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THE INFLUENCE OF THE FORM OF THE LOG-CONDUCTIVITY COVARIANCE ON NON-FICKIAN DISPERSION IN RANDOM PERMEABILITY FIELDS

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SUMMARY

The paper deals with non-Fickian dispersion of inert solutes in random permeability fields. Attention is focused critically on the statistical characterization of the porous medium which affects pollutant dispersion in groundwater. After a brief account of recent results of stochastic theories of transport in porous media and of the fundamental indications of large-scale field experiments, it is inferred from numerical studies that the particular choice of an analytical form of covariance of log-conductivity has a poor influence on the overall dispersion process. In fact, different covariance structures with the same macroscale (a measure of the distance between two points beyond which the permeability ceases to be correlated) yield very similar dispersion processes. The result has a noteworthy bearing on field studies of pollutant dispersion in groundwater because it underlines the reliability of exponential correlation structures yielding analytical expression for time-varying macrodispersion coefficients.

INTRODUCTION

Recent studies on dispersion in random permeability fields[1–3] have shown the validity of Dagan's theory[4–6] of stochastic transport in groundwater in comparison with the results of the large-scale field study, known as the Borden site experiment.[1,7,8]

The theory hinges on the relationship between the Eulerian velocity field and the heterogeneous structure and yields the dependence of the concentration expected values upon the formation structure via the covariance of the log-conductivity of the medium,[5] which is modelled by a second-order stationary random field. This paper focusses on the effects of different correlation structures of the random permeability field on the overall dispersion process. A consistency requirement is posed in that all covariances are assumed to yield the same integral scale (macroscale).

The paper is organized as follows. An introductory section recalls the main findings of stochastic theory of transport in groundwater. A section follows on the computation of dispersion coefficients of an isotropic 2-D random permeability field, which is the thickness-averaged model of a layered system. This is considered representative[1,5,6] of a stratified natural formation in

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which the horizontal macroscales are similar, and much larger than the vertical one. A discussion on the results closes the paper.

LAGRANGIAN AUTOCORRELATION TENSOR AND THE STRUCTURE OF THE RANDOM PERMEABILITY FIELDS

We consider a porous formation and a solute body of concentration C_0 introduced at time $t=t_0$ in a volume V_0; the ambient concentration is $C=0$. A solute particle is viewed as a indivisible infinitesimal body of mass $\mathrm{d}M=n_0 C_0 \mathbf{da}$ that moves along a trajectory of equation $\mathbf{x}=\mathbf{X}(t;\mathbf{a},t_0)$. The concentration distribution ΔC associated with the particle is proportional to Dirac's distribution

$$\Delta C(\mathbf{x},t;\mathbf{a},t_0)=\frac{n_0}{n}C_0\,\mathbf{da}\,\delta(\mathbf{x}-\mathbf{X}) \tag{1}$$

Since the porosity n changes very little as compared with the conductivity, we assume that it is constant, i.e. $n=n_0$.

Let $f(\mathbf{X};t,t_0,\mathbf{a})\,\mathrm{d}\mathbf{X}$ be the probability of a particle originating at $\mathbf{x}=\mathbf{a}$ at time t_0 to be within $\mathrm{d}\mathbf{X}$ at time t. By the definition of the expected value we obtain from (1) that

$$\langle \Delta C\rangle=\frac{n_0}{n}C_0\,\mathbf{da}\,f(\mathbf{x};t,t_0,\mathbf{a}) \tag{2}$$

This fundamental result, obtained by Taylor,[9] can be described as follows: the concentration expected value is given by the probability density function (pdf) of the particle's trajectory, which is regarded as a function of $\mathbf{x}$ and t.

It is readily seen that $\langle C\rangle$ is obtained from (2) by integration over the volume V_0 with respect to $\mathbf{a}$:

$$\langle C(\mathbf{x},t;t_0)\rangle=\int_{V_0}\langle \Delta C(\mathbf{x},t;\mathbf{a},t_0)\rangle\,\mathbf{da} \tag{3}$$

We can think of the random particle's trajectory $\mathbf{x}=\mathbf{X}(t;\mathbf{a},t_0)$ as a sum of a large number of independent infinitesimal small steps: for the central limit theorem in statistics the pdf of $\mathbf{X}$ would be the stationary multivariate normal

$$f(\mathbf{X})=\frac{1}{(2\pi)^{m/2}|\mathbf{R}|^{1/2}}\exp\left[-\tfrac{1}{2}(\mathbf{X}-\langle\mathbf{X}\rangle)^{\mathrm{T}}\cdot\mathbf{R}^{-1}\cdot(\mathbf{X}-\langle\mathbf{X}\rangle)\right] \tag{4}$$

where $\mathbf{X}'=\mathbf{X}-\langle\mathbf{X}\rangle$ is the residual, and $\mathbf{R}$ is the covariance matrix of the displacements about the mean (a moment of inertia), whose j, lth element is $X_{jl}(t;\mathbf{a},t_0)=\langle X'_j X'_l\rangle$, dependent only, for the stationary case, on the time lag $t-t_0$. If we take $t_0=0$ then $X_{jl}=X_{jl}(t)$. Power to -1 denotes inverse and $|\cdot|$ denotes determinant.

It is well known that, for the Gaussian pdf (4), $\langle\Delta C\rangle$, equation (2), satisfies the convection diffusion-type equation

$$\frac{\partial\langle\Delta C\rangle}{\partial t}+V_j\frac{\partial\langle\Delta C\rangle}{\partial x_j}=D_{jl}(t)\frac{\partial^2\langle\Delta C\rangle}{\partial x_j\partial x_l} \tag{5}$$

where the velocity V_j and the hydrodynamic dispersion coefficients D_{jl} are

$$V_j=\left\langle\frac{\mathrm{d}X_j}{\mathrm{d}t}\right\rangle \quad\text{and}\quad D_{jl}(t)=\frac{1}{2}\cdot\frac{\mathrm{d}X_{jl}}{\mathrm{d}t} \tag{6}$$

Let $\mathbf{V}(\mathbf{x}, t)$ be the Eulerian velocity field, with $\mathbf{V}=\mathbf{U}+\mathbf{u}(\mathbf{x}, t)$, $\mathbf{U}=\langle\mathbf{V}\rangle$, and $\mathbf{u}$ a random space function[5] deterministic in t. The total displacement $\mathbf{X}_t$ is related to $\mathbf{u}$ by

$$\frac{\mathrm{d}\mathbf{X}_t}{\mathrm{d}t}=\mathbf{U}+\mathbf{u}(\mathbf{X}, t)+\frac{\mathrm{d}\mathbf{X}_\mathrm{d}}{\mathrm{d}t} \tag{7}$$

where $\mathbf{X}_\mathrm{d}$ is associated with a 'Brownian motion' type of transport, such that $\mathbf{X}_{\mathrm{d}jl}=2D_{\mathrm{d}jlt}$, and the remaining part of (7) is related to displacement originating from convection by the fluid.

By employing a first-order perturbation method and a generalized Fourier transform, Dagan[5] obtains the fundamental result

$$\frac{\mathrm{d}^2X_{jl}}{\mathrm{d}t^2}=\frac{2}{(2\pi)^{m/2}}\int \hat{u}_{jl}(\mathbf{k}, t)\exp[\mathrm{i}\mathbf{k}\cdot\langle\mathbf{X}\rangle-\mathbf{k}^\mathrm{T}\cdot\mathbf{D}_\mathrm{d}\cdot\mathbf{k}t]\,\mathrm{d}\mathbf{k} \tag{8}$$

rendering the displacement covariance in terms of Eulerian velocity covariance transform $\hat{u}_{jl}$, by means only of the hypothesis that $\mathbf{X}_\mathrm{d}$ is a Gaussian process.[10] In (8) $\mathbf{k}$ is the wave-number vector and integration ranges from $-\infty$ to $+\infty$.

For a constant hydraulic gradient and stationary log-conductivity Y of the permeability field, the velocity covariance transform can be expressed[4,5] in terms of $\hat{C}_Y$ (the Fourier–Stieltjes transformed covariance of Y) by the linearized expression

$$\hat{u}_{jl}(\mathbf{k})=\sum_p\sum_q U_pU_q\left(\delta_{pj}-\frac{k_jk_p}{|\mathbf{k}|^2}\right)\left(\delta_{ql}-\frac{k_lk_q}{|\mathbf{k}|^2}\right)\hat{C}_Y(\mathbf{k}) \tag{9}$$

where $\hat{C}_Y(\mathbf{k})$ is the log-conductivity covariance transform, δ is the Kronecker 'function', $p, q=1, m$, and m is the space dimensionality. From (8) and (9) we obtain the expression for X_{jl} in terms of $\hat{C}_Y(\mathbf{k})$ as follows:[5]

$$\frac{\mathrm{d}^2X_{jl}}{\mathrm{d}t^2}=\frac{2}{(2\pi)^{m/2}}\cdot\int\sum_p\sum_q U_pU_q\left(\delta_{pj}-\frac{k_jk_p}{|\mathbf{k}|^2}\right)\left(\delta_{ql}-\frac{k_lk_q}{|\mathbf{k}|^2}\right)\hat{C}_Y(\mathbf{k})$$
$$\times\exp[\mathrm{i}\mathbf{k}^\mathrm{T}\cdot\mathbf{U}t-\mathbf{k}\cdot\mathbf{D}_\mathrm{d}\cdot\mathbf{k}t]\,\mathrm{d}\mathbf{k} \tag{10}$$

Solution of (10), given a transform covariance structure $\hat{C}_Y(\mathbf{x})$ of the log-conductivity field, yields the time-varying dispersion coefficients $D_{jl}(t)$ in equation (5), whose general solution (for the pulse boundary condition at $t=0$ and centred at the origin of the Cartesian co-ordinate system) is furnished by (4) apart from constants.

Dagan[4] has given the solution to (10) in the case of exponential covariance ($C_Y(\mathbf{x})=\sigma_Y^2\exp(-|\mathbf{x}|/l_Y)$. The 2-D results for the constant velocity field $\mathbf{V}=(v, 0)$ are[2]

$$D_{11}(t)=vl_Y\sigma_Y^2\left[1-\frac{3}{2\tau}-3\frac{\exp(-\tau)}{\tau^2}+\frac{3}{\tau^3}(1-\exp(-\tau))\right]+D_{\mathrm{d}11} \tag{11}$$

$$D_{22}(t)=\frac{vl_Y\sigma_Y^2}{2\tau}\left[1-\frac{6}{\tau^2}+2\exp(-\tau)\left(1+\frac{3}{\tau}+\frac{3}{\tau^2}\right)\right]+D_{\mathrm{d}22} \tag{12}$$

where $\tau=vt/l_Y$.

These last results are used to calibrate the computational procedure.

Solution to (3) and (5) yields, for the impulse at $t_0=0$ in the 2-D case (11), (12)

$$\langle C(x_1, x_2, t)\rangle=\frac{1}{4\pi(\Phi_1\Phi_2)^{1/2}}\iint_{V_0} C_0(a_1, a_2)\exp\left[-\frac{(x_1-a_1-vt)^2}{4\Phi_1}-\frac{(x_2-a_2)^2}{4\Phi_2}\right]\mathrm{d}a_1\,\mathrm{d}a_2 \tag{13a}$$

where Φ_i, $i=1, 2$, is given by

$$\Phi_i(t)=\int_0^t D_{ii}(t')\,\mathrm{d}t' \tag{13b}$$

Equations (13a) and (13b) are integrated for the final comparisons.

THE COMPUTATION OF DISPERSION COEFFICIENTS

Integrating (10) once, we have

$$\frac{\mathrm{d}X_{jl}}{\mathrm{d}t}=\frac{2}{(2\pi)^{m/2}}\int\frac{\sum_p\sum_q U_p U_q\left(\delta_{pj}-\frac{k_j k_p}{|\mathbf{k}|^2}\right)\left(\delta_{ql}-\frac{k_l k_q}{|\mathbf{k}|^2}\right)}{\mathrm{i}\mathbf{k}\cdot\mathbf{U}-\mathbf{k}^{\mathrm{T}}\cdot\mathbf{D}_{\mathrm{d}}\cdot\mathbf{k}}\hat{C}_Y(\mathbf{k})$$
$$\times\exp[\mathrm{i}\mathbf{k}\cdot\mathbf{U}t-\mathbf{k}^{\mathrm{T}}\cdot\mathbf{D}_{\mathrm{d}}\cdot\mathbf{k}t-1]\,\mathrm{d}\mathbf{k} \tag{14}$$

If we neglect $\mathbf{D}_{\mathrm{d}}$ in (14)[5] and for the 2-D constant velocity field $\mathbf{V}=(v, 0)$, the hydrodynamic dispersion coefficients are from (14), (6) and (7)

$$D_{11}=\frac{1}{2}\frac{\mathrm{d}X_{11}}{\mathrm{d}t}+D_{\mathrm{d}11}=\frac{1}{2\pi}\iint\left(1-\frac{k_1^2}{k_1^2+k_2^2}\right)^2\frac{\hat{C}_Y(k_1, k_2)[\exp(\mathrm{i}k_1 vt)-1]}{\mathrm{i}k_1 v}\mathrm{d}k_1\,\mathrm{d}k_2+D_{\mathrm{d}11} \tag{15}$$

$$D_{22}=\frac{1}{2}\frac{\mathrm{d}X_{22}}{\mathrm{d}t}+D_{\mathrm{d}22}=\frac{1}{2\pi}\iint\left(\frac{k_1 k_2}{k_1^2+k_2^2}\right)^2\frac{\hat{C}_Y(k_1, k_2)[\exp(\mathrm{i}k_1 vt)-1]}{\mathrm{i}k_1 v}\mathrm{d}k_1\,\mathrm{d}k_2+D_{\mathrm{d}22} \tag{16}$$

The longitudinal and transversal dispersion coefficients are numerically evaluated from (15) and (16) for several different forms of the isotropic correlation function $C_Y(\mathbf{x})$ outlined below:

(a)
$$C_Y(\mathbf{x})=\sigma_Y^2\exp(-|\mathbf{x}|/l_{Y1}) \tag{17}$$

(b)
$$C_Y(\mathbf{x})=\begin{cases}\sigma_Y^2(1-|\mathbf{x}|/l_{Y2}) & \text{for } |\mathbf{x}|\leqslant l_{Y2}\\ 0 & \text{for } |\mathbf{x}|>l_{Y2}\end{cases} \tag{18}$$

(c)
$$C_Y(\mathbf{x})=\begin{cases}\sigma_Y^2(1+\cos(\pi|\mathbf{x}|/l_{Y3}))/2 & \text{for } |\mathbf{x}|\leqslant l_{Y3}\\ 0 & \text{for } |\mathbf{x}|>l_{Y3}\end{cases} \tag{19}$$

(d)
$$C_Y(\mathbf{x})=\begin{cases}\sigma_Y^2 & \text{for } |\mathbf{x}|\leqslant l_{Y4}\\ 0 & \text{for } |\mathbf{x}|>l_{Y4}\end{cases} \tag{20}$$

Equation (20) is the limit case of the covariance structures used, in which the formation has been regarded as a collection of equal blocks of independent properties. The exclusion of uncorrelated components of Y ('nugget' effects) is inconsequential because variability at other scales is assumed negligible. Hole effects in the covariance structure do not appear in experimental analyses.[8]

The covariances (17), (18), (19) and (20) are all isotropic and the symmetry reduced the computation of transform and of integrals (15), (16). The calculations are performed only for the real part: the formulas employed (enforcing symmetry of the spectra and complex conjugation of real data) are

$$\frac{\mathrm{d}X_{11}}{\mathrm{d}t}=\frac{4v}{\pi}\int_0^\infty\int_0^\infty\frac{\sin(k_1 vt)}{k_1}\left(1-\frac{k_1^2}{k_1^2+k_2^2}\right)^2\hat{C}_Y(k_1, k_2)\,\mathrm{d}k_1\,\mathrm{d}k_2 \tag{21}$$

$$\frac{\mathrm{d}X_{22}}{\mathrm{d}t}=\frac{4v}{\pi}\int_0^\infty\int_0^\infty\frac{\sin(k_1 vt)}{k_1}\left(\frac{k_1 k_2}{k_1^2+k_2^2}\right)^2\hat{C}_Y(k_1, k_2)\,\mathrm{d}k_1\,\mathrm{d}k_2 \tag{22}$$

It is emphasized that the numerical procedure of integration of (21) and (22) is a delicate one, since $\mathbf{k}$ starts from zero: yet limits for $\mathbf{k}\to 0$ are finite. The treatment of the sine function is delicate too, because the period of the function decreases as time increases: if time-adjusted shorter integration steps Δk were not employed, a large error would occur. On the other hand, a fixed larger Δk is sufficient for a correct evaluation of numerical transform of the covariance $C_Y(\mathbf{x})$: to perform varying steps of integration, the covariance matrix $\hat{C}_Y(\mathbf{k})$ is interpolated by linear piecewise polynomial functions.[11] Limits for $t\to 0$ of sine functions are trivial.

The case of exponential covariance is solved numerically to provide a measure of the accuracy of the procedure upon comparison with the closed-form solutions (11) and (12). Numerical accuracy proves to be within 1 per cent.

To well-pose the comparison, the isotropic integral scale

$$I_h = \left[\frac{2}{\sigma_Y^2}\int_0^\infty C_Y(r)r\,\mathrm{d}r\right]^{1/2} \tag{23}$$

has been fixed so as to study the possible influence of the form of the correlation function for Y. If we impose $l_{Y1}=2{\cdot}7$ m (Reference 1) the remaining coefficients for (18), (19) and (20) are

$$l_{Y2}=6{\cdot}6\,\mathrm{m} \quad l_{Y3}=7{\cdot}0\,\mathrm{m} \quad l_{Y4}=3{\cdot}8\,\mathrm{m}$$

Figures 1 and 2 illustrate the time evolution of the dispersion coefficients D_{11} and D_{22} for all the cases (17) to (20). Figures 3 and 4 show the comparison between the computed covariance of longitudinal and transversal displacements of the plume (the moments of inertia) with that measured at the Borden site for the case of inorganic inert solute,[1] where the experimental characteristics of the permeability field have been employed.

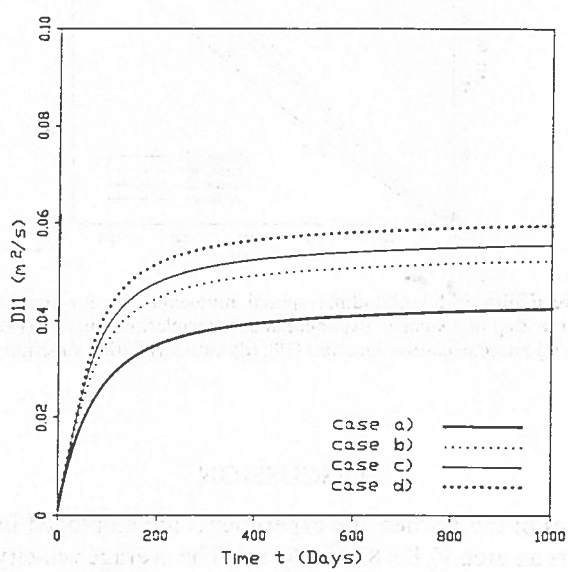

Figure 1. Longitudinal dispersion coefficients D_{11} as a function of residence time t in the random permeability field: (a) Dagan's[4] exponential autocorrelation function (17); (b) autocorrelation function (18); (c) autocorrelation function (19); (d) autocorrelation function (20)

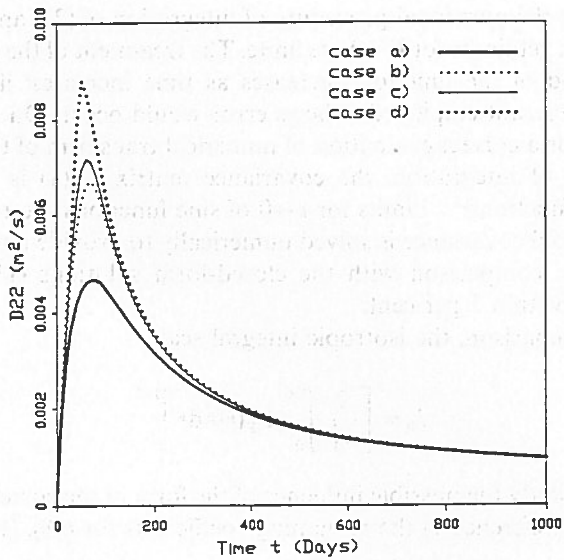

Figure 2. Same as Figure 1 for transversal dispersion coefficients D_{22}

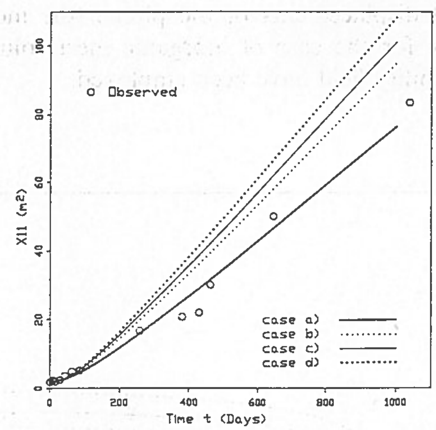

Figure 3. Comparison between observed longitudinal spatial moments X_{11} for the Borden site experiment (after Freyberg[1]) and computed curve X_{11}: (a) Dagan's[4] exponential autocorrelation function (17); (b) autocorrelation function (18); (c) autocorrelation function (19); (d) autocorrelation function (20)

DISCUSSION

The characteristic values of the Borden site experiment[1] are employed in the example. Here the initial solute body covers an area V_0 $8 \times 8\ m^2 = 64\ m^2$. The average velocity oriented along the X_1-axis is $v = 0{\cdot}091$ m/day: the variance of log-conductivity $\sigma_Y^2 = 0{\cdot}74 \times 0{\cdot}24 = 0{\cdot}1776$.[1] The spatial correlation scales are $I_{x1} = I_{x2} = I_h = 3{\cdot}82$ m. Solute injection is, at initial concentration $C_0 = 60$ mg/l.

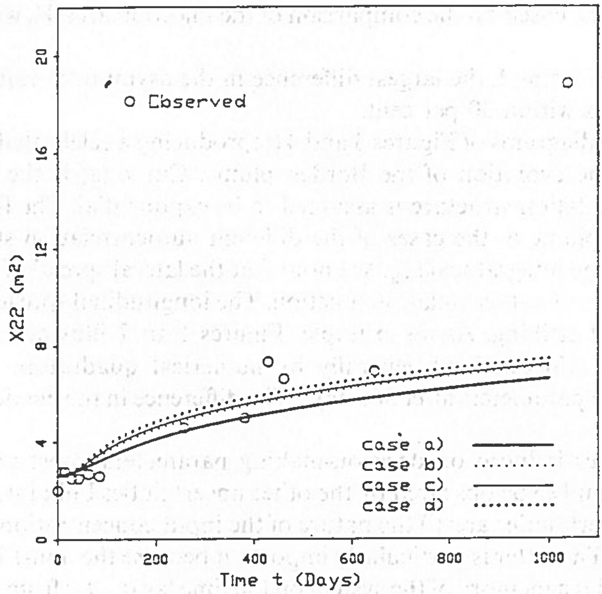

Figure 4. Same as Figure 3 for the lateral spatial moment X_{22} (observed X_{22} after Freyberg[1])

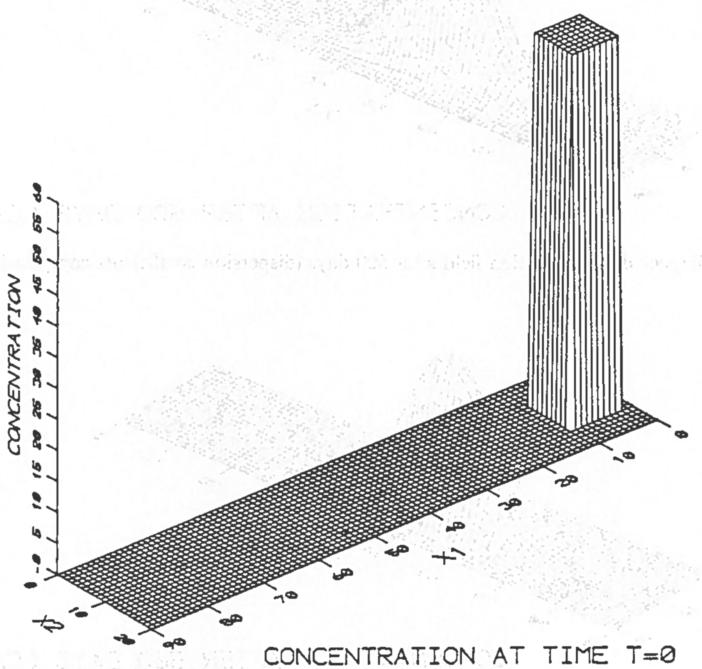

Figure 5. Initial concentration field for the numerical experiment. Units are [mg/l] for concentration and [m] for X_1, X_2

Ergodic requirements, based on the comparison of the injection area V_0 with the integral scales, are seemingly met.[4]

As shown in Figures 1 and 2, the largest difference in the asymptotic value of the longitudinal dispersion coefficient is within 30 per cent.

We observe that the diagrams of Figures 3 and 4 (reproducing a celebrated graph by Freyberg[1]) synthetize very well the evolution of the Borden plume. Curve (a) is the outcome of Dagan's theory, where the correlation structure is assumed to be exponential. The lines (b) to (d) portray the evaluation of the plume in the cases of the different autocorrelation structures (17) to (20), which maintain the same integral scale I_h. We note that the lateral spread of the plume is virtually unaffected by the choice of autocorrelation function. The longitudinal spread is more affected, but the differences are not striking. As an example, Figures 5 to 7 illustrate the plume evolution (solution to equation (13) obtained generally by numerical quadrature via a 3-point Gauss scheme) with the above parameters after 500 days. The difference in the maximum concentration is 17 per cent.

Hence the differences induced on decision-making parameters (most notably the maximum concentration) are bound to be obscured by the other uncertainties built into field-scale transport phenomena. Such uncertainties are: (i) the nature of the input concentration; and (ii) the real time sequence of injection. The latter is particularly important because the non-Fickian structure of the macrodispersion implies a memory of the system on the time lag $(t-t_0)$ from injection time t_0. As a

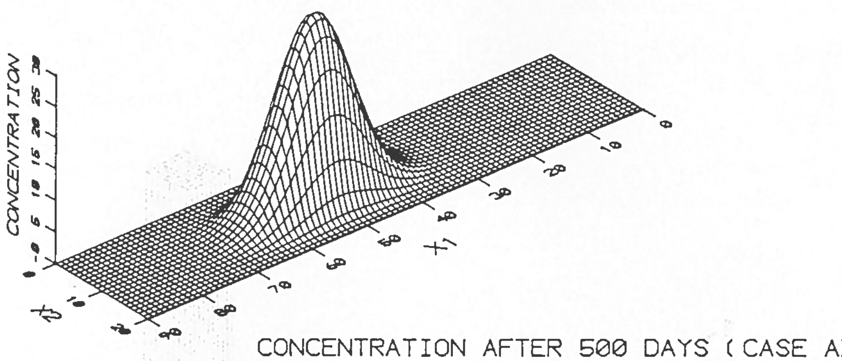

Figure 6. Expected concentration field after 500 days (dispersion coefficients computed as in case (a))

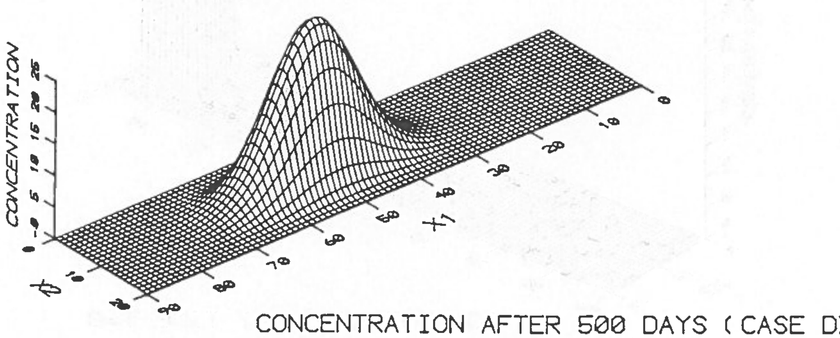

Figure 7. Expected concentration field after 500 days (dispersion coefficients computed as in case (d))

consequence, non-Fickian processes result in a convoluted structure for the dispersion coefficients, whenever the mass injected $\dot{M}(t_0, \mathbf{a})\,\mathrm{d}\mathbf{a}\,\mathrm{d}t_0$ is not instantaneously forced in the system. Real life settings (waste repositories or injection wells) almost inevitably fall into this case unless for special test setups.

We therefore conclude that the choice of analytical expressions for the autocorrelation structure of random permeability fields is quite irrelevant, provided that the integral scale of correlation is properly defined.

This amounts to a clear picture of the macroscopic scale of heterogeneity in the formation which turns out to be the dominant factor in the establishment of a macrodispersive regime in groundwater. This has important practical implications. In fact, this conclusion yields to a generalized use of Dagan's model with exponential autocorrelation function, which allows the closed-form solutions (11) and (12) for the time-varying dispersion coefficients.

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