{\exp\left\{-\left(\frac{\xi-b}{a^{1/2}}\right)\left[a\left(\frac{1-a}{2a}\right)^2 + 1\right]^{1/2}\right\} \cdot \operatorname{erfc}\left[\frac{\frac{\xi-b}{a^{1/2}} - \left\{4\left[a\left(\frac{1-a}{2a}\right)^2 + 1\right]\tau^2\right\}^{1/2}}{(4\tau)^{1/2}}\right] + \exp\left\{\left(\frac{\xi-b}{a^{1/2}}\right)\left[a\left(\frac{1-a}{2a}\right)^2 + 1\right]^{1/2}\right\} \cdot \operatorname{erfc}\left[\frac{\frac{\xi-b}{a^{1/2}} + \left\{4\left[a\left(\frac{1-a}{2a}\right)^2 + 1\right]\tau^2\right\}^{1/2}}{(4\tau)^{1/2}}\right]\right\} \tag{26}$$

where erfc( ) denotes the "error function complement."

Case 2: Instantaneous Point Source at the Left Boundary

Using (15), $C_0 = 0$ and $c_2 = 0$ in (22). The particular solution for the transformed equation is

$$\hat{C}(\xi) = \int_b^\infty e^{m(\xi-\gamma)} \int_b^{\xi-\gamma} \frac{\exp\{[(1/a) - 2m]\rho\}}{\rho} \cdot C_i\delta(\gamma - b)\, d\rho\, d\gamma. \tag{27}$$

Substituting (17) for m with the minus option for the external integral and with the plus option for the internal integral (the only combination of options which makes the integrands bounded), solving the external integral, and taking the inverse Laplace transform, (27) can be written as

$$C(\xi, \tau) = l^{-1}\{\hat{C}(\xi)\} = C_i \exp\left[\left(\frac{1-a}{2a}\right)(\xi - b)\right] \cdot \int_b^{\xi-b} \frac{e^\rho}{\rho}\, l^{-1}\left\{\exp\left[-(\xi - b + 2\rho) \cdot \left(\frac{1}{a}\right)^{1/2}\left(a\left(\frac{1-a}{2a}\right)^2 + 1 + s\right)^{1/2}\right]\right\} d\rho \tag{28}$$

This equation can be easily inverted with the use of standard Laplace transform tables. Equation (28) reduces to

$$C(\xi, \tau) = \frac{C_i}{(4\pi a\tau^3)^{1/2}} \exp\left\{\left(\frac{1-a}{2a}\right)(\xi - b) - \left[a\left(\frac{1-a}{2a}\right)^2 + 1\right]\tau\right\} \int_b^{\xi-b} \left(\frac{\xi - b + 2\rho}{\rho}\right) \cdot \exp\left\{-\left[\frac{(\xi - b + 2\rho)^2}{4a\tau} - \rho\right]\right\} d\rho. \tag{29}$$

5. Application Examples and Comparison With Existing Results

In this section the solution of the VDE for cases 1 and 2, (26) and (29) respectively, will be used to illustrate the effect of aquifer hydraulic and hydrologic parameters on the spatial distribution of contaminants within the aquifer. We will also attempt a comparison between the well-known CDE with constant coefficients and the VDE. In the CDE the effect of recharge rates and other hydrologic-hydraulic elements is neglected, the pore velocity is assumed constant throughout the aquifer, and the dispersion coefficient is constant and usually estimated as a "calibration" parameter. Since in the VDE the dispersion parameters are explicit functions of the recharge rate and other hydrologic-hydraulic elements, the objective of a comparison between the CDE and the VDE is to observe the sensitivity of the concentration field to those elements, and to assess the magnitude of the error generated when the hydrologic regime is not included in the model. In order to establish a uniform basis for comparison between the CDE and the VDE, we will try to derive the constant dispersion parameters of the CDE in terms similar to those of the VDE. The classical CDE written for the same hypothetical aquifer under constant dispersion coeffcient, $\bar{D}$, and constant pore velocity, $\bar{u}$, resulting from neglecting recharge is given by [*Bear*, 1979]

$$C_t - \bar{D}C_{xx} + \bar{u}C_x = 0 \qquad 0 \le x < \infty,\ 0 \le t \le \infty. \tag{30}$$

$$C(0, t) = C_0 \qquad C(\infty, t) = 0 \qquad C(x, 0) = C_i\delta(x). \tag{31}$$

For comparison purposes, and for consistency, we will use the same expressions for pore velocity and dispersion coefficient derived in sections 3 and 4. Since the CDE assumes these parameters as constants, we will define their values at a typical fixed distance, $\bar{x}$. Thus from (6), $\bar{u} = (1/n)(I\bar{x} - h_0'T)$, and from (7), $\bar{D} = (\alpha/n)$, $(I\bar{x} - h_0'T)$. Thus the CDE

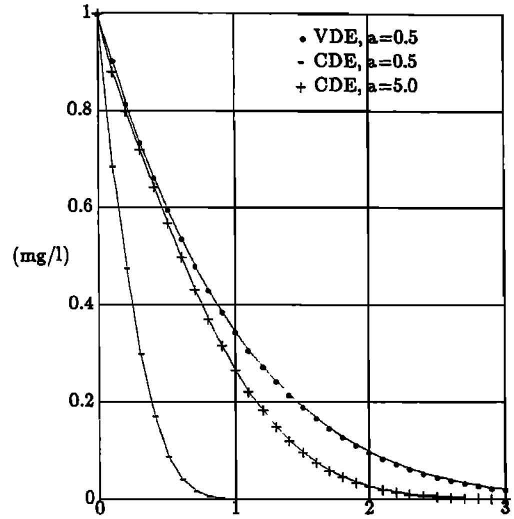

Fig. 1. Comparison between the CDE and the VDE for case 1.

with parameters in terms of aquifer hydraulic and hydrologic properties becomes

$$C_t - \frac{\alpha}{n}(I\bar{x} - h_0'T)C_{xx} + \frac{1}{n}(I\bar{x} - h_0'T)C_x = 0. \tag{32}$$

This is an improved version of the CDE since it uses the aquifer recharge, average thickness, average porosity, and average transmissivity in the definition of its parameters.

In order to preserve dynamic similitude between the CDE and the VDE we reduce (32) into a dimensionless from by defining again $\tau = It/nh_0$, $\eta = x/L$, $\bar{\eta} = \bar{x}/L$, $T^* = T/L$, $\xi = \eta - (h_0'T^*/I)$, $\bar{\xi} = \bar{\eta} - (h_0'T^*/I)$, $a = \alpha/L$, and $b = -h_0'T^*/I$. Thus the dimensionless version of (32) is

$$C_\tau - a\bar{\xi}C_{\xi\xi} + \bar{\xi}C_\xi = 0 \qquad b \le \xi < \infty,\ 0 \le \tau < \infty. \tag{33}$$

$$C(b, \tau) = f \qquad C(\infty, \tau) = 0 \qquad C(\xi, 0) = 0,\ \xi > b, \tag{34}$$

where f will vary for cases 1 and 2.

Case 1: Constant Source Boundary Condition

In this case $f = C_0$ in (34) and the well-known solution to the CDE, (33), is [*Ogata and Banks*, 1961]

$$C(\xi, \tau) = \frac{C_0}{2}\left\{\operatorname{erfc}\left[\frac{\xi - \bar{\xi}\tau}{(4a\bar{\xi}\tau)^{1/2}}\right] + e^{\xi/a}\operatorname{erfc}\left[\frac{\xi + \bar{\xi}\tau}{(4a\bar{\xi}\tau)^{1/2}}\right]\right\}. \tag{35}$$

Next a comparison between the VDE, (26), and the CDE, (35), was done by assuming typical values for the aquifer hydrologic and hydraulic properties and then calculating breakthrough curves of concentration versus distance at specified times. Figure 1 illustrates one of those tests with the following adopted parameters: I = 20.0 mm/month, which is a moderate recharge rate; t = 24.0 months; h_0 = 1.0 m; h_0' = −0.001 m/m; T^* = 1.0 m^2 m^{-1} month^{-1}; a = 0.5, which is by design a high relative dispersivity; and C_0 = 1.0 mg/L. For the CDE, besides the above values, the pore velocity was taken as that at $\bar{x}$ = 0.0 m. Since our objective is to compare the VDE and the classical CDE, which neglects recharge, the obvious choice that eliminates the recharge is $\bar{x}$ = 0.0. This implies that the pore velocity and the dispersion coefficient in the CDE is based on a constant (and linear) hydraulic gradient.

From the simulations a few points should be noted, as follows.

1. The CDE largely underestimates the concentration, especially at large distances and long simulation times. In Figure 1, the CDE only approaches the VDE after the relative dispersivity, a, has been increased by a factor of 10. These observations coincide with recent results of the CDE which state that the values of dispersivity in the CDE must be increased several orders of magnitude when attempting to simulate field concentrations.

2. Hydraulic gradients, aquifer thickness, aquifer transmissivity, and especially infiltration rates have an important effect on the contaminant distribution, because of the functional relationship between these parameters and the flow velocities. This is illustrated more in detail in case 2. In particular, recharge rates drastically increase the velocities with distance, making the migration of solutes more efficient. The effect of these hydrogeological characteristics on contaminant transport has been known for a long time, only here the VDE numerically and specifically accounts for them.

3. The calculation of concentration breakthrough curves using the VDE requires a similar effort as that used for the CDE. In fact, a simple microcomputer routine will do the job. An important advantage with the VDE is the definition of the parameters in terms of measurable aquifer properties and the hydrologic regime. This should make the simulation efforts a little more objective, and a little easier, than trying to obtain the values of dispersion coefficients by conventional estimation techniques. By using a transport model, such as the VDE, traditional transmissivity values derived from pumping tests, recharge estimations based on rainfall measurements, and hydraulic gradients based on piezometric monitoring may be incorporated into the transport model. Furthermore, those characteristics could be directly related to the contaminant distribution.

4. An interesting feature of the VDE is that it uses a constant dispersivity value and yet the breakthrough curves reflect the evolving nature of the velocity field and its effect on the concentration distribution observed via typical applications of the CDE with arbitrary fitted dispersivities which increase with the domain scale. The difficulty in defining the relationship between scale and dispersivity has prompted much research in the last 20 years. A question naturally arises here, Is the dispersivity a true function of scale or is the relationship a practical necessity when using the CDE without recharge? Field verifications of the VDE will have to be done before any attempt is made at answering this question, but for the moment the VDE poses an open alternative which suggests that the use of a constant, laboratory scale (only related to the chemical constituent in question) dispersivity may prove a fruitful modeling solution.

5. The use of a dimensionless differential equation for the solution is a convenient device to assure dynamic similitude between prototype and model, and a useful technique to generalize the model to multiple dimensions.

6. One limitation of the VDE, as with any other model, is

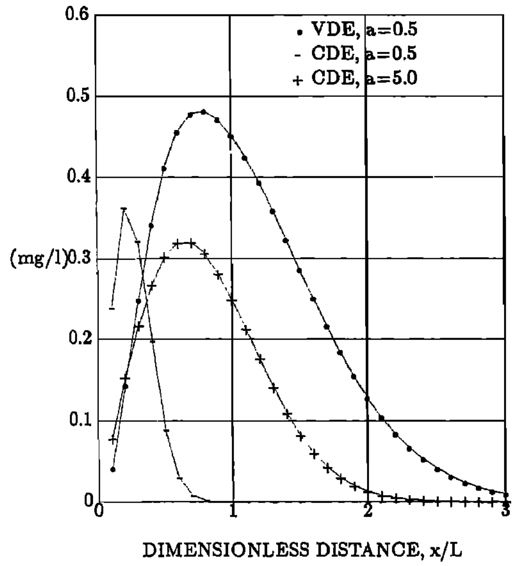

Fig. 2. Comparison between the CDE and the VDE for case 2.

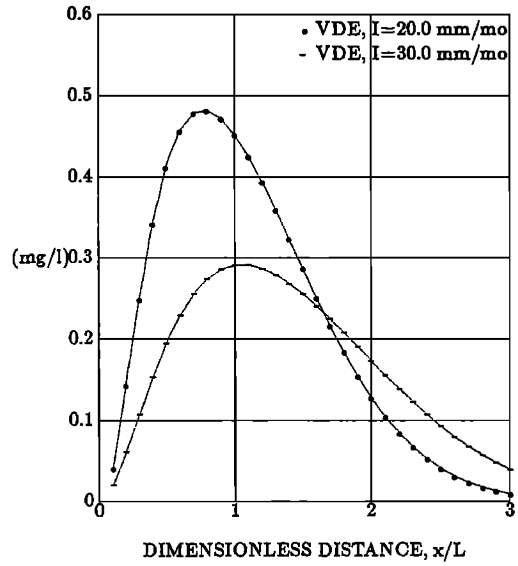

Fig. 3. Effect of infiltration rate on contaminant distribution.

that the choice of the parameters should satisfy certain stability constraints. Although a stability analysis was not done, preliminary observations indicate that the values of the parameters must not be unbounded, as one might expect. For instance, it is known that the values of transmissivity are a direct function of the typical domain scale and if, for example, a transmissivity of 1000.0 m^2/month is measured in the field, it should be related to a typical length $L = 1000.0$ m to obtain a parameter $T^* = 1.0$ m^2 m^{-1} month^{-1}.

Case 2: Instantaneous Point Source at the Left Boundary

In this case $f = C_i\delta(\tau)$ in (34), and the solution to the classical CDE is given by [*Serrano*, 1988*a*]

$$C(\xi, \tau) = \frac{\xi - b}{(4\pi a\bar{\xi})^{1/2}}$$

$$\cdot \int_0^\tau \exp\left\{-\frac{(\xi - b - \bar{\xi}(\tau - \rho))^2}{4a\bar{\xi}(\tau - \rho)}\right\} \frac{C_i\delta(\rho)}{(\tau - \rho)^3}\, d\rho. \quad (36)$$

Solving,

$$C(\xi, \tau) = \frac{C_i(\xi - b)}{(4\pi a\bar{\xi}\tau^3)^{1/2}} \exp\left\{-\frac{(\xi - \bar{\xi}\tau - b)^2}{4a\bar{\xi}\tau}\right\} \quad (37)$$

Once again, a comparison between the VDE, (29), and the CDE, (37), was done along with an investigation of the sensitivity of the contaminant distribution to the individual hydrologic and hydraulic properties. The parameter values assumed were the same as those adopted for case 1, except that $t = 12.0$ month.

From the simulations a few points very similar in nature from the ones drawn for case 1 should be noted.

1. The CDE tends to underestimate the concentration at large distances and long simulation times. Figure 2 shows a comparison between the CDE and the VDE. Note that the CDE only approaches the VDE after the relative dispersivity, a, has been increased by a factor of 10.

2. Infiltration rate increases the efficiency in which the contaminant migrates through the aquifer. Figure 3 is an example illustrating the concentration distribution after increasing the recharge rate to 30.0 mm/month as compared to that for a 20.0 mm/month rate of recharge.

3. The dispersivity tends to behave as a scaling parameter of the concentration distribution, reflecting the ability of a key contaminant to travel in porous media. Figure 4 shows the concentration distributions for relative dispersivities $a = 0.5$ and $a = 0.1$ respectively.

4. Higher transmissivity tends to increase the migration efficiency of the contaminant. Figure 5 shows the concentration distributions for relative transmissivity values of $T^* = 1.0$ m^2 m^{-1} month^{-1} and $T^* = 0.5$ m^2 m^{-1} month^{-1}.

5. Higher hydraulic gradients also tend to increase the velocities of flow and therefore the efficiency of migration of the contaminant. Figure 6 is an example of the effect of increasing the hydraulic gradient by an order of magnitude from $h'_0 = -0.0001$ m/m to $h'_0 = -0.001$ m/m. Clearly, all of

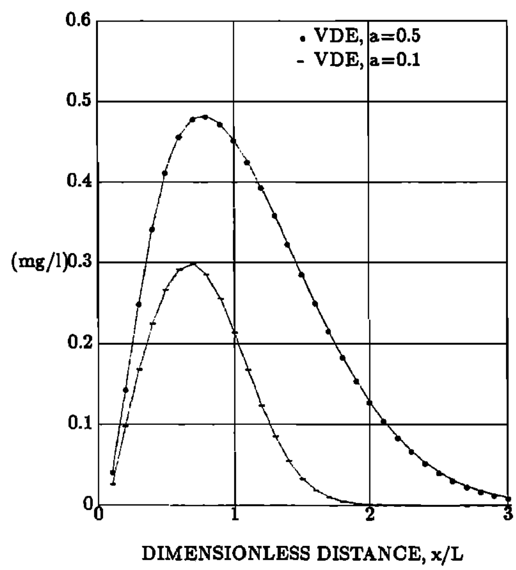

Fig. 4. Effect of aquifer dispersivity on contaminant distribution.

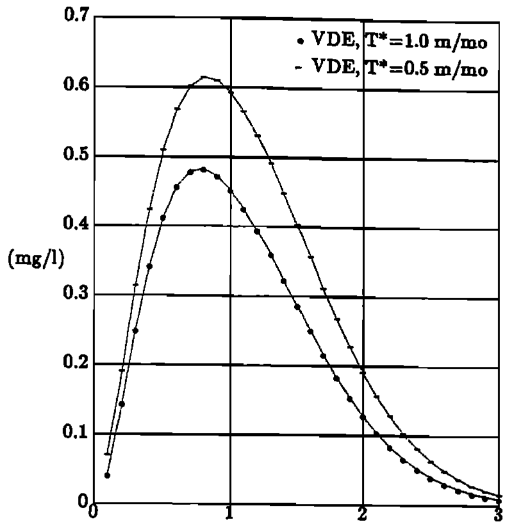

Fig. 5. Effect of aquifer transmissivity on contaminant distribution.

these hydraulic and hydrologic properties of the aquifer have a direct impact on the concentration distribution because of the intrinsic relationship between them and the spatial distribution of groundwater velocities (i.e., (6)).

6. The calculation of concentration breakthrough curves using the VDE requires a simple numerical integration procedure, which can be easily implemented with a microcomputer. In the present example a 24-point Gaussian quadrature was employed in the approximation of (26) with a short code in C requiring minimal computer space and execution time. This is to say that, as for comment 3 in case 1, the use of the VDE as a transport model does not require much extra effort and yet the advantages of having a model with parameters defined in terms of aquifer hydrologic and hydraulic properties could be beneficial.

7. All of the calculations for case 2, as well as for case 1, assumed a constant recharge rate through the period of simulation. Given the important effects of recharge rate, as well as those of other hydraulic parameters, on the time and space distribution of the contaminant, one should conclude that there is a need for an investigation into the effects of time and space variability of these parameters on transport models. Including the effects of spatial variability as well as the true transient behavior of the groundwater flow system on the analysis of solute transport should prove a most interesting research aim for the future.

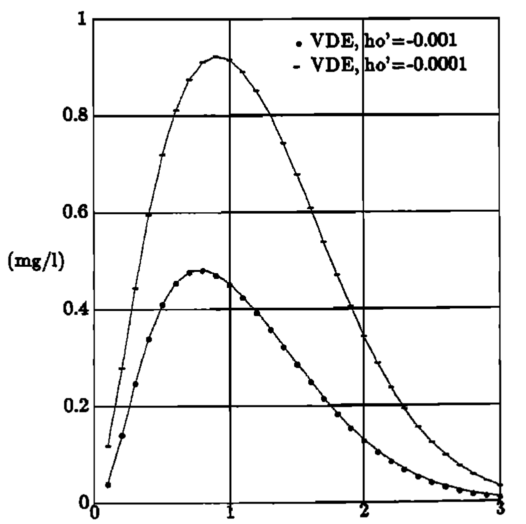

Fig. 6. Effect of hydraulic gradient magnitude on contaminant distribution.

6. Summary and Conclusions

An investigation of the effect of aquifer hydrologic and hydraulic parameters (such as recharge rate, transmissivity, hydraulic gradients, and aquifer thickness) on the time and space evolution of solute concentration at the field scale was conducted. The investigation involved a solution of the groundwater flow equation for the velocity field in terms of relevant aquifer properties, the definition of dispersion parameters as functions of the same aquifer properties, the derivation of the corresponding transport differential equation, its analytical solution, and a few application examples and comparison with the classical CDE. The results of the research could be summarized as follows.

1. Hydrologic and hydraulic aquifer properties, and in particular recharge, have a strong effect on the magnitude and distribution of the groundwater velocity field. It was found that even moderate recharge rates generate a variable velocity field, one with an increasing magnitude with distance, which significantly impacts the solute transport conditions in the aquifer.

2. Aquifers subject to natural recharge, which in turn generate variable velocity fields, exhibit evolving (increasing) dispersion coefficients with distance, even if constant (laboratory scale) values of dispersivities and homogeneity assumptions are adopted. This may be one of the reasons, along with the aquifer heterogeneities at the field scale, for the increasing value of the dispersion coefficient with the spatial and temporal scale so frequently reported in the literature. In the present study a physical interpretation based on a hydrologic-hydraulic functional dependence is given.

3. The form of the dispersion equation in aquifers subject to recharge exhibits a dispersion coefficient and advection as variable (increasing) functions of space (VDE), and an extra term involving the dependent variable with a coefficient given by the recharge rate. Stable solutions of this equation can be obtained, in particular after transforming it into a dimensionless equation, which at the same time helps in the reproduction of the model dynamic similitude. Although the solution of the VDE is more involved than that for the CDE, its implementation in practical simulation models does not appear to require much more computational effort, and yet the advantages of having a dispersion equation in terms of measurable hydrologic and hydraulic properties may prove beneficial.

4. It was found that higher transmissivity values and higher hydraulic gradient values tend to increase the velocities of flow and therefore the solute transport efficiency as expected. On the other hand, values of dispersivity tend to have a scaling effect on the entire contaminant plume.

5. The results indicated that the VDE with constant

dispersivity values may be able to reproduce the evolving nature of the velocity field and its effect on the concentration distribution observed via typical applications of the CDE with arbitrary fitted dispersivities which increase with the domain scale. This suggests that a constant, laboratory scale, dispersivity included in a dispersion equation which accounts for other aquifer hydraulic properties might be sufficient to model dispersion at the field scale. Substantial research and field verification will have to be done in order to determine if this is the case, but for the moment the possibility of using laboratory tests of dispersivity and their association with individual contaminants is encouraging.

6. Comparisons between the VDE and the classical CDE under similar conditions indicated that the CDE largely underestimates concentration values, especially as distance and time increase. Dispersivity values in the CDE must be increased substantially in order to make its concentration distribution comparable to that of the VDE.

7. The effect of regional hydrologic and hydraulic parameters on the evolution of contaminants is important since they substantially affect the magnitude and distribution of the velocity and that of the concentration. Even moderate recharge rates drastically increase the efficiency of the flow and that of the contaminant evolution. Given the apparent absence of recharge considerations in most of the existing field investigations on the scale dependence of transport parameters, and the fact that the scale dependence could partially be explained by the influence of this important input function, the present study suggests that the aquifer hydrologic regime should be included in the analyses. The relative importance of the hydrologic regime with respect to the field heterogeneity in explaining the scale dependence of aquifer parameters remains to be investigated. Because of the sensitivity of contaminant migration to recharge and to other hydrologic-hydraulic parameters, future research should be devoted to the inclusion of temporal and spatial variability of these parameters in the form of the dispersion equation (i.e., the effect of time-space variability of recharge).

8. The above results are based on the adoption of Dupuit assumptions in the flow field. Since the governing differential equation is different in a deep aquifer, and since the presence of a nonlinear dynamic free surface boundary condition constitutes a new element in the analysis, efforts should be directed toward the theoretical analysis of three-dimensional flow problems and their effect on contaminant transport.

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S. E. Serrano, Department of Civil Engineering, University of Kentucky, Lexington, KY 40506.

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