An effective scale-dependent dispersivity deduced from a purely convective flow field

HUBERT J. MOREL-SEYTOUX &
MAHMOOD NACHABE
Department of Civil Engineering, Colorado State University, Fort Collins, Colorado 80523, USA

Abstract In the case of straight flow but with hydraulic conductivity varying in a transverse direction, the distribution of hydraulic conductivity has been determined for which the breakthrough curve due to convection only will have the same analytical form as the one-dimensional convection/dispersion equation solution at the outlet end of a porous medium. That distribution is found exactly and it is very similar to the lognormal distribution. This result is significant since field evidence indicates that the logarithm of hydraulic conductivity is normally distributed. For the case considered, a simple relation between dispersivity and the coefficient of variation of hydraulic conductivity is found. One can thus determine very simply dispersivity in terms of the parameters of the distribution of hydraulic conductivity. This is particularly useful to estimate dispersivity in various cells of finite difference or finite element models when the distribution of hydraulic conductivity is not stationary, i.e. varies in space.

Dérivation d'une dispersivité équivalente, fonction de l'échelle, à partir d'un champ d'écoulement purement convectif

Résumé Dans le cas d'un écoulement droit mais avec variation de conductivité hydraulique dans la direction transversale, on a obtenu la distribution pour laquelle l'écoulement purement convectif et l'écoulement convectif/diffusif dans une seule dimension donnent la même courbe de concentration avec le temps à la sortie du milieu poreux. Cette distribution théorétique se confond presque avec la loi normale logarithmique, qui a été retenue pour caractériser la variation aléatoire de la conductivité sur le terrain. Le résultat est donc pratique et significatif. On a de plus obtenu une relation simple entre la dispersivité et le coefficient de variation de la conductivité. On peut ainsi déterminer de façon très simple la dispersives en termes de paramètres de la distribution de la conductivité hydraulique. Cette relation permet d'estimer différentes dispersivités dans les mailles d'un réseau de différences finies quand la distribution de la conductivité n'est pas stationnaire dans l'espace, ni dans sa moyenne ni dans sa variance.

INTRODUCTION

It is a well-known fact that the phenomenon of dispersion is caused not only by heterogeneity of media properties at a variety of scales (Bear, 1972;

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Konikow & Bredehoeft, 1978; Dagan, 1990) but also by heterogeneity of boundary conditions (Daly & Morel-Seytoux, 1985; Morel-Seytoux & Rathnayake, 1988). Under special conditions it has been shown (Bear, 1972) that the dispersion caused by heterogeneity of media properties can be represented by the convection/dispersion equation which in one dimension may be written in the form (Konikow & Bredehoeft, 1978):

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(C\bar{V}) - \frac{\partial}{\partial x}\left[D\frac{\partial C}{\partial x}\right] = 0 \tag{1}$$

In equation (1) C is solute concentration (solute mass per unit volume of solution); t is time, $\bar{V}$ is the mean particle velocity (also known as the seepage velocity); x is the Cartesian coordinate in the direction of flow; and D is the dispersion coefficient (dimension of area per unit time). Typically, one is interested in predicting the breakthrough curve of concentration at some distance L from an injection of a concentration pattern, for example a step of concentration. Clearly, without the dispersion term in equation (1), the step of concentration injected at one end (at $x = 0$) will propagate as a step and the breakthrough curve, i.e. the time pattern of concentration at $x = L$, will also be a step function.

In reality, the flow is two-dimensional, though on the average essentially one-dimensional, due to variations in hydraulic conductivity, which may be organized or random. One expects the magnitude of D to depend upon the degree of heterogeneity of that hydraulic conductivity. The development of this type of relationship is the purpose of this article.

PROBLEM GEOMETRY AND BOUNDARY CONDITIONS

The flow domain is a rectangle as shown in Fig. 1. Water flows steadily from left to right under a constant head drop ΔH over the length L. The mean of the hydraulic conductivity is $\bar{K}$. The thickness of the flow is assumed uniform (of value unity) and so is the porosity, ϕ. Initially the concentration is uniform of value zero. Starting at time zero, the concentration in the entering water is maintained at a value C_B.

Solution of the one-dimensional convection/dispersion equation

The analytical solution to this problem (Ogata, 1970) for the breakthrough curve is:

$$\bar{C}/C_B = ½\{erfc[(L-\bar{V}t)/(4Dt)^{½}] + \exp(\bar{V}L/D)erfc[(L+\bar{V}t)/(4DT)^{½}]\} \tag{2}$$

where $erfc(x)$ is the complementary error function, a well tabulated function

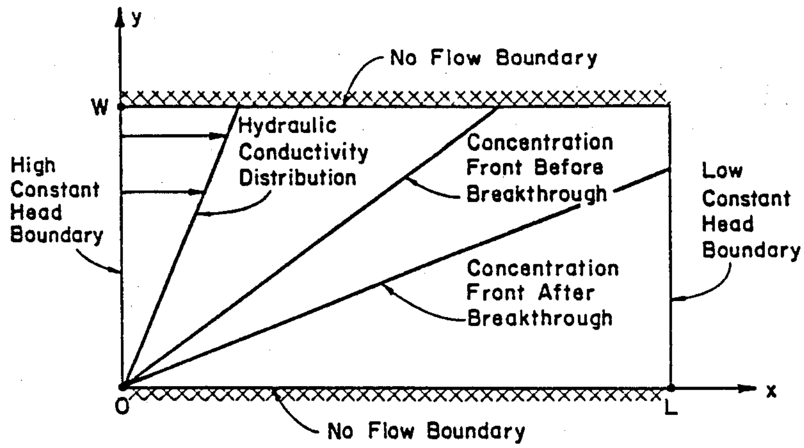

Fig. 1 Geometry and boundary conditions of problem: positions of concentration front at various times; hydraulic conductivity pattern in the transverse direction.

(Abramowitz & Stegun, 1972). $\bar{C}$ is the mean concentration over the width of flow at $x = L$, i.e. generally:

$$\bar{C} = \int_0^W \frac{C(L,y,t)\mathrm{d}y}{W} \tag{3}$$

For purely one-dimensional flow, C at $x = L$ does not depend on y. In equation (2), $\bar{V}$ is related to $\bar{K}$, ΔH, L and ϕ by Darcy's law, namely:

$$\bar{V} = \bar{K}\Delta H/\phi L \tag{4}$$

For practical conditions with L typically large, the second term on the right-hand side of equation (2) is negligible (Freeze & Cherry, 1979) and equation (2) reduces to:

$$\bar{C}/C_B = 1 - F_N[(L-\bar{V}t)/(2Dt)^{1/2}] \tag{5}$$

where $F_N(u)$ is the cumulative distribution function (cdf) for the standard normal variate (Abramowitz & Stegun, 1972).

Solution to the two-dimensional convection equation

If the medium is heterogeneous with respect to hydraulic conductivity, the flow will generally be two-dimensional and its equation, under steady-state conditions, is:

$$\frac{\partial}{\partial x}\left[K(x,y)\frac{\partial h}{\partial x}\right] + \frac{\partial}{\partial y}\left[K(x,y)\frac{\partial h}{\partial y}\right] = 0 \tag{6}$$

where h is the hydraulic head.

If the hydraulic conductivity pattern is of a separable form i.e. $K(x,y) = K(x)K(y)$, it is straightforward to show that the streamlines are straight regardless of the nature of the functions $K(x)$ and $K(y)$. The case when K varies only with y is investigated.

Let $F(K)$ represent the cumulative distribution function (cdf) of K. It is immaterial at this point to specify whether the spatial pattern of variation of K is organized or random. Since the process is purely convective, the concentration step will propagate as a step in each stream tube. The mean concentration at $x = L$ at time t will simply be the product of the fraction of the stream tubes that have broken through and C_B, namely $C_B[1 - F(K)]$ where K is the hydraulic conductivity of the stream tube that has broken through at time t precisely. This K value must be such that Vt along the stream tube equals L. In other words, the relation between K and t is:

$$t = L/V = L/(K\Delta H/\phi L) = (\phi L^2/K\Delta H) = (\phi L^2/\bar{K}\Delta H)(\bar{K}/K) = (L/\bar{V})(\bar{K}/K) \tag{7}$$

The breakthrough curve is given by the expression:

$$\bar{C}/C_B = [1-F(K)] = [1-F_K(L\bar{K}/\bar{V}t)] \tag{8}$$

If K_M, the maximum value of K, is finite then breakthrough will not occur until a time t_{B0} such that:

$$t_{B0} = L\bar{K}/\bar{V}K_M$$

On the other hand, if the minimum value of K is K_m, breakthrough will have occurred for all layers at time t_{BF} such that:

$$t_{BF} = L\bar{K}/\bar{V}K_m$$

One may thus rewrite equation (8) more specifically:

$$\bar{C}/C_B = 0 \qquad \text{for } 0 \le t \le t_{B0} \tag{8a}$$

$$\bar{C}/C_B = 1-F_K(L\bar{K}/\bar{V}t) \qquad \text{for } t_{B0} \le t \le t_{BF} \tag{8b}$$

$$\bar{C}/C_B = 1 \qquad \text{for } t \ge t_{BF} \tag{8c}$$

With the deterministic spatial interpretation of the cdf of hydraulic conductivity, the distribution of K with y is simply:

$$y/W = F(K)$$

To obtain K as a function of y, this expression would have to be inverted.

The purpose here is to define an equivalence between the two approaches. In the process a dispersivity will be derived in terms of the mean of the hydraulic conductivity and its variance. However, the dispersivity in this paper is not defined in the traditional way. For this reason, it is useful to review that concept and the concept of equivalence, as presented by other authors.

THE FICKIAN DIFFUSIVE (DISPERSIVE) BEHAVIOUR

Equation (1) with the interpretation of D as the molecular diffusion is the one-dimensional form of the advection/diffusion equation. The simplicity of this equation (with a uniform $\bar{V}$ and a constant D) and its convenient mathematical properties have motivated many researchers to find ways to reduce the more complex advective/diffusive (or locally dispersive) equation to the form of equation (1) with an "effective" value for the dispersion coefficient and a uniform value for the velocity.

Equation (1), with a constant $\bar{V}$ and a constant D, has the fundamental solution:

$$C(x,t) = M/(4\pi Dt)\exp[(-x-\bar{V}t)^2/(4Dt)] \qquad (9)$$

where M has the physical significance of a mass of solute introduced into the system at $t = 0$ and at $x = 0$. Due to the linear character of equation (1), any solution can be obtained by weighted linear combinations of equation (9). Because equation (9) at a given time has the analytical form of a normal (Gaussian) distribution, it follows that: (a) any initial spatial distribution of concentration will eventually evolve into a Gaussian shape; and (b) the temporal rate of increase of the variance of the spatial distribution of concentration is a constant independent of its initial spatial shape. Symbolically, the second property may be written:

$$\frac{1}{2}\,\frac{d\sigma_x^2}{dt} = Q = \text{constant} \qquad (10)$$

where σ_x^2 is the variance of the concentration distribution in space at a given moment in time. These two properties (Fischer *et al.*, 1979) characterize the so-called Fickian behaviour and fully characterize equation (1). In other words, if a dispersing plume satisfies these two properties, its evolution is governed by equation (1) for constant $\bar{V}$ and D. Because it is not known *a priori* whether the plume behaviour is Fickian or not, these properties must be checked based on observations. To check the first property (Gaussian shape in space) one must compute high order moments of the concentration profile. This is rarely done, with few exceptions (e.g. Gelhar *et al.*, 1979). Investigators justify the presumption of normality by invoking the central limit theorem.

In fact, the observations indicate that Q as defined by equation (1) varies with x (abscissa of the centre of gravity of the distribution). It is scale-dependent.

A legitimate question to ask is: if the rate of change with time of the spatial variance of the plume concentration is a function of x, does an equation of the form:

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(C\bar{V}) - \frac{\partial}{\partial x}\left[Q(x)\frac{\partial C}{\partial x}\right] = 0 \tag{11}$$

represent the behaviour of the dispersing plume? That equivalence has not been shown. In fact, in the authors' opinion, it cannot be shown. Indeed, Matheron & de Marsily (1980, p.910) showed that Fickian behaviour will "not occur and that the usual convection/diffusion equation should not be used". It can be used only for one particular time, say t_1, with an "equivalent macro-dispersion coefficient" calculated as:

$$D_E(t_1) = \sigma_{x1}^2(t_1)/2t_1 \tag{12}$$

with $x_1 = \bar{V}t_1$. Such a procedure has no predictive capability since it requires the knowledge of $\sigma_{x1}(t_1)$, say from observations, and cannot be used for any other time. Others have used equation (11) as if representing dispersion (Pickens & Grisak, 1981; Yates, 1990) with a dispersivity function of space (or equivalently time). Either procedure is an approximation as equation (1) or (11) is not applicable.

For example, Güven *et al.* (1984), using the method of moments, showed that for an essentially longitudinal one-dimensional flow with both Fickian longitudinal and transverse components (with local dispersion coefficient values) the equivalent scale-dependent dispersivity for a strictly one-directional equation such as equation (1) is:

$$\alpha = D/V = (\sigma_K/\bar{K})^2\bar{V}t \tag{13}$$

with $\bar{K}$ the mean hydraulic conductivity and σ_K^2 its variance, valid for large time or even small time if longitudinal and lateral local Fickian dispersion is neglected (Güven *et al.*, 1984, p.1342, equation (46)). Again, the dispersion coefficient is defined by equation (10) which in no way proves that equation (1) is applicable at the larger scale. Indeed, in some other work (Molz *et al.*, 1983) the same authors used a constant value of D, that obtained for a time t yielding breakthrough at a distance, L. Their conclusion (*ibidem*, pp. 717 and 719) is that asymptotic Fickian behaviour for the particular aquifer they studied would not obtain until the plume had travelled 109 km. In other words, if the plume starts to disperse in Beirut, one needs to track it all the way to Damascus before Fickian behaviour obtains! In this article one does not start with a convective/dispersive equation at a smaller scale and integrate it to a larger scale. The governing starting equation is purely convective. Also very importantly, dispersivity (or dispersion) is not defined by equation (10), but by the requirement that the two-dimensional purely convective equation and the one-dimensional convective/diffusive equation give the same breakthrough curve solution at distance L from the injection source.

RELEVANT LITERATURE

The most relevant article is one by Mercado (1967), studying the "spreading pattern of injected water in a permeability stratified aquifer". His starting assumptions (Mercado, 1967, p.24) are the same as the authors'. However, in addition, Mercado assumed that the variations of K were small relative to its mean (an assumption which is not made in this article) and that it has a normal distribution (another assumption not made in this article). As a result, the breakthrough curve, i.e., the variation of $\bar{C}/C_B$ with time at $x = L$ is given by equation (8) assuming a normal cdf for K, but is not the solution given by equation (5). Since the hydraulic conductivity distribution is assumed normal, the concentration distribution in space at a fixed time (not the breakthrough curve) will be Gaussian because the x coordinate of the front in one layer is directly proportional to its K. Thus, there will be a perfect match in space between the solution of the convective/diffusive equation (with the proper dispersivity) and the solution of the purely convective equation with spatial variation in K. On the other hand, for that same value of dispersivity, the corresponding breakthrough curves in time by the two approaches will not match identically.

Güven *et al.* (1984) solved the stratified aquifer problem, starting with a convective/diffusive equation with both local longitudinal and transverse Fickian terms, using the method of moments. They derived an expression for the dispersion coefficient, but again that defined by equation (10). They showed that, except if the local longitudinal and transverse Fickian terms are negligible, their derived dispersivity is essentially valid for all times and is identical to the expression obtained by Mercado (1967). Their derivation makes no assumption regarding the magnitudes of K. They also obtain a large time approximation for the equivalent dispersion coefficient which is a constant. However, as previously mentioned, that Fickian behaviour obtains only for practically useless times and distances (109 km for the aquifer of interest).

In contrast to the two articles just discussed, Gelhar *et al.* (1979) considered the governing equation as a stochastic differential equation. As a result, a cross-correlation function between velocity and concentration perturbations appears. Neglecting second order terms, the solution to the concentration perturbation is obtained. However, for the asymptotic value of the dispersion coefficient to be a constant, the autocorrelation function of the conductivity should have a "hole effect" (*ibidem*, p.1390). For small times, the expression for the dispersivity is the same as that obtained by Güven *et al.* (1984), and Mercado (1967). In passing, it should be mentioned that an autocorrelation function with a hole effect is not a very realistic one.

EQUIVALENCE OF TWO SOLUTIONS

The case investigated in this section is the one when K varies only with y (i.e., stratification in one direction, homogeneity in the other direction). The question to be addressed is: is there a particular distribution of K for which the two solutions as given by equations (5) and (8) are identical for all times?

Determination of the distribution yielding equivalence

This will be the case if:

$$F(K) = F_N[(L - Vt)/(2Dt)^{1/2}] \tag{14}$$

It is always possible to find a function (transformation) of K, say $g(K)$, or its standardized form $g^*(K)$, such that $g^*(K)$ will be normally distributed even though (and because) K itself is not. The problem reduces to finding $g^*(K)$ such that:

$$g^*(K) = (L - \bar{V}t)/(2Dt)^{1/2} \tag{15}$$

The right-hand side of equation (15) can be expressed in terms of K, given the relation for breakthrough time of a particular layer represented by equation (7), with the result:

$$g^*(K) = u = \frac{L(1 - \bar{K}/K)}{(2DL/\bar{V})^{1/2}(\bar{K}/K)^{1/2}} = \frac{L[(K/\bar{K})^{1/2} - (\bar{K}/K)^{1/2}]}{(2DL/\bar{V})^{1/2}} \tag{16}$$

Equation (16) is manipulated so that the numerator of the last right-hand side term has the dimension of K. This may be carried out by multiplying it by $\bar{K}/\bar{K}$, with the result, after division by L in both numerator and denominator:

$$g^*(k) = \frac{(K\bar{K})^{1/2} - \bar{K}(\bar{K}/K)^{1/2}}{(2D\bar{K}^2/L\bar{V})^{1/2}} \tag{17}$$

Defining dispersivity as $\alpha = D/\bar{V}$, then finally one obtains:

$$g^*(K) = \frac{(K\bar{K})^{1/2} - \bar{K}(\bar{K}/K)^{1/2}}{(2\alpha\bar{K}^2/L)^{1/2}} \tag{18}$$

Since $g^*(K)$ is a standard variate, its value must be zero at $g(K) = \overline{g(K)}$. Because $g^*(K)$ equals zero for $K = \bar{K}$ one can take $\overline{g(K)} = g(\bar{K}) = 0$. This gives the result that:

$$g^*(K) = \frac{g(K)}{\sigma_g} = \frac{(K\bar{K})^{1/2} - \bar{K}(\bar{K}/K)^{1/2}}{(2\alpha\bar{K}^2/L)^{1/2}} = u \tag{19}$$

where u is the standardized normal variate. It can be verified that for $K = 0$,

$u = -\infty$, and for $K = \infty$, $u = +\infty$.

Relation between dispersion coefficient and variance of K

It remains to find the relation between $\sigma_g = (2\alpha\bar{K}^2/L)^{½}$ and σ_K. First, $(K/\bar{K})^{½} = x$ is expressed as a function of u from equation (19) leading to a quadratic expression in x, namely:

$$x^2 - u(2\alpha/L)^{½}x - 1 = 0$$

which solved for x and then for K yields:

$$K = \bar{K}\{1 + u^2\alpha/L + u/2[(2\alpha/L)(2\alpha u^2/L+4)]^{½}\} \quad (20)$$

From the definition of the variance and expressing K in terms of u, it follows that:

$$\mathrm{var}(K) = \int_{-\infty}^{\infty} \bar{K}^2\{u^2\alpha/L + u/2[(2\alpha/L)(2\alpha u^2/L+4)]^{½}\}^2 f_N(u)\ du \quad (21)$$

where $f_N(.)$ is the standard normal density function. More explicitly one has:

$$\mathrm{var}(K) = (\alpha\bar{K}/L)^2E(U^4) + \bar{K}^2\int_{-\infty}^{\infty}(\text{odd function of } u)\ f_N(u)\ du + (\bar{K}\alpha/L)^2\ E(U^4) + 2\bar{K}^2(\alpha/L)E(U^2) \quad (22)$$

For a standard normal distribution, the expected value of an odd function is zero, $E(U^4)$ is the kurtosis of value 3 and $E(U^2) = 1$. The expression for the variance reduces to the simple form:

$$\sigma_K^2 = \bar{K}^2[6(\alpha/L)^2 + 2\alpha/L] \quad (23)$$

which can be solved for α with the result:

$$\alpha = [(1 + 6C_{v,K}^2)^{½} - 1]L/6 \quad (24)$$

or equivalently:

$$D = \alpha\bar{V} = \bar{K}\Delta H[(1 + 6C_{v,K}^2)^{½} - 1]/6\phi \quad (25)$$

where $C_{v,K}$ is the coefficient of variation of the hydraulic conductivity. As expected, α and D will be zero if there is no variation in hydraulic conductivity. Also equation (24) shows that the dispersivity increases with the distance at which the breakthrough curve is desired.

Practical realism of derived distribution of K

As stated earlier, the results apply whether the distribution of hydraulic conductivity is organized (deterministic) or random. In practice, the distribution of hydraulic conductivity tends to be random and many observations (Nielsen *et al.*, 1973; Russo & Bresler, 1981; Sudicky, 1986) tend to support the hypothesis that it is lognormal. Figure 2 displays the derived distribution of K/K for various coefficients of variation on lognormal paper. Rather clearly, the derived distribution does not deviate appreciably over a wide range of values from the lognormal distribution since the curves are straight. A Taylor series expansion of both distributions indicates that the two series deviate little from each other. It is inferred that the observations could have been fitted just as well by the derived distribution.

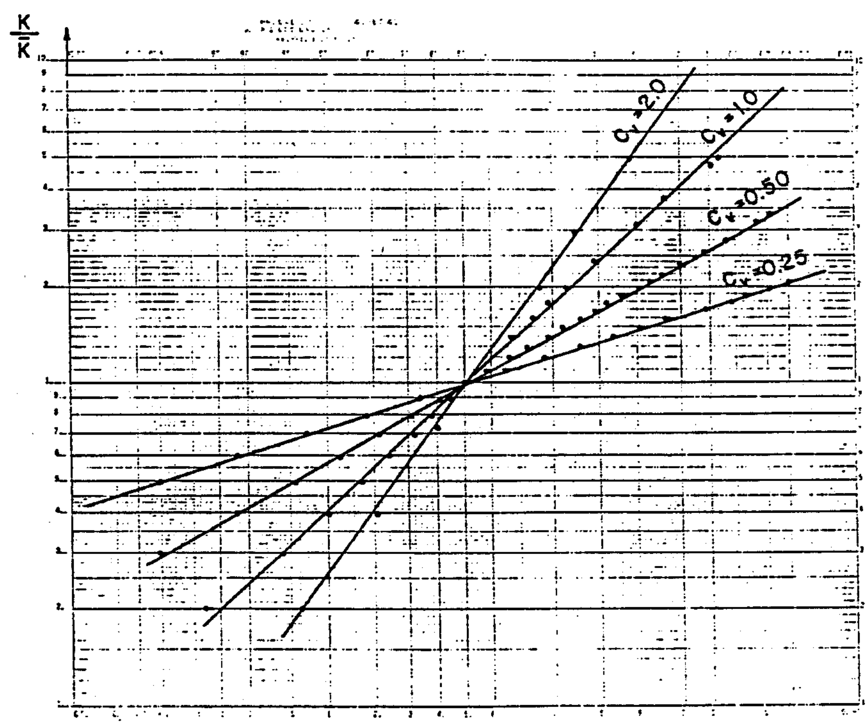

Fig. 2 Plot of the "dispersion equivalent" cumulative distribution function on lognormal probability paper.

Implications

It has been shown that a purely convective process in a particular heterogeneous medium can reproduce exactly the solution of the convection/dispersion equation as far as the breakthrough curve is concerned. This is especially significant because the distribution required for the exact equivalence is in practice the one observed in the field. It is usually very difficult to calibrate a dispersion coefficient and typically a unique value of the dispersivity is used for the entire field (Rathnayake & Morel-Seytoux, 1989). Equation (24), on the other hand, allows one to calculate the value of the dispersivity as a function of length and coefficient of variation of the hydraulic conductivity, thus allowing for variation in the dispersion coefficient from cell to cell in a finite-difference grid system. However, the relationship was developed for the restricted situation of steady-state and homogeneous boundary conditions. On the other hand, the two-dimensional purely convective flow approach is valid under transient conditions and for heterogeneous boundary conditions. It would, therefore, be safer to describe the phenomenon of dispersion with a two-dimensional purely convective equation.

It should be noted that had $K(x,y)$ been chosen to be a function only of x, say $K(x)$, then the dispersion coefficient would have been zero. The coefficient of dispersion thus depends upon the angle between the direction of flow and the gradient of hydraulic conductivity. Equation (25) applies only when that angle is 90°.

CONCLUSION

The fact that laboratory experiments in columns have shown that breakthrough curves could be well fitted by a one-dimensional solution to the convection/dispersion equation appears as no surprise. The same result could be obtained with a purely convective process using a distribution of hydraulic conductivity which is practically the lognormal one, the very one that has been observed in the field. The formula for scale-dependent dispersivity is valid for all practical times. It does not reduce to Mercado's formula for two reasons. First, it does not assume a normal distribution for the hydraulic conductivity (which is not realistic as no negative values are possible), but a special distribution which is very close to the lognormal one. Second, the dispersion coefficient is not defined as the rate of change with time of the spatial variance of concentration profiles at a fixed time. It is defined as the value that will provide full equivalence of the breakthrough curves at a fixed location. Equivalence is strictly possible only for a special distribution of hydraulic conductivity which was derived in this paper, is given by equation (19) and turns out to be very close to the lognormal one.

With the derived simple relation between the dispersivity and the coefficient of variation of the hydraulic conductivity it is possible to estimate the dispersion coefficient and its variation in space as a result of the variation of conductivity in space. This is particularly useful for the modelling of solute transport with the traditional convection/dispersion approach in a regional aquifer system which is highly heterogeneous. However, this procedure is not really recommended. Instead, one can describe in detail the flow field and no dispersion term is needed in the solute transport equation (Daly & Morel-Seytoux, 1985; Morel-Seytoux & Rathnayake, 1988; Rathnayake & Morel-Seytoux, 1989). Possibly, then, the most useful result is the calibration of D on an observed breakthrough curve and use of the relation between D and the coefficient of variation of the hydraulic conductivity to estimate that variability. One can then use the purely convective model to describe the concentration profile at any abscissa or time. That model applies for all times.

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