Large-time behavior of macrodispersion in heterogeneous trending aquifers

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[1] This paper presents a stochastic analysis of the large-time behavior of macrodispersion in a three-dimensional heterogeneous aquifer with a linear trend in the mean log hydraulic conductivity. To solve the problem analytically, focus is placed on the particular case where the linear trend is aligned in the direction of mean hydraulic head gradient. A spectral approach based on Fourier-Stieltjes representations for the perturbed quantities is used to develop closed-form expressions that describe variability of flow velocity, the second-order mean flow, and asymptotic macrodispersion. The impact of the mean log hydraulic conductivity gradient on these results is examined. It is found that the asymptotic longitudinal and transverse macrodispersion coefficients decrease with the increasing trend gradient of mean log hydraulic conductivity in the case of finite Peclet numbers. This feature is a consequence of the reduction in variability of flow velocity with the trend gradient.

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1. Introduction

[2] The presence of a trend in the mean log hydraulic conductivity induces nonstationarity in the statistics of random velocity fields in heterogeneous aquifers, thereby affecting the behavior of solute transport [e.g., *Rehfeldt et al.*, 1992; *Eggleston and Rojstaczer*, 1998; *Seong and Rubin*, 1999]. For such a nonstationary condition, most stochastic analyses of field-scale solute transport [e.g., *Rubin and Seong*, 1994; *Indelman and Rubin*, 1996; *Eggleston and Rojstaczer*, 1998] assume that large-scale velocity variations, reflecting the effects of log hydraulic conductivity trends, would not enhance spreading. The small-scale velocity variations, caused by small-scale hydraulic conductivity fluctuations, contribute the most to spreading. Therefore, in the analysis of macrodispersion, the trends must be removed from the log hydraulic conductivity field in order to relate the spatial covariances of the velocity field to those of the local log hydraulic conductivity fluctuations [e.g., *Rubin and Seong*, 1994; *Indelman and Rubin*, 1995, 1996].

[3] Existing stochastic studies of field-scale solute transport in trending media [e.g., *Rubin and Seong*, 1994; *Indelman and Rubin*, 1996; *Eggleston and Rojstaczer*, 1998] have built on the Lagrangian methodology. The application of the Eulerian concept to the investigation of the impact of the trend gradient in the mean log hydraulic conductivity on the behavior of solute transport by groundwater has so far not been attempted, and this is the task undertaken here. This task will be performed using a spectral approach [e.g., *Bakr et al.*, 1978; *Gelhar and Axness*, 1983; *Li and McLaughlin*, 1991, 1995] based on Fourier-Stieltjes representations for the perturbed quantities.

[4] The numerical investigation of field-scale spreading of solute transport by *Rubin and Seong* [1994] for a two-dimensional system suggests that the impact of the linear log hydraulic conductivity trend on the process of solute transport through the trending formations becomes noticeable at very large travel time. Motivated by this, this paper therefore focuses only on analysis of the asymptotic behavior of field-scale solute transport in heterogeneous trending media. It presents closed-form expressions for the mean and variances of flow velocity, and the asymptotic macrodispersion coefficients in a three-dimensional statistically homogenous medium where the mean log hydraulic conductivity displays a linear trend aligned in the direction of mean head gradient. The closed-form results, to the best of our knowledge, have never before been presented. It concludes by examining the impact of the mean log hydraulic conductivity gradient on these results.

2. Problem Formulation

[5] We start by considering steady state transport of conservative solutes in heterogeneous porous media displaying a linear trend in the mean log hydraulic conductivity. The flow domain under consideration is of a sufficiently large extent. The log hydraulic conductivity (ln*K*) field is modeled as a random process, and may be represented as the sum of a constant, *F*, a linear ln*K* trend gradient vector, $\boldsymbol{\mu}$, and a zero mean perturbation, *f*: [e.g., *Loaiciga et al.*, 1993; *Rubin and Seong*, 1994; *Li and McLaughlin*, 1995]

$$\ln K = \langle \ln K \rangle + f = F + \boldsymbol{\mu} \bullet \boldsymbol{X} + f \qquad (1)$$

where $\langle\ \rangle$ stands for the expected value operator and the ln*K* perturbation field *f* is assumed to be a second-order

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stationary random field with known covariance function or spectral density function. For convenience, the positive X_1 coordinate axis is selected to be in the direction of the mean hydraulic gradient vector $\boldsymbol{J}$ so that $\boldsymbol{J} = -\nabla\langle H\rangle = (J(X), 0, 0)$, where H is the hydraulic head; consequently, the mean flow is parallel to the X_1 coordinate axis, i.e., $\boldsymbol{U} = \langle \boldsymbol{u}\rangle = (U, 0, 0)$, where $\boldsymbol{u}$ is the fluid velocity.

[6] It is apparent that the spatial variability of flow velocities strongly influenced by spatial variations in hydraulic conductivity is responsible for the field-scale dispersion in heterogeneous media. *Neuman and Zhang* [1990] have derived a quasi-linear stochastic model relating the macrodispersion of conservative solutes to the local flow variation. We will use their macrodispersion model to investigate the large-time behavior of macrodispersion in medium of trending mean log hydraulic conductivity. From *Neuman and Zhang* [1990], under the unidirectional mean fluid flow condition, the macrodispersion tensor, $\overline{\boldsymbol{D}}_{ij}$, at large times is given by

$$\overline{\boldsymbol{D}}_{ij} = \int_{-\infty}^{\infty} \frac{\boldsymbol{R}\cdot\boldsymbol{dR}}{(\boldsymbol{R}\cdot\boldsymbol{dR})^2+(\boldsymbol{R}\cdot\boldsymbol{U})^2} S_{u_j u_i}(\boldsymbol{R})d\boldsymbol{R} \tag{2}$$

where $\boldsymbol{R} = (R_1, R_2, R_3)$ is the wave number vector, $S_{ujuj}(\boldsymbol{R})$ is the cross spectrum of the j and i components of the velocity, and $\boldsymbol{d}$ is a diagonal dispersion tensor whose components are equal to d_1 (the longitudinal dispersion coefficient) parallel to u_1, and d_2, d_3 (the dispersion transverse coefficients) parallel to u_2, u_3, respectively.

[7] To proceed with the evaluation of (2) in trending formations, one needs to establish the relationship between $S_{ujuj}(\boldsymbol{R})$ and the spectrum of the local log hydraulic conductivity field, $S_{ff}(\boldsymbol{R})$, by taking account of the impact of coefficient $\boldsymbol{\mu}$, the trend gradient of mean log hydraulic conductivity. The scope of this study is limited to the case where the trend in the mean log conductivity is parallel to the mean hydraulic head gradient, i.e., $\boldsymbol{\mu} = (\mu, 0, 0)$.

3. Flow Analysis

3.1. Flow Perturbation

[8] Using the Fourier-Stieltjes representations of the random fields the spectra of the local flow variation in (2) and hydraulic conductivity are directly related through the linearized first-order perturbation approximation of Darcy's law [*Gelhar and Axness*, 1983]. The first-order equation for the velocity perturbation in trending media derived from the Darcy equation is of the form [e.g., *Rubin and Seong*, 1994; *Indelman and Rubin*, 1995]

$$u_i' = K_g(X)\left[J_i\delta_{i1}f - \frac{\partial h}{\partial X_i}\right] \tag{3}$$

where $K_g = \exp[\langle \ln K\rangle] = \exp[F + \mu X_1]$, and h is a zero mean head perturbation, related to the log hydraulic conductivity perturbation f by the following first-order perturbation approximation of the flow equation [*Rubin and Seong*, 1994; *Li and McLaughlin*, 1995]

$$\frac{\partial^2 h}{\partial X_i^2} + \mu\frac{\partial h}{\partial X_1} = J(X_1)\frac{\partial f}{\partial X_1} \tag{4}$$

It is noteworthy that the presence of the trend gradient produces a space-dependent mean hydraulic head gradient, and consequently, results in a nonstationary solution, h, to (4). To evaluate the flow velocity spectrum in (2), equation (4) must be solved first in order to relate the gradient of the hydraulic head perturbation field in (3) to the local log hydraulic conductivity perturbations.

[9] In the case where the trend gradient is in the direction of the mean hydraulic head gradient, the spectral representation solution for the head perturbations to (4) can be expressed as, according to [*Li and McLaughlin*, 1995]

$$h(\boldsymbol{X}) = -\int_{-\infty}^{\infty} \exp[iR\cdot\boldsymbol{X}]\frac{iR_1}{R^2 + i\mu R_1}J(X_1)dZ_f(\boldsymbol{R}) \tag{5}$$

with the mean hydraulic head gradient $J(X_1)$ quantified as

$$J(X_1) = J_o\exp[-\mu(X_1 - X_o)] \tag{6}$$

where $dZ_f(\boldsymbol{R})$ is the complex Fourier-Stieltjes increment, $R^2 = R_1^2 + R_2^2 + R_3^2$, and J_0 is the known value of J at $X_1 = X_0$. Using their result, we can start to investigate the characteristics of the velocity variation, which are important in the analysis of field-scale solute transport.

[10] From (5) we immediately have

$$\frac{\partial h(\boldsymbol{X})}{\partial X_1} = \int_{-\infty}^{\infty} \exp[i\boldsymbol{R}\cdot\boldsymbol{X}]\frac{R_1^2 + i\mu R_1}{R^2 + i\mu R_1}J(X_1)dZ_f(\boldsymbol{R}) \tag{7a}$$

$$\frac{\partial h(\boldsymbol{X})}{\partial X_2} = \int_{-\infty}^{\infty} \exp[i\boldsymbol{R}\cdot\boldsymbol{X}]\frac{R_1R_2}{R^2 + i\mu R_1}J(X_1)dZ_f(\boldsymbol{R}) \tag{7b}$$

$$\frac{\partial h(X)}{\partial X_3} = \int_{-\infty}^{\infty} \exp[i\boldsymbol{R}\cdot\boldsymbol{X}]\frac{R_1R_3}{R^2 + i\mu R_1}J(X_1)dZ_f(\boldsymbol{R}) \tag{7c}$$

Substituting (7a)–(7c) and the Fourier-Stieltjes representations of velocity perturbations, i.e.,

$$u_i' = \int_{-\infty}^{\infty} \exp[i\boldsymbol{R}\cdot\boldsymbol{X}]dZ_{u_i}(\boldsymbol{R})$$

into the velocity perturbation equation (3) and invoking the uniqueness of the spectral representation gives the following velocity spectra

$$S_{u_1u_1}(\boldsymbol{R}) = \left(K_gJ\right)^2\frac{R^4 - 2R^2R_1^2 + R_1^4}{R^4 + \mu^2R_1^2}S_{ff}(\boldsymbol{R}) \tag{8a}$$

$$S_{u_2u_2}(\boldsymbol{R}) = \left(K_gJ\right)^2\frac{R_1^2R_2^2}{R^4 + \mu^2R_1^2}S_{ff}(\boldsymbol{R}) \tag{8b}$$

$$S_{u_3u_3}(\boldsymbol{R}) = \left(K_gJ\right)^2\frac{R_1^2R_3^2}{R^4 + \mu^2R_1^2}S_{ff}(\boldsymbol{R}) \tag{8c}$$

[11] The velocity spectra (8a)–(8c) are the generalization of the corresponding spectra given by Equation (23) in *Rubin and Seong* [1994] to the case of a three-dimensional flow domain.

[12] Recalling that $\langle \ln K \rangle = F + \mu X_1$, the first term on the right hand side of (8) can be rewritten, using (6), as

$$K_g J = \exp[F + \mu X_1] J_o \exp[-\mu(X_1 - X_o)] = \exp[F + \mu X_o] J_o \tag{9}$$

For consistence with the order of the derivation of (8), (9) may be interpreted as the mean fluid velocity at zero order and implies that the mean fluid velocity at zero order can be determined from a reference velocity, i.e., $U_0 = \exp[F + \mu X_0] J_0 = K_g J$. This leads (8) to

$$S_{u_1 u_1}(\boldsymbol{R}) = U_0^2 \frac{R^4 - 2R^2 R_1^2 + R_1^4}{R^4 + \mu^2 R_1^2} S_{ff}(\boldsymbol{R}) \tag{10a}$$

$$S_{u_2 u_2}(\boldsymbol{R}) = U_0^2 \frac{R_1^2 R_2^2}{R^4 + \mu^2 R_1^2} S_{ff}(\boldsymbol{R}) \tag{10b}$$

$$S_{u_3 u_3}(\boldsymbol{R}) = U_0^2 \frac{R_1^2 R_3^2}{R^4 + \mu^2 R_1^2} S_{ff}(\boldsymbol{R}) \tag{10c}$$

3.2. Velocity Variances

[13] The variance of flow velocity can now be computed by integrating (10) over the wave number domain, according to

$$\sigma_{u_i}^2 = \int_{-\infty}^{\infty} S_{u_i u_i}(\boldsymbol{R}) d\boldsymbol{R} \tag{11}$$

The form of the ln$K$ spectrum in (10) must be selected to evaluate (11).

[14] The evaluation of (11) cannot be performed analytically for the general case of statistically anisotropic ln$K$ distribution. However, to take the advantage of closed-form expressions, which provide a clear insight of the impact of trend gradient on the variation of flow velocity, we assume statistical isotropy of the ln$K$ field. The random ln$K$ perturbation field f under consideration is characterized by the following spectral density function [e.g., *Bakr et al.*, 1978; *Gelhar and Axness*, 1983; *Neuman and Zhang*, 1990]

$$S_{ff}(\boldsymbol{R}) = \frac{\sigma_f^2 \lambda^3}{\pi^2 \left(1 + \lambda^2 R^2\right)^2} \tag{12}$$

where σ_f^2 is the variance of ln$K$ and λ is the correlation scale of ln$K$.

[15] The closed-form expressions for variations in longitudinal and transverse flow velocities can be derived by substituting (10) and (12) into (11) and integrating over the wave number domain, respectively,

$$\sigma_{u_1}^2 = U_0^2 \sigma_f^2 \left[-\frac{6}{\mu^4 \lambda^4} + \frac{3}{\mu^3 \lambda^3} + \frac{6}{\mu^2 \lambda^2} - \frac{5}{2} \frac{1}{\mu \lambda} + \left(\frac{6}{\mu^5 \lambda^5} - \frac{8}{\mu^3 \lambda^3} + \frac{2}{\mu \lambda} \right) \ln(1 + \mu\lambda) \right] \tag{13a}$$

$$\sigma_{u_2}^2 = \sigma_{u_3}^2 = U_0^2 \sigma_f^2 \left[\frac{3}{\mu^4 \lambda^4} - \frac{3}{2} \frac{1}{\mu^3 \lambda^3} - \frac{1}{\mu^2 \lambda^2} + \frac{1}{4} \frac{1}{\mu \lambda} + \left(-\frac{3}{\mu^5 \lambda^5} + \frac{2}{\mu^3 \lambda^3} \right) \ln(1 + \mu\lambda) \right] \tag{13b}$$

with the corresponding limits for the no-trend case ($\mu\lambda \to 0$)

$$\sigma_{u_1}^2 = \frac{8}{15} U_0^2 \sigma_f^2 \tag{14a}$$

$$\sigma_{u_2}^2 = \sigma_{u_3}^2 = \frac{1}{15} U_0^2 \sigma_f^2 \tag{14b}$$

where $\sigma_{u_1}^2$ is the variance of longitudinal flow velocity and $\sigma_{u_2}^2$, $\sigma_{u_3}^2$ are the variances of transverse flow velocity. Equations (14a) and (14b) are the well known results [e.g., *Winter et al.*, 1984; *Gelhar*, 1987] in the no-trend case.

[16] In Figures 1a and 1b the behavior of the velocity variances as a function of the trend gradient are illustrated respectively in the longitudinal and transversal directions. The variance of velocity decreases with increasing trend gradient, because of the fact that the larger trend gradient results in longer correlation distance of hydraulic head and hence the smaller variability of the flow velocity.

3.3. Note on the Mean Velocity at Second Order

[17] Following *Rubin and Seong* [1994], the mean velocity at the second order for the case of parallel $\boldsymbol{\mu}$ and $\boldsymbol{J}$ is approximated as

$$U = K_g J \left[1 + \frac{1}{2} \sigma_f^2 - \frac{1}{J} \left\langle f \frac{\partial h}{\partial X_1} \right\rangle \right] \tag{15}$$

The cross-correlation term in (15) is evaluated using (7a) and the representation theorem for f such that

$$\frac{1}{J} \left\langle f \frac{\partial h}{\partial X_1} \right\rangle = \int_{-\infty}^{\infty} \frac{R^2 R_1^2 + \mu^2 R_1^2}{R^4 + \mu^2 R_1^2} S_{ff}(\boldsymbol{R}) d\boldsymbol{R} \tag{16}$$

Introducing the statistically isotropic input spectrum (12), the integral of (16) takes the following form:

$$\frac{1}{J} \left\langle f \frac{\partial h}{\partial X_1} \right\rangle = \left[-\frac{4}{\mu^2 \lambda^2} + \frac{2}{\mu \lambda} + 1 + \left(\frac{4}{\mu^3 \lambda^3} - \frac{2}{\mu \lambda} \right) \ln(1 + \mu\lambda) \right] \sigma_f^2 \tag{17}$$

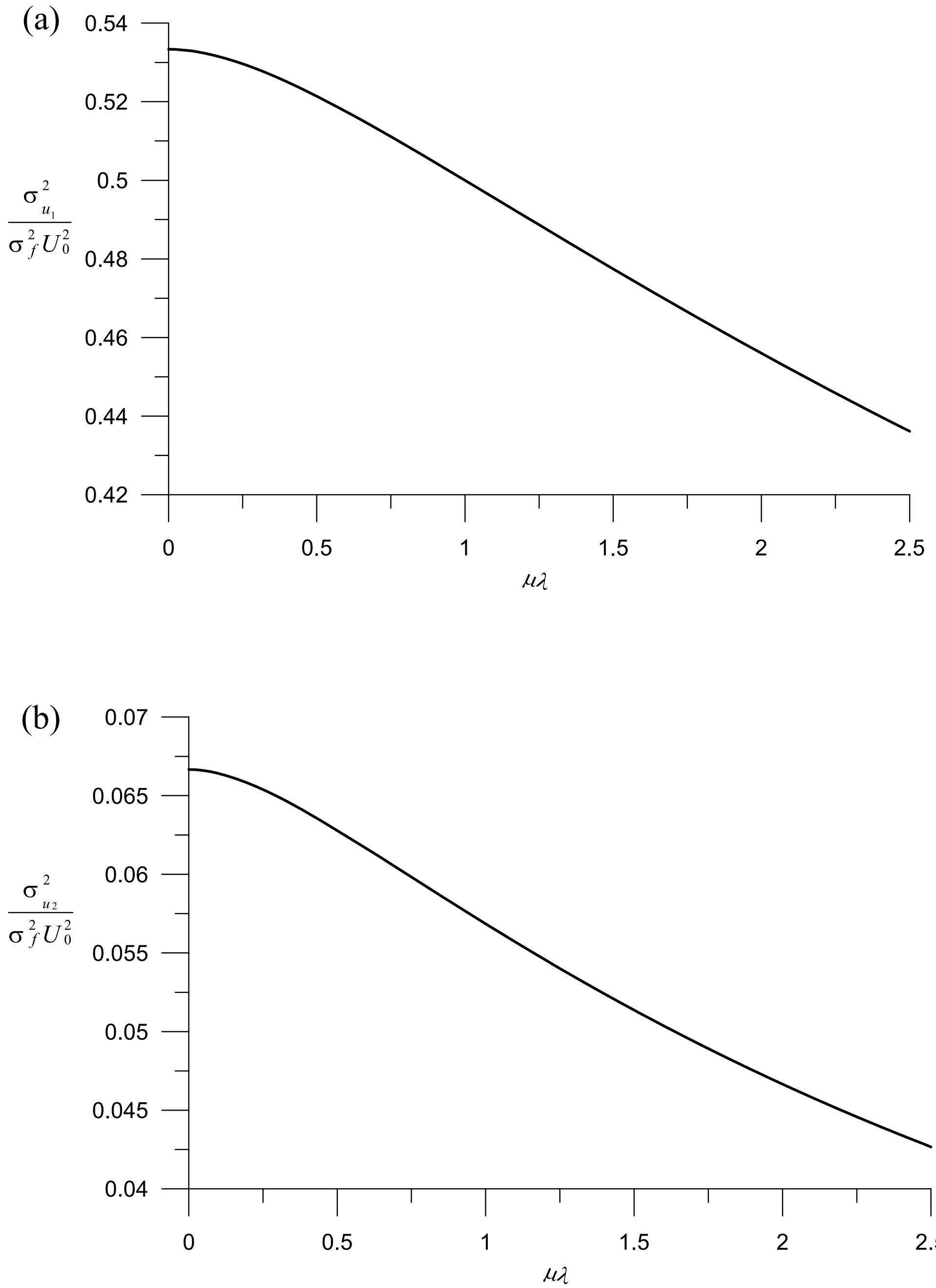

Figure 1. Dimensionless variance of the (a) longitudinal and (b) transverse velocity versus dimensionless trend gradient.

On the basis of (9) and (17), the second-order approximation for the mean velocity in (15) becomes

$$U = U_0\left\{1 + \frac{1}{2}\sigma_f^2 - \left[-\frac{4}{\mu^2\lambda^2} + \frac{2}{\mu\lambda} + 1 + \left(\frac{4}{\mu^3\lambda^3} - \frac{2}{\mu\lambda}\right) \cdot \ln(1+\mu\lambda)\right]\sigma_f^2\right\} \quad (18)$$

where $U_0 = \exp[F + \mu X_0]J_0$.

[18] The second-order result for the mean velocity is independent of position for the case where the trend gradient is aligned in the direction of mean hydraulic head gradient, as indicated by (18). This qualitatively agrees with the earlier finding of the numerical simulations by *Rubin and Seong* [1994] for a two-dimensional system. The result of (18) is presented graphically in Figure 2, which shows the decrease in the mean velocity as a function of the trend gradient. In the limit of $\mu\lambda \rightarrow 0$, the last term in brackets in (18) approaches 1/3 and the mean velocity converges to

$$U = U_0\left[1 + \frac{1}{2}\sigma_f^2 - \frac{1}{3}\sigma_f^2\right] = U_0\left[1 + \frac{1}{6}\sigma_f^2\right] \quad (19)$$

which is a well-known expression reported in the literature.

4. Asymptotic Macrodispersion

[19] Once the spectrum of the fluid velocity accounting for the impact of trend gradient is obtained, we are in a

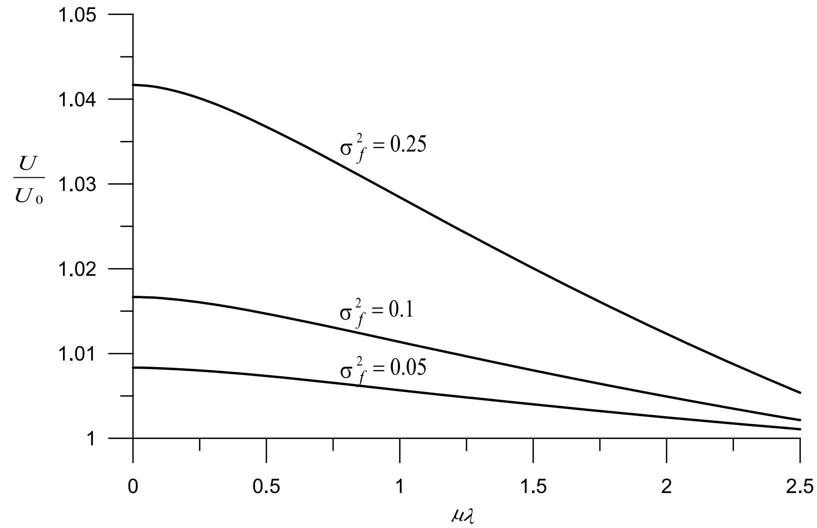

Figure 2. Dimensionless mean velocity versus dimensionless trend gradient for various ln$K$ variance.

position to investigate the asymptotic behavior of field-scale solute transport spreading in media displaying a linear trend in the mean log hydraulic conductivity. Substituting (10) and (12) into (2) leads to the following results for the large time limit of longitudinal and transverse macrodispersion coefficients:

$$\overline{D_{11}} = \frac{U_o\sigma_f^2\lambda}{P\left(1-\mu^2\lambda^2/P^2\right)}\left\{\left[\frac{4}{P^2}-\frac{2}{P}+P+4\left(-\frac{1}{P^3}+\frac{1}{P}\right)\ln(1+P)\right] - \left[\frac{4}{\mu^2\lambda^2}-\frac{2}{\mu\lambda}+\mu\lambda+4\left(-\frac{1}{\mu^3\lambda^3}+\frac{1}{\mu\lambda}\right)\ln(1+\mu\lambda)\right]\right\} \quad (20a)$$

$$\overline{D_{22}} = \overline{D_{33}} = \frac{U_o\sigma_f^2\lambda}{P\left(1-\mu^2\lambda^2/P^2\right)}\left\{\left[-\frac{2}{P^2}+\frac{1}{P}+\left(\frac{2}{P^3}-\frac{1}{P}\right)\ln(1+P)\right] - \left[-\frac{2}{\mu^2\lambda^2}+\frac{1}{\mu\lambda}+\left(\frac{2}{\mu^3\lambda^3}-\frac{1}{\mu\lambda}\right)\ln(1+\mu\lambda)\right]\right\} \quad (20b)$$

where $P = U_o\lambda/d$.

[20] Taking the limit of (20a) and (20b) as $\mu\lambda \to 0$, we thus have

$$\overline{D_{11}} = \frac{U_o\sigma_f^2\lambda}{P}\left[\frac{4}{P^2}-\frac{2}{P}+P-\frac{8}{3}+4\left(-\frac{1}{P^3}+\frac{1}{P}\right)\ln(1+P)\right] \quad (21a)$$

$$\overline{D_{22}} = \overline{D_{33}} = \frac{U_o\sigma_f^2\lambda}{P}\left[-\frac{2}{P^2}+\frac{1}{P}+\frac{1}{3}+\left(\frac{2}{P^3}-\frac{1}{P}\right)\ln(1+P)\right] \quad (21b)$$

These are equivalent to the results of *Neuman and Zhang* [1990, (50a) and (50b)] after rearranging their rational expressions as partial fractions.

[21] Figures 3a and 3b show how longitudinal and transverse macrodispersion coefficients, respectively, vary with the trend gradient for various P values. As expected, the larger the trend gradient, the less the plume spreads, as implied by Figure 1. A larger trend gradient results in reductions in the variation of flow velocity and, consequently, results in less spreading of the solute. Also, from Figures 3a and 3b, the longitudinal macrodispersion coefficient becomes a constant, $\sigma_f^2U_0\lambda$, and the transverse macrodispersion coefficient tends to zero in the case when the local dispersion coefficient $d = 0$ (i.e., $P \to \infty$). In other words, the large-time limit of the macrodispersion becomes independent of the trend gradient for very small local dispersion. So it would not be appropriate to assume advection-dominated transport in approximating the large-time asymptotic limit of macrodispersion coefficients in nonstationary velocity fields.

5. Conclusions

[22] We have presented closed-form expressions for the mean and variances of flow velocity, and the asymptotic macrodispersion coefficients in a three-dimensional statistically homogenous medium where the mean log hydraulic conductivity displays a linear trend aligned in the direction of mean head gradient. These expressions are derived directly from the spectrum of the Eulerian velocity including the log hydraulic conductivity trend effects, based on the nonstationary representation for head perturbation [*Li and McLaughlin*, 1995].

[23] It was found that the inclusion of a trend gradient of mean log hydraulic conductivity parallel to the mean head gradient reduces both the asymptotic longitudinal and transverse macrodispersion coefficients. This feature is a consequence of the reduction in variability of flow velocity with a trend gradient. The prediction of the large-time behavior of macrodispersion made by assuming advec-

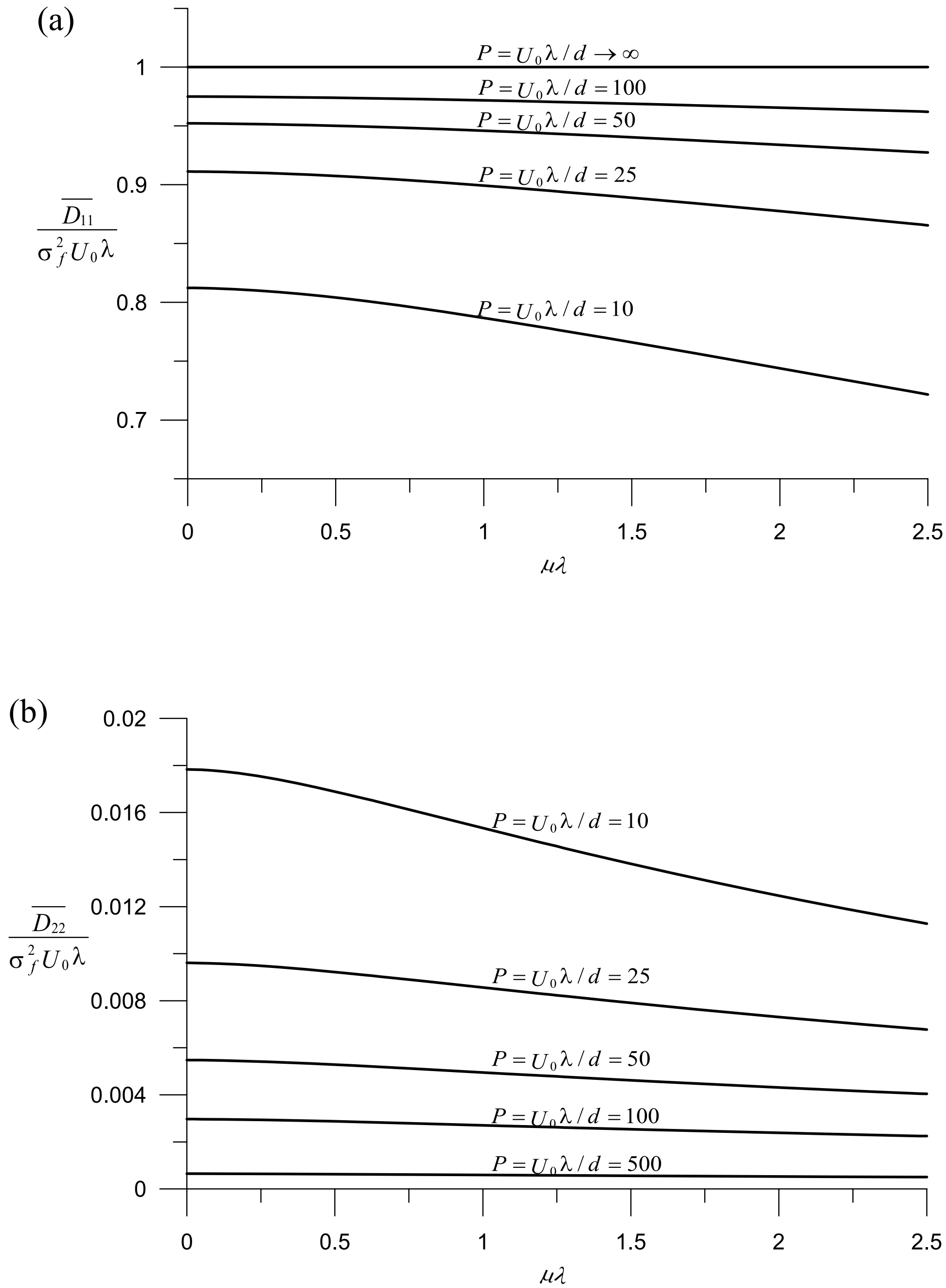

Figure 3. Dimensionless (a) longitudinal and (b) transverse macrodispersion versus dimensionless trend gradient for various *P*.

tion-dominated transport, which is in disregard of pore-scale dispersion, will not provide a good asymptotic approximation in nonstationary velocity field.

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