Impact of Human Activity on Groundwater Dynamics (Proceedings of a symposium held during the Sixth IAHS Scientific Assembly at Maastricht, The Netherlands, July 2001). IAHS Publ. no. 269, 2001.

Analysis of the longitudinal dispersion of non-reactive solutes in long-range correlated permeability fields

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Abstract The concept of porous formations characterized by long-range correlated permeability fields has been introduced in recent years in order to explain the observed increase in dispersive parameters as a function of the observation scale, often coined as anomalous transport. One of the main purposes of the present study is to analyse the combined effects of the field and the local scales of heterogeneity in determining the transport properties of non-reactive solutes. The permeability field is assumed to be a space random function, lognormally distributed, and the transport parameters are obtained through a Lagrangian formulation of transport, by means of a few simplifying assumptions. The validity of the results obtained in the past, in particular concerning the occurrence of anomalous transport, is also checked. The results show that longitudinal dispersivity grows unbounded with the observation scale when local-scale dispersion is present, indicating that transport is always anomalous for the random fields considered. The results are at variance with those obtained in the past, under both the ergodic and the non-ergodic assumptions, which neglect local-scale dispersion.

Key words anomalous transport; dispersion; heterogeneous formations; porous media

INTRODUCTION

Recent transport theories indicate that the heterogeneous permeability field plays a fundamental role in transport through natural porous formations. The transport problem has often been solved in the past by modelling the permeability K as a stationary space random function; the latter is assumed to be log-normally distributed, and fully characterized by a few statistical moments, such as the mean $\langle Y \rangle$, the variance σ_Y^2 and the integral scale I_Y, with $Y = \ln K$. In particular, the permeability integral scale I_Y seems to be one of the most important parameters controlling dispersion.

In recent years, many theoretical and experimental studies have argued that in natural aquifers the conductivity field is long-range correlated, characterized by an integral scale of the hydraulic properties of the soils that increase unbounded with the observation scale. Among the arguments supporting such models are: (a) the apparent increase of dispersivities with the observation scale (e.g. Neuman, 1990), often coined as anomalous transport, and (b) the dependence of the variability in permeability on the observation scale recorded in a number of studies based on the analysis of field data (e.g. Hewett, 1986; Desbarats & Bachu, 1994; Liu & Molz, 1997).

Out of the various models proposed for the long-range correlated $Y = \ln K$, a relevant one is the case of stationary log-conductivity of finite variance σ_Y^2 and of unbounded integral scale. The covariance function $C_Y = \langle Y'(\mathbf{x})Y'(\mathbf{x}+\mathbf{r})\rangle$, where the prime denotes fluctuation around the mean and $\mathbf{r}$ is the distance vector between two points, can be approximated for large lag distances as a power law of the distance $r = |\mathbf{r}|$ (Glimm & Sharp, 1991):

$$C_Y = ar^{\beta} \qquad (-1 \le \beta \le 0) \tag{1}$$

where a and β are constants.

The aim of the present study is the determination of the actual longitudinal dispersion coefficient D_L for transport in formations of long-range permeability fields by considering both large-scale advection, which is ruled by the spatial variability of K, and local-scale dispersion, which is defined at a smaller scale; the non-ergodicity of the plume will be considered throughout the work. The scope is twofold: (a) to analyse the mutual role played by both scales of heterogeneity (the field and the local scale) in determining the overall transport properties, and (b) to check the validity of the results obtained in the past, in particular concerning the occurrence of anomalous transport.

MATHEMATICAL BACKGROUND

We consider the transport of a conservative solute in a two-dimensional formation of local-scale dispersion (assumed here as isotropic) coefficient D_d. The mean hydraulic gradient is uniform, with mean velocity U aligned with the longitudinal direction x_1, and x_2 is the transverse coordinate. At time $t = 0$, a conservative solute of mass M, with concentration $C_0(\mathbf{a})$, is released across the area A. By adopting a Lagrangian representation, the expected concentration spatial moments $\langle S_{ij}(t)\rangle$ can be calculated as follows (see Dagan, 1989):

$$\langle S_{ij}(t)\rangle = \frac{1}{M}\left\langle \int n(x_i - R_i)(x_j - R_j)C(\mathbf{x},t)\mathrm{d}\mathbf{x}\right\rangle = S_{ij}(0) + X_{ij}(t) + 2D_d t - R_{ij}(t) \tag{2}$$

where n is the constant porosity. In equation (2) $\mathbf{R}(t)$ is the centroid of the plume, defined by:

$$\mathbf{R}(t) = \frac{1}{M}\int n\mathbf{x}C(\mathbf{x},t)\mathrm{d}\mathbf{x} \tag{3}$$

where $X_{ij} = \langle X_i'(t;\mathbf{a})X_j'(t;\mathbf{a})\rangle$ represents the generic component of the covariance tensor of the trajectory $\mathbf{X}(t;\mathbf{a})$ of a solute particle injected at $\mathbf{x} = \mathbf{a}$ at $t = 0$, while $R_{ij} = \langle R_i'(t)R_j'(t)\rangle$ represents the covariance tensor of the plume centroid trajectory, defined by equation (3); $S_{ij}(0)$ is the second moment of the initial plume.

The component $R_{ij}(t)$ is calculated by integration of the two-particles covariance $Z_{ij}(t;\mathbf{a}-\mathbf{b}) = \langle X_i'(t;\mathbf{a})X_j'(t;\mathbf{b})\rangle$ (Dagan, 1989). For a rectangular injection area A, of dimensions l_1 and l (longitudinal and transverse, respectively), the resulting expression is:

$$R_{ij}(t) = \frac{1}{(l_1 l)^2} \int_{-l_1/2}^{l_1/2} \int_{-l_1/2}^{l_1/2} \int_{-l/2}^{l/2} \int_{-l/2}^{l/2} Z_{ij}(t; \mathbf{r} - \mathbf{r}') \mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}' \tag{4}$$

The terms X_{ij} and Z_{ij}, which are crucial in the determination of the concentration moments, equation (2), were derived in the past by adopting a first-order approximation of the log-conductivity variance σ_Y^2 as a function of the particular structure of the velocity covariance (e.g. Dagan, 1991; Fiori & Dagan, 2000). The resulting expressions are given in Fiori & Dagan (2000, equations 14 and 15) in terms of a Fourier transform of the covariance velocity spectrum.

The longitudinal macrodispersion coefficient D_L, whose computation is the main objective of this study, is defined as $D_L = (1/2)\mathrm{d}\langle S_{11}\rangle/\mathrm{d}t - D_d$, is obtained by a simple derivation in equation (2). After insertion of the expressions for X_{ij}, Z_{ij} reproduced in Fiori & Dagan (2000), in equation (4) and subsequently in equation (2), manipulation of the resulting expression yields (the detailed derivations are given in Fiori (2001)):

$$D_L(t) = \frac{1}{2}\frac{\mathrm{d}\langle S_{11}\rangle}{\mathrm{d}t} - D_d = \frac{1}{2}\int_0^{Ut} \{\xi(Ut, x) + \xi(x, Ut)\}\mathrm{d}x \tag{5}$$

with:

$$\xi(x,x') = \frac{1}{4\pi U (l_1 l)^2} \int_{-l_1/2}^{l_1/2} \int_{-l_1/2}^{l_1/2} \int_{-l/2}^{l/2} \int_{-l/2}^{l/2} \int \int \Big\{u_{11}\Big(x + x' + z'\sqrt{D_d|x-x'|/U}, z\sqrt{D_d|x-x'|/U}\Big) - u_{11}\Big(x + x' + y_1 - y_1' + z'\sqrt{D_d(x-x')/U}, y - y' + z\sqrt{D_d(x-x')/U}\Big)\Big\} \cdot \exp\left(-\frac{z^2 + z'^2}{4}\right)\mathrm{d}z\mathrm{d}z'\mathrm{d}y_1\mathrm{d}y_1'\mathrm{d}y\mathrm{d}y' \tag{6}$$

DISCUSSION OF RESULTS AND CONCLUSIONS

The longitudinal dispersion coefficient for a stationary random log-permeability field characterized by the covariance structure of equation (1) was evaluated by Glimm & Sharp (1991), who however have implicitly assumed $R_{11} = 0$ in equation (2). The assumption is that the plume centroid moves like a straight line $R_1 = Ut$. We shall denote this result as "ergodic", as opposed to the non-ergodic one where $R_{11} \neq 0$ (Dagan, 1991); the ergodic dispersion coefficient will be indicated hereinafter with the symbol d_L, to be distinguished from the non-ergodic one D_L. In the range $-1 < \beta < 0$, the ergodic dispersion coefficient d_L grows proportional to $t^{1+\beta}$ when time is large, leading to anomalous transport (Glimm & Sharp, 1991).

Results obtained by adopting the non-ergodic approach (Dagan, 1994; Bellin *et al.*, 1996) show that for any value of β, the actual dispersion coefficient D_L tends to a constant value when time is large; hence transport is always "Fickian". The latter result was obtained by means of a first-order approximation in the log-permeability variance, and neglecting the effects of local-scale dispersion.

We wish now to determine D_L in the presence of local-scale dispersion under non-ergodic conditions, using expression (5). The latter requires the velocity covariance $u_{11}(\mathbf{r})$ as a function of the two-points distance $\mathbf{r}(x,y)$, with the coordinates x and y longitudinal and transverse to the mean flow direction, respectively. The velocity covariance was obtained in the past by means of a first-order approximation in the log-permeability variance (Dagan, 1994). We reproduce here, for completeness, the final expression for u_{11} :

$$u_{11}(x,y)=\frac{U^2 a}{(2+\beta)(4+\beta)}\left[(1+\beta)(3+\beta)r^{\beta}-2\beta(1+\beta)r^{\beta-2}x^2+\beta(\beta-2)r^{\beta-4}x^4\right] \tag{7}$$

with $r^2=x^2+y^2$.

The integrations in equation (5) cannot be carried out in an analytical form; we therefore assess the asymptotic behaviour of D_L by adopting some simplifying assumptions in equation (5). First, if $D_d t >> l^2, l_1^2$, we can assume $y, y', y_1, y_1' \cong 0$ in equation (6) and eliminate the integrations over l, l_1. Then, for $U^2 t >> D_d$, we split the integral over x in equation (5) into one over $x \approx (D_d t)^{1/2}$ and the remaining contribution up to $x >> (D_d t)^{1/2}$. For the latter interval, the term can be evaluated by a Taylor expansion of u_{11} around the transverse displacement. We finally obtain for D_L the following asymptotic, large-time expression:

$$D_L=\frac{15 a D_d (Ut)^{\beta}}{4(1-\beta)(2+\beta)(4+\beta)}+\mathrm{O}\left(aU(D_d t)^{(1+\beta)/2}\right) \tag{8}$$

Considering the range of possible values for β, the dispersion coefficient approaches the following asymptotic, large-time limit, valid when $tD_d >> l^2$ and $U^2 t >> D_d$:

$$D_L \approx aU(D_d t)^{\frac{1+\beta}{2}} \qquad (-1<\beta<0) \tag{9}$$

The important result is that in the range $-1 < \beta < 0$ the non-ergodic dispersion coefficient does not tend to a constant value, as predicted by the zero local-scale result, but increases with time, leading to anomalous diffusion. The macrodispersion coefficient d_L predicted by the ergodic formulation is proportional to $t^{1+\beta}$, i.e. the growth is faster with time.

Next, some results for D_L based on direct numerical integration of equation (5) are presented. In order to reduce the required five quadratures, the problem is simplified as follows: (a) the longitudinal local-scale component, which has a negligible influence on the trajectory moments compared to the transverse component (Fiori, 1996), is suppressed, and (b) the initial plume is of vanishing longitudinal dimension l_1, the transverse dimension l being the most important component (Dagan, 1991). Consequently, expression (5) simplifies as follows:

$$D_L(t) = \frac{1}{l^2 U \sqrt{\pi}} \int_0^l \int_0^{Ut} \int_0^\infty (l-y) \Big\{ 2u_{11}\left(x, z\sqrt{D_d x/U}\right) - u_{11}\left(x, y + z\sqrt{D_d(2t - x/U)}\right) - u_{11}\left(x, y - z\sqrt{D_d(2t - x/U)}\right) \Big\} \exp\left(-\frac{x^2}{4}\right) \mathrm{d}z\, \mathrm{d}x\, \mathrm{d}y \tag{10}$$

The dispersion coefficient D_L is calculated by numerical quadrature of the latter expression.

Figure 1 represents the dimensionless longitudinal dispersion coefficient as a function of the dimensionless travel distance tU/l for a few values of the Peclet number, defined as $Pe = Ul/D_d$ (usually $Pe >> 1$) and $\beta = -0.5$. The figure shows that for $Pe = \infty$, D_L tends to a constant limit, as predicted by the non-ergodic, pure advective formulation of Dagan (1994). No matter how large, but finite, is the Peclet number, the dispersion coefficient will depart from the infinite Peclet result and increase with time, to reach the asymptotic value, equation (9) (for the examined case, $D_L \approx t^{0.25}$) for $tU/l >> Pe$. It should be noted that the latter condition is satisfied at times which might be large in real systems.

The behaviour at early and intermediate times is strongly affected by the competing mechanisms of large-scale advection and local-scale dispersion. At early times ($tU/l << 1$), advection dominates and D_L tends to assume the constant value predicted by Dagan (1994). Consistent with the analysis of Fiori (1996) for finite-range permeability fields, in this regime D_L decreases with the Peclet number. At intermediate times ($tU/l = \mathrm{O}(1) \div \mathrm{O}(Pe)$) local-scale dispersion starts to play a role and competes with advection, resulting in a deviation from the purely advective result.

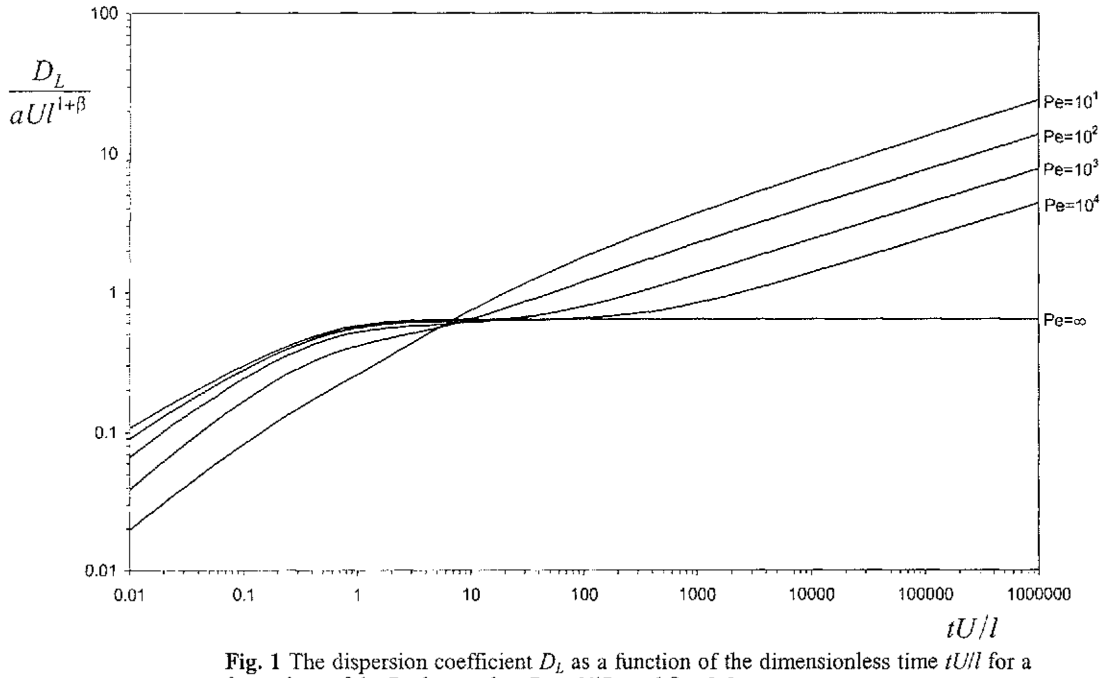

Fig. 1 The dispersion coefficient D_L as a function of the dimensionless time tU/l for a few values of the Peclet number $Pe = U/D_d$ and $\beta = 0.5$.

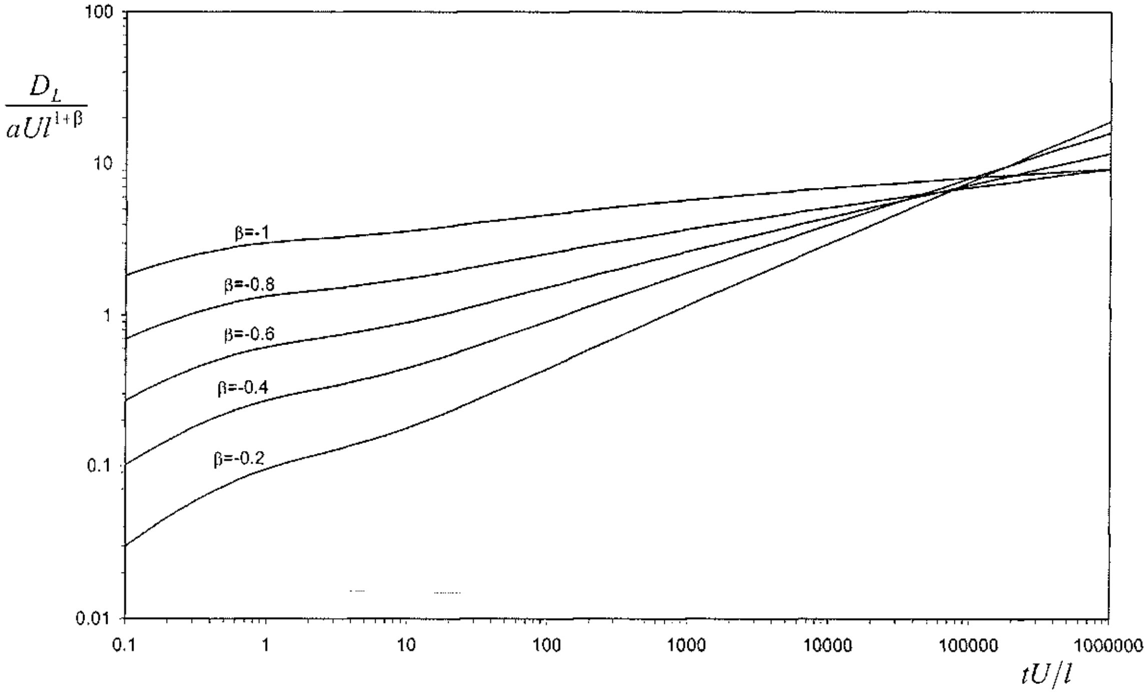

Fig. 2 The dispersion coefficient D_L as a function of the dimensionless time tU/l for a few values of β, and for $Pe = Ul/D_d = 100$.

To further illustrate results, Fig. 2 reproduces D_L as a function of tU/l for a fixed Peclet number (Pe = 100) and a few values of β. The behaviour at early and intermediate times is the same as that illustrated above. At late times ($tU/l >> Pe$), the slope of the curves is equal to the exponent in equation (9) $(1 + \beta)/2$. As the coefficient β drops to zero, transport is characterized by decreasing values of the longitudinal dispersion coefficient. When $\beta = 0$, D_L vanishes because at this limit the entire solute body translates without dispersing.

We conclude that the interplay between large-scale, advective displacement and local-scale dispersion has a fundamental impact on the occurrence of anomalous transport in random long-range correlated permeability fields. Such an impact is manifested, however, at time scales of the order of $t >> l^2/D_d$ which may be large for practical applications.

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