The influence of the log-conductivity autocovariance structure on macrodispersion coefficients

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Abstract

Macrodispersion coefficients are derived for heterogeneous porous media under ergodic and nonergodic conditions. Influences of the log-conductivity autocovariance function on macrodispersion are investigated through six commonly used isotropic log-conductivity autocorrelation models. They are the exponential, Gaussian, spherical, linear, Whittle and Mizell A-type models. Analytical expressions for ergodic macrodispersion coefficients for each of these models are presented. The results for nonergodic macrodispersion coefficients are calculated numerically. The results show that the various autocovariance functions, which display slight differences in the preasymptotic region, have little effect on the ultimate macrodispersion coefficient. The effect of nonergodicity is more significant than the log-conductivity autocovariance function for the aquifers exhibiting unimodal log-conductivity distribution.

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1. Introduction

Naturally occurring porous media usually display heterogeneity that renders the processes of groundwater flow and solute transport complicated. The stochastic approach treats the hydraulic parameters of the porous medium as random variables in the spatial domain, and therefore, distributions of the seepage velocity and the solute concentration are also random. To analyze solute transport in randomly heterogeneous porous media, a perturbation analysis is commonly applied (Gelhar, 1993; Dagan, 1989). This analysis,
valid for small log-conductivity variance, has the convenience that enables one to derive closed-form expressions of the Eulerian velocity covariance for uniform average flow. For the solute transport, the required partial differential equations that describe the expected concentration and its associated variance in heterogeneous porous media are derived by Dagan and Fiori (1997) as

\[
\frac{\partial \langle c \rangle}{\partial t} = -V_i \frac{\partial \langle c \rangle}{\partial x_i} + (D'_{ij} + D''_{ij}) \frac{\partial^2 \langle c \rangle}{\partial x_i \partial x_j} \tag{1}
\]

\[
\frac{\partial \sigma^2_c}{\partial t} = -V_i \frac{\partial \sigma^2_c}{\partial x_i} + (D'_{ij} + D''_{ij}) \frac{\partial^2 \sigma^2_c}{\partial x_i \partial x_j} + 2D'_{ij} \frac{\partial \langle c \rangle}{\partial x_i} \frac{\partial \langle c \rangle}{\partial x_j} - 2D''_{ij} \left\langle \frac{\partial c'}{\partial x_i} \frac{\partial c'}{\partial x_j} \right\rangle \tag{2}
\]

respectively. Here \( \langle c \rangle \) is the expected concentration, \( \sigma^2_c \) is the concentration variance, \( c' \) is the concentration fluctuation, \( V_i \) is the mean of seepage flow velocity in \( i \) direction, \( D'_{ij} \) is the macrodispersion coefficient while \( D''_{ij} \) is the pore scale or local dispersion. In most groundwater applications, the Peclet number, defined as \( Pe_{ij} = \frac{V_i k}{D''_{ij}} \), is in the range of \( 10^2 \) – \( 10^4 \), where \( k \) is the integral scale of the log-hydraulic conductivity. The effect of the local dispersion for the small scale mixing process is therefore negligible. Solving Eqs. (1) and (2) requires the knowledge of the macrodispersion coefficient. As pointed out by Dagan et al. (1992), ‘the derivation of the macrodispersion coefficient in terms of the velocity field statistics is one of the central issues of transport theory’.

Analytical studies on macrodispersion coefficients have been carried out with the ergodic theory (Dagan, 1982, 1984, 1987, 1988; Gelhar and Axness, 1983; Neuman et al., 1987; Neuman and Zhang, 1990; Hsu et al., 1996) and nonergodic theory (Kitanidis, 1988; Dagan, 1990, 1991; Rajaram and Gelhar, 1993a,b; Zhang et al., 1996). The ergodic condition applies when the length scale of the initial solute body is large while the nonergodic condition is valid for the plume source small compared to the correlation scale of the log-conductivity field. Dagan (1982, 1984, 1987, 1988) was able to show that the macrodispersion is time-dependent and it may take exceedingly larger distances to reach the field-scale Fickan dispersion. Gelhar and Axness (1983) and Neuman et al. (1987) have derived the asymptotic macrodispersion by mixed-order and first-order approximations, respectively. Zhang and Neuman (1990) investigated the nonlinear effect on macrodispersion using Corrsin’s conjecture while Hsu et al. (1996) utilized a perturbation method. Hsu et al. (1996) found that the higher order effect is more profound in the transverse macrodispersion than in the longitudinal direction. The effect of nonergodicity on macrodispersion has been investigated just recently. Kitanidis (1988) first investigated nonergodic transport analytically and compared his fist-order solution to a numerical solution. Dagan (1990, 1991) extended his Lagrangian analysis of the ergodic theory to nonergodic transport. The first two moments of solute concentration are related to the motion of two particles. His results illustrated that the effective dispersion coefficient depends on the initial size of the solute body and on travel time. Rajaram and Gelhar (1993a,b) conducted Eulerian and Lagrangian analyses on the plume scale-dependent dispersion. They applied the theoretical result to the Borden tracer test and showed a better fit to the field data. Zhang et al. (1996) applied Dagan’s theory to three-dimensional statistical isotropic aquifers. The comparison of their result with the numerical simulation
shows good agreement between the calculated and simulated longitudinal second spatial moments.

The studies reviewed above have established a theoretical background for transport and have significantly enhanced our understanding of solute transport in heterogeneous porous media. However, the results are based on specific forms of the spatial log-conductivity field such as the exponential or Gaussian forms. There are several other autocovariance functions available in geostatistical literatures that present meaningful spatial correlation of the log-conductivity field (Dagan, 1989). The dependence of ergodic and nonergodic macrodispersion on the spatial log-conductivity function has not been investigated in the literature. The present study follows Dagan’s (1984, 1990) first-order approach and utilizes Hsu’s (2000) evaluation for the macrodispersion coefficient to investigate such effects in two-dimensional domain for regional transport.

2. Solute transport

The approach used to derive the macrodispersion is the Lagrangian one (Dagan, 1982). If a conservative solute particle is injected into the field at the origin at time $t=0$ and is then swept by the random groundwater velocity field, the time-dependent trajectory $X(t)$ of the solute particle is related to the velocity $u(X)$ via

$$X(t) = \int_0^t u[X(\tau)]d\tau$$

Defining $X = \langle X \rangle + X'$, where $\langle X \rangle$ is the expected location of the particle at time $t$ and $X'$ is its fluctuation. The first two moments of the particle displacement become

$$\langle X(t) \rangle = \int_0^t \langle u[X(\tau)] \rangle d\tau$$

$$X_{jk}(t) = \langle X_j(t)X_k(t) \rangle = \int_0^t \int_0^t \langle u_j[X(\tau)]u_k[X(\tau')] \rangle d\tau d\tau'$$

Since the Lagrangian velocity moment in Eq. (5) is difficult to obtain, Dagan (1984) approximated it by the Eulerian moments, i.e. replacing the particle displacement $X$ by its mean value $\langle X \rangle$ to obtain a first-order analytical solution for $X_{jk}$. For steady state and the uniform mean flow in the $x_1$ direction, Dagan (1982) gives the statistical first two moments of solute particle displacement as

$$\langle X_1 \rangle = Vt = L, \quad \langle X_2 \rangle = 0$$

$$X_{jk}(L) = \frac{1}{V^2} \int_0^L \int_0^L u_{jk}[r-r']drdr = \frac{2}{V^2} \int_0^L (L-r)u_{jk}(r)dr$$

where $V=K_gJ/n$ is the uniform mean seepage velocity, $K_g$ is the geometric mean of hydraulic conductivity $K$, $J$ is the uniform mean driving force, $u_{jk}$ is the velocity
covariance and \( n \) is the porosity. Neglecting the pore-scale dispersion effect, the macrodispersion coefficient in the ergodic condition becomes (Dagan, 1989)

\[
D_{jk}(L) = \frac{1}{2} \frac{dX_{jk}}{dr} = \frac{1}{V} \int_0^L u_{jk}(r) dr
\]  

(8)

Under nonergodic conditions, there exists an uncertainty about the actual location of the plume center of mass. Assuming the initial plume center is at the origin, the first two moments of the centroid longitudinal trajectory are given by (Dagan, 1990)

\[
\langle R_j \rangle = V_j t
\]  

(9)

\[
R_{ij} = \langle (R_i - \langle R \rangle)(R_j - \langle R \rangle) \rangle = \frac{1}{A^2_0} \int_{A_0} \int_{A_0} X_{ij}(t, \mathbf{b}) \, d\mathbf{a} \, d\mathbf{a}''
\]  

(10)

where \( \mathbf{b} = \mathbf{a}'' - \mathbf{a}' \) is the distance vector between two points located in the plume source. Dagan (1990) defined the effective dispersion coefficient \( D_{ij} \) as

\[
D_{ij}(t, l) = \frac{1}{2} \frac{dX_{ij}(t, 0)}{dr} - \frac{1}{2} \frac{dR_{ij}(t, l)}{dr} = D_{ij} - \beta_{ij}
\]  

(11)

where \( D_{ij}' \) is calculated from Eq. (8) and \( \beta_{ij} = (1/2)(dR_{ij}/dt) \) depends on the geometry of the plume source. For a rectangular source defined by \( 0 < x_1 < l_1, \ 0 < x_2 < l_2, \) \( \beta_{ij} \) can be calculated as (Dagan, 1991)

\[
\beta_{ij} = \frac{2}{l_1 l_2} \int_0^{l_1} \int_0^{l_2} (l_1 - b_1)(l_2 - b_2) \left[ u_{ij}(Vt + b_1, b_2) + u_{ij}(Vt - b_1, b_2) \right] \, db_2 \, db_1
\]  

(12)

Eq. (12) will be numerically evaluated by using Gaussian quadratures because of its complicated form.

3. Effects of the log-conductivity autocovariance structure on macrodispersion

The velocity covariance plays the key role in deriving the macrodispersivity (as shown in Eqs. (8) and (12). By assuming (1) infinite domain, (2) steady and uniform mean flow in the \( x_1 \) direction, (3) natural log hydraulic conductivity \( Y \) as a stationary homogeneous, multivariate Gaussian random field with a constant mean, variance \( \sigma^2 \) and a statistically isotropic autocovariance structure in the spatial domain, the general expression for the velocity covariances in two dimensions have been shown to be (Hsu, 1999)

\[
u_{11}(r) = V^2 \sigma^2 \left[ \frac{3}{8} \rho(r) - \frac{1}{2} \left( \rho(r) - \frac{2T(r)}{r} \right) \cos2\theta 
+ \left( \frac{1}{8} \rho(r) + \frac{1}{2} \frac{T(r)}{r} - \frac{3}{2} U(r) \right) \cos4\theta \right]
\]  

(13)
\[ u_{12}(r) = V^2 \sigma^2 \left[ -\frac{1}{4} \left( \rho(r) - \frac{2T(r)}{r} \right) \sin 2\theta \right. \]
\[ + \left( \frac{1}{8} \rho(r) + \frac{1}{2} \frac{T(r)}{r} - \frac{3}{2} \frac{U(r)}{r} \right) \sin 4\theta \left. \right] \]  

(14)

\[ u_{22}(r) = V^2 \sigma^2 \left[ \frac{1}{8} \rho(r) - \left( \frac{1}{8} \rho(r) + \frac{1}{2} \frac{T(r)}{r} - \frac{3}{2} \frac{U(r)}{r} \right) \cos 4\theta \right] \]  

(15)

Here \( u_{jk} \) is the first order groundwater velocity covariance, \( r \) is the separation vector with magnitude of \( r \) and angle \( \theta \) to the \( x_1 \) direction, and the auxiliary functions \( T \) and \( U \) are related to the correlation function \( \rho \) for \( Y \) according to

\[ T(r) = \frac{1}{r} \int_0^r r' \rho(r') dr' \]  

(16)

\[ U(r) = \frac{1}{r^4} \int_0^r r^3 \rho(r') dr' \]  

(17)

Since functions \( T \) and \( U \) are easy to derive through Eqs. (16) and (17), the macrodispersion coefficients (Eqs. (8) and (11)) associated with velocity covariance (Eqs. (13)–(15)) form a convenient tool for deriving the analytical expressions of macrodispersion coefficients for any statistically isotropic log-conductivity autocovariance structure.

Six commonly used statistically isotropic, stationary log-conductivity correlation functions were utilized to calculate the macrodispersion coefficients. They are the exponential model

\[ \rho(r) = e^{-r/\lambda} \]  

(18)

the Gaussian model

\[ \rho(r) = e^{-\pi r^2/4\lambda^2} \]  

(19)

the spherical model

\[ \rho(r) = 1 - \frac{9}{16} \left( \frac{r}{\lambda} \right) + \frac{9}{128} \left( \frac{r}{\lambda} \right)^2 \quad \text{for} \quad \frac{3}{8} \frac{r}{\lambda} < 1; \quad \rho(r) = 0 \quad \text{for} \quad \frac{3}{8} \frac{r}{\lambda} > 1 \]  

(20)

the linear model

\[ \rho(r) = 1 - \frac{1}{2} \left( \frac{r}{\lambda} \right) \quad \text{for} \quad \frac{1}{2} \frac{r}{\lambda} < 1; \quad \rho(r) = 0 \quad \text{for} \quad \frac{1}{2} \frac{r}{\lambda} > 1 \]  

(21)

Whittle model (Whittle, 1954)

\[ \rho(r) = \frac{r\pi}{2\lambda} K_1 \left( \frac{r\pi}{2\lambda} \right) \]  

(22)

and Mizell A-type model (Mizell et al., 1982)

\[ \rho(r) = \frac{r\pi}{4\lambda} K_1 \left( \frac{r\pi}{4\lambda} \right) - \frac{1}{2} \left( \frac{r\pi}{4\lambda} \right)^2 K_0 \left( \frac{r\pi}{4\lambda} \right) \]  

(23)
where $K_i$ is the modified Bessel function of the second kind, $i$th order and $r$ is the separation distance defined as $r = \sqrt{x_1^2 + x_2^2}$. Fig. 1 shows how the dimensionless correlation functions vary with the dimensionless separation distance which is normalized with respect to the integral scale $\lambda$. Among the six models, the exponential, Gaussian and Whittle models are monotonically decreasing functions. The spherical and linear models monotonically decrease first and remain zero after $8/3\lambda$ and $2\lambda$, respectively. The Mizell A-type model shows a hole behavior with slightly negative value after about $3\lambda$. The hole type of autocovariance function represents the geological formation associated with pseudo-periodicity (Kitanidis, 1997). All of the six correlation functions of log-conductivity are stationary but only the Mizell A-type model yields stationary head variance (Mizell et al., 1982).

3.1. Velocity covariance

Applying Eqs. (18)–(23) to Eqs. (13)–(15), the velocity covariances can be calculated for the required auxiliary functions $T$ and $U$ as shown in Table 1. Fig. 2 shows the dimensionless longitudinal and transverse velocity covariances for the separation vector in the mean flow direction versus the dimensionless separation distance. The dimensionless velocity covariance is normalized with respect to $V^2\sigma^2$. All the longitudinal velocity covariance functions monotonically decrease and reach zero. For both longitudinal and transverse directions, the exponential model drops fastest near the origin and the Gaussian model has the mildest slope near the zero separation distance. All the models start to show the slight negative transverse velocity covariance around a value of 2 dimensionless

![Fig. 1. Isotropic hydraulic conductivity correlation functions versus dimensionless separation distance.](image-url)
Table 1
Functions $T$ and $U$ for two dimensions

<table>
<thead>
<tr>
<th>Correlation function</th>
<th>$T(r)$</th>
<th>$U(r)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exponential</td>
<td>$\frac{2^2}{\tau} \left[ 1 - \left( \frac{r}{\tau} \right)^2 \right]$</td>
<td>$- \frac{6^2}{\tau^2} + \frac{6^2}{\tau^3} - 3^2 \frac{r}{\tau} + \frac{2}{\tau^2} \left( \frac{r}{\tau} \right)^2 + \frac{2^2}{\tau^3}$</td>
</tr>
<tr>
<td>Gaussian(^a)</td>
<td>$\frac{1}{2\pi} \left( 1 - e^{-\frac{2r}{\beta}} \right)$</td>
<td>$\left( \frac{1}{2\pi \beta} \right)^2 \left[ \frac{2^2}{\beta^2} + \frac{2^2}{\beta^3} - \frac{2}{\beta^2} r + \frac{2}{\beta^3} \left( \frac{r}{\beta} \right)^2 - \frac{1}{2\pi \beta^4} \right]$</td>
</tr>
<tr>
<td>Spherical</td>
<td>$r \left( \frac{1}{2} - \frac{1}{3} \frac{r^2}{\sigma^2} + \frac{27}{5120} \frac{r^4}{\sigma^4} \right)$ for $\frac{r^2}{\sigma^2} &lt; 1$;</td>
<td>$\frac{1}{4} - \frac{1}{3} \frac{r^2}{\sigma^2} + \frac{27}{5120} \frac{r^4}{\sigma^4}$ for $\frac{r^2}{\sigma^2} &lt; 1$;</td>
</tr>
<tr>
<td></td>
<td>$\frac{32^2}{\sigma^2}$ for $\frac{r^2}{\sigma^2} &gt; 1$</td>
<td>$\frac{1024 \beta^4}{2\pi \sigma^2}$ for $\frac{r^2}{\sigma^2} &gt; 1$</td>
</tr>
<tr>
<td>Linear</td>
<td>$\frac{1}{4} \left( \frac{r}{\beta} \right)^2$ for $\frac{r^2}{\beta^2} &lt; 1$;</td>
<td>$\frac{1}{4} - \frac{1}{3} \frac{r^2}{\beta^2}$ for $\frac{r^2}{\beta^2} &lt; 1$;</td>
</tr>
<tr>
<td></td>
<td>$\frac{4}{5} \frac{r^2}{\beta^2}$ for $\frac{r^2}{\beta^2} &gt; 1$</td>
<td>$\frac{4}{5} \frac{r^2}{\beta^2}$ for $\frac{r^2}{\beta^2} &gt; 1$</td>
</tr>
<tr>
<td>Whittle</td>
<td>$\frac{1}{4} \left( \frac{2}{\beta} \right)^2 K_1 \left( \frac{2r}{\beta} \right)$</td>
<td>$\frac{2}{\beta^2} \left[ 16 - \left( \frac{2}{\beta} \right)^4 K_2 \left( \frac{2r}{\beta} \right) \right.$</td>
</tr>
<tr>
<td></td>
<td>$+ \frac{2}{\beta^3} K_3 \left( \frac{2r}{\beta} \right) + \frac{2}{\beta^2} K_2 \left( \frac{2r}{\beta} \right) + \frac{1}{\beta^2} K_1 \left( \frac{2r}{\beta} \right) \right]$</td>
<td></td>
</tr>
<tr>
<td>Mizell A-type(^b)</td>
<td>$\frac{1}{2\pi} \left( \frac{2}{\beta} \right)^2 K_1 \left( \frac{2r}{\beta} \right)$</td>
<td>$\frac{2}{\beta^2} \left[ -16 + 2 \left( \frac{2}{\beta} \right)^4 K_3 \left( \frac{2r}{\beta} \right) \right.$</td>
</tr>
<tr>
<td></td>
<td>$+ \frac{2}{\beta^2} K_2 \left( \frac{2r}{\beta} \right) + \frac{1}{\beta^2} K_1 \left( \frac{2r}{\beta} \right) \right]$</td>
<td></td>
</tr>
</tbody>
</table>

\(^a\) $\beta = \pi \sqrt{2};$

\(^b\) $K_1$, $K_2$, and $K_3$ are modified Bessel functions of second kind, first, second and third order, respectively.

Fig. 2. Dimensionless velocity covariance versus dimensionless separation distance in two dimensions: (A) longitudinal direction; (B) transverse direction.
separation distance whether they are of hole type in the log-conductivity covariance function or not. The hole behavior of transverse velocity covariance can be explained as the tendency of groundwater to converge in high permeable zone or diverge in low permeable zones. These phenomena persist for a larger area when the Mizell A-type autocovariance model is used.

3.2. Macrodispersion coefficient

For ergodic transport, we have derived the analytical expressions for macrodispersion given by Eq. (8) for the six models under consideration. These analytical expressions are presented in Table 2. The expressions of macrodispersion coefficient for the exponential, Gaussian, spherical and linear models of log-conductivity autocovariance structure have been derived by Hsu (2000), and the expressions for Whittle and Mizell A-type models are presented here for the first time. The macrodispersion coefficient for the exponential model is the same expression as that derived by Sposito and Barry (1987). Fig. 3 shows how the dimensionless macrodispersion coefficients vary with the dimensionless particle travel distance. The macrodispersion coefficient is normalized with respect to \( \lambda V \sigma^2 \). It is clear that, quantitatively, in both longitudinal and transverse directions, the exponential model rises most slowly and takes the longest particle travel distance (time) to reach the Fickian macrodispersion coefficient, while the Mizell A-type model has the shortest traveling distance to reach the asymptotic macrodispersion coefficient. In the transverse macrodispersion coefficient, the Mizell A-type has the highest peak value about 0.127.

Table 2

<table>
<thead>
<tr>
<th>Function</th>
<th>( D_{11} )</th>
<th>( D_{22} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exponential</td>
<td>( D_{11} = \frac{\lambda V \sigma^2}{\varphi} \left[ 2 - \frac{5}{12} + \frac{2\lambda}{7} - \frac{3\lambda^2}{12} \right] )</td>
<td>( D_{22} = \frac{\lambda V \sigma^2}{\varphi} \left[ \frac{5}{12} - \frac{2\lambda}{7} + 2\lambda \left( 1 + \frac{\lambda}{3} + \frac{3\lambda^2}{12} \right) e^{-\lambda/2} \right] )</td>
</tr>
<tr>
<td>Gaussian</td>
<td>( D_{11} = \frac{\lambda V \sigma^2}{4\sqrt{\pi} \varphi} \left[ \left( \frac{5}{3} - \frac{\lambda}{3} + \frac{\lambda^2}{30} \right) e^{-\lambda/2} \right] + 2\sqrt{\pi} \text{Erf} \left( \sqrt{\lambda} \right) )</td>
<td>( D_{22} = \frac{\lambda V \sigma^2}{4\sqrt{\pi} \varphi} \left[ \frac{5}{12} - \frac{\lambda}{3} + \frac{\lambda^2}{30} \right] e^{-\lambda/2} + \frac{2\lambda}{3} e^{-\lambda/2} )</td>
</tr>
<tr>
<td>Spherical</td>
<td>( D_{11} = \frac{\lambda V \sigma^2}{\varphi} \left[ 1 - \frac{5}{12} + \frac{\lambda^2}{12} \right] ) for ( L &lt; \frac{3}{7} \lambda ); ( D_{22} = \frac{\lambda V \sigma^2}{\varphi} \left[ 1 - \frac{5}{12} + \frac{\lambda^2}{12} \right] ) for ( L &gt; \frac{3}{7} \lambda )</td>
<td>( D_{22} = \frac{16\lambda V \sigma^2}{9\sqrt{\pi} \varphi} \left[ \frac{4}{15} + \frac{\lambda^2}{30} \right] ) for ( L &gt; \frac{3}{7} \lambda )</td>
</tr>
<tr>
<td>Linear</td>
<td>( D_{11} = LV \sigma^2 \left( \frac{1}{2} - \frac{\lambda}{20} \right) ) for ( L &lt; 2\lambda ); ( D_{22} = LV \sigma^2 \left( \frac{1}{2} - \frac{\lambda}{20} \right) ) for ( L &lt; 2\lambda )</td>
<td>( D_{22} = \frac{2\lambda V \sigma^2}{\pi} \left( \frac{2}{3} - \frac{\lambda}{\pi} \right) ) for ( L &gt; 2\lambda )</td>
</tr>
<tr>
<td>Whittle</td>
<td>( D_{11} = \frac{3\lambda V \sigma^2}{\varphi} \left[ \frac{8}{5} - K_2 \left( \frac{1}{3} \right) + \frac{2}{5} K_1 \left( \frac{1}{3} \right) - \frac{3}{5} K_3 \left( \frac{1}{3} \right) \right] )</td>
<td>( D_{22} = \frac{2\lambda V \sigma^2}{\pi} \left[ 2K_3 \left( \frac{1}{3} \right) + \frac{5}{3} - 16 \left( \frac{1}{3} \right)^3 \right] )</td>
</tr>
<tr>
<td>Mizell A-type</td>
<td>( D_{11} = \frac{2\lambda V \sigma^2}{\varphi} \left[ \frac{44}{27} + 2K_1 \left( \frac{1}{3} \right) + 2K_3 \left( \frac{1}{3} \right) \right] - 16 \left( \frac{1}{3} \right)^3 )</td>
<td>( D_{22} = \frac{2\lambda V \sigma^2}{\pi} \left[ 2K_3 \left( \frac{1}{3} \right) + \frac{5}{3} K_1 \left( \frac{1}{3} \right) \right] + \left( \frac{4}{3} \right) K_0 \left( \frac{1}{3} \right) - 16 \left( \frac{1}{3} \right)^3 )</td>
</tr>
</tbody>
</table>

*a* \( \varphi = \pi/4\lambda^2 \).

*b* \( S(x) = xK_0(x) + (1/2)\pi x \left[ L_0(x)K_0(x) + L_1(x)K_0(x) \right] \); \( L_i \) and \( K_i \) are modified Struve and Bessel functions, respectively (Abramowitz and Stegun, 1972).
while the exponential model has the lowest peak value of 0.096. The ultimate longitudinal and transverse macrodispersion coefficients are model-independent and their values are $kVr^2$ and 0, respectively.

For the nonergodic transport, three square source areas are considered. They are $1k/C^2$, $10k/C^2$, and $100k/C^2$. Fig. 4 shows the variation of dimensionless longitudinal macrodispersion coefficients versus the dimensionless traveling distance of the plume center of mass for the different source sizes and different log-conductivity covariance models. In Fig. 4(A), when the source area is $1k/C^2$, the different autocorrelation functions show little difference in longitudinal macrodispersion coefficients. The asymptotic dimensionless longitudinal macrodispersion coefficients of the six models are only about 0.11, which is much smaller than the ergodic case. The value is also smaller than 0.2 obtained from the three-dimensions with isotropic exponential model and a cubic source volume of $1k/C^2$ (Zhang et al., 1996). When the source area increases, the ultimate macrodispersion coefficients rise from between 0.7 and 0.9 for different models with a source area $10k/C^2$ to approach the ergodic condition for a source area of $100k/C^2$ as shown in Fig. 4(B) and (C), respectively. Fig. 5(A–C) is the same as Fig. 4(A–C) but for the dimensionless transverse macrodispersion coefficients with square source areas of $1k/C^2$, $10k/C^2$, and $100k/C^2$, respectively. When the source area is $1k/C^2$, the peaks of all models happen within 2 dimensionless traveling

Fig. 3. Dimensionless longitudinal and transverse dispersion coefficients versus dimensionless particle traveling distance under ergodic conditions. (A) Longitudinal direction; (B) transverse direction.
distances and their values are about 1/10 of the peak value for ergodic conditions. The peak values are above 0.01 which are higher than the value of about 0.007 obtained from the three-dimensional cubic source of side $1\lambda$ with the isotropic exponential model (Zhang et al., 1996). As the source area increases, the peak values increase and approach the values for the ergodic condition. In the cases of $10\lambda \times 10\lambda$ and $100\lambda \times 100\lambda$ source areas, the Mizell A-type model has the highest peak value and reaches the asymptotic value most

Fig. 4. Dimensionless longitudinal macrodispersion coefficient versus dimensionless particle traveling distance in a two-dimensional domain for various isotropic correlation models with plume source of (A) $1\lambda \times 1\lambda$, (B) $10\lambda \times 10\lambda$ and (C) $100\lambda \times 100\lambda$. 
rapidly while the exponential model behaves in the opposite manner. The ergodic transport provides the upper bound for the nonergodic transport in both longitudinal and transverse directions. The macrodispersion coefficient for nonergodic transport for rectangular shape of source area has been calculated but not presented here. Similar to the results in three dimensions (Zhang et al., 1996), negative transverse macrodispersion coefficients were
found when the rectangular source area is parallel to the mean flow. This unphysical result requires further exploration.

4. Summary and discussion

The influences of autocovariance structure on the solute transport for ergodic and nonergodic conditions are investigated using six commonly used statistically isotropic log-conductivity correlation functions. They are exponential, Gaussian, spherical, linear, Whittle and Mizell A-type models. Each model corresponds to different random processes presented in geological formations. For example, the Gaussian model represents a smooth and differential regionalized variable; the hole models like the Mizell A-type function represent the geological structure associated with pseudo-periodicity; and the Whittle model arises from a diffusion process in a plane (Whittle, 1954). Linkages between the different models may exist. Ritzi (2000) was able to show the similarity of the hole model and exponential (or spherical) model by changing the geometry of a facies and its associated variability in geometry. We present the analytical expressions of the ergodic macrodispersions corresponding to these six models. The result shows that the dimensionless longitudinal and transverse macrodispersion coefficients have the same ultimate Fickian values but they are slightly different in the preasymptotic region. While the size of source area significantly affects the ultimate nonergodic longitudinal macrodispersion and the peak transverse macrodispersion, the choice of autocovariance function has little effect on the ultimate macrodispersion coefficient and peak values. The macrodispersions presented in this study are suitable for the aquifers with unimodal spatial structure defined by a covariance and a single, finite length scale. This kind of aquifer commonly exists and has been reported in the literature (Gelhar, 1993). One conclusion that can be drawn from this study is that the effect of nonergodicity is more significant than the lnK autocovariance function for the unimodal aquifers. Recently, there have been a few investigations on the bimodal structure (Desbarats, 1990; Rubin and Journel, 1991; Rubin, 1995) and multiscale model (Neuman, 1995; Rajaram and Gelhar, 1995). Their results show that the choice of model structure is also an important factor for evaluating the macrodispersion besides the nonergodic assumption. Therefore, the choice of a suitable model structure will be one of the important tasks in characterizing the hydraulic conductivity field. It should be emphasized that a reliable macrodispersion estimate cannot be obtained without reliable statistically characterization of site-specific lnK heterogeneity.

References