Using the nonstationary spectral method to analyze asymptotic macrodispersion in uniformly recharged heterogeneous aquifers

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Summary   This paper describes an investigation of the influence of uniformly distributed groundwater recharge on asymptotic macrodispersion in two-dimensional heterogeneous media. This is performed using a nonstationary spectral approach [Li, S.-G., McLaughlin, D., 1991. A nonstationary spectral method for solving stochastic groundwater problems: unconditional analysis. Water Resour. Res. 27 (7), 1589–1605; Li, S.-G., McLaughlin, D., 1995. Using the nonstationary spectral method to analyze flow through heterogeneous trending media. Water Resour. Res. 31 (3), 541–551] based on Fourier–Stieltjes representations for the perturbed quantities. To solve the problem analytically, focus is placed on the case where the local longitudinal dispersivity α_L is much smaller than the integral scale of log transmissivity λ (i.e., $\alpha_L/\lambda \ll 1$). The closed-form expressions are obtained for describing the spectrum of flow velocity, the variability of flow velocity and asymptotic macrodispersion, in terms of the statistical properties and the integral scale of log transmissivity, local transport parameters and a parameter β [Rubin, Y., Bellin, A., 1994. The effects of recharge on flow nonuniformity and macrodispersion. Water Resour. Res. 30 (4), 939–948] used to characterize the degree of flow nonuniformity due to the groundwater recharge. The impact of β on these results is examined.
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Introduction

The field-scale spreading of nonreactive solutes in porous formations is largely determined by the spatial variability in groundwater flow velocities. From the stochastic point of view, the velocity variability is directly related to the cross-correlation between the log hydraulic conductivity perturbation and the perturbation in the hydraulic head. Therefore, the quantification of this relationship is the key in the prediction of field-scale transport processes in heterogeneous media.

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Li and McLaughlin (1995) used the nonstationary spectral method to analyze flow in nonstationary velocity fields and concluded that the stationary spectral method (Bakr et al., 1978) fails to capture the log conductivity-head cross covariance. Therefore, this excludes the direct applicability of the stationary spectral method to solve the problem of transport of solutes in random nonstationary velocity fields. Motivated by this, this study is devoted to the quantification of the nonstationarity in the statistics of random velocity fields using the nonstationary spectral approach (Li and McLaughlin, 1991, 1995).

Groundwater recharge causes nonuniformity in the mean gradient of hydraulic head, and results in nonstationarity in the statistics of random velocity fields, thereby affecting the behavior of solute transport in heterogeneous aquifers (e.g., Rubin and Bellin, 1994; Li and Graham, 1998; Butera and Tanda, 1999; Zhu and Satish, 1999; Destouni et al., 2001; Maugis et al., 2002). This characteristic allows us to use the nonstationary spectral approach (Li and McLaughlin, 1991, 1995) to analyze the field-scale spreading process.

Many studies within the framework of stochastic theory have been devoted to the investigation of field-scale solute transport in nonuniform groundwater flow (e.g., Rubin and Bellin, 1994; Li and Graham, 1998; Butera and Tanda, 1999; Zhu and Satish, 1999; Destouni et al., 2001; Maugis et al., 2002). The works of Rubin and Bellin (1994) and Butera and Tanda (1999) are more directly relevant to our concern. Their investigation was carried out using the Lagrangian transport formalism in a near-source region where the effect of the pore-scale dispersion is not felt and the advective transport is strictly dominated. In other words, the effect of the pore-scale dispersion is negligible in the evaluation of their numerical results. However, in this study, focus is placed on the influence of nonuniformity in the mean flow caused by the uniform groundwater recharge on the asymptotic behavior of field-scale solute transport, which is strongly affected by the pore-scale dispersion. Chang and Yeh (2007) have shown that the prediction of the large-time behavior of macrodispersion in nonstationary velocity field made by using the advection-dominated transport theory, which is useful to quantify the near source transport characteristics, will not provide a good asymptotic approximation. Therefore, the effect of the pore-scale dispersion will be included in the following analysis of the field-scale solute transport in nonstationary velocity field.

The application of the nonstationary spectral approach (Li and McLaughlin, 1991, 1995) to the investigation of the influence of uniformly distributed groundwater recharge on asymptotic macrodispersion is the task undertaken here. This will be performed by developing the closed-form expressions for the asymptotic macrodispersion coefficients within an Eulerian transport framework under consideration of the effect of the pore-scale dispersion. To the best of our knowledge, the large-time closed-form expressions have never before been presented. It is hoped that our finding will be useful for the prediction of large-time behavior of macrodispersion in nonuniform groundwater flow.

Statement of the problem

In this study we consider the problem of transport of a conservative contaminant in a two-dimensional aquifer subject to uniformly distributed recharge where the transmissivity is a stationary random space function. The spatial persistence of the random field of the log transmissivity can be fully characterized in terms of the covariance between two locations. The theoretical analysis is developed herein for unidirectional mean flow with two-dimensional perturbations in transmissivity and hydraulic head. For convenience the coordinate axis X_1 is selected to be in the direction of the mean groundwater flow so that $U = <u> = (U, 0)$, where $u = (u_1, u_2)$ is the groundwater flow velocity vector and $<\ >$ stands for the expected value operator. The governing equation for hydraulic head distribution in a two-dimensional uniformly recharged aquifer can be written as (e.g., Gelhar, 1993; Graham and Tankersley, 1994)

$$\frac{\partial}{\partial X_i}\left[T(X)\frac{\partial \phi}{\partial X_i}\right] + Q_R = 0 \qquad (1)$$

where ϕ is the hydraulic head, T is the transmissivity and Q_R is the constant recharge rate. Assume that recharge and $\ln T$ processes are uncorrelated (e.g., Rubin and Bellin, 1994; Butera and Tanda, 1999). In the analysis that follows, $\ln T(X)$ and $\phi(X)$ are considered to be random functions.

Gelhar and Axness (1983) presented an Eulerian approach to analyze the field-scale spreading of solute transport in heterogeneous media. In this approach the macrodispersion coefficients are determined by constructing the macroscopic dispersive flux and relating it to the Fickian-type gradient transport relationship. This approach has proven useful in characterizing the larger-time behavior of the field-scale solute transport. We will adopt the formalism outlined by Gelhar and Axness (1983) along with (1) to investigate the influence of recharge on asymptotic macrodispersion in two-dimensional heterogeneous media.

Head perturbation

The evaluation of asymptotic macrodispersion coefficients (Gelhar and Axness, 1983) in heterogeneous media would require relating the variability of the groundwater flow velocity to that of the local log transmissivity field. Toward the determination of the variability of the flow velocity we start with developing the hydraulic head perturbation which describes the variability of hydraulic head. We then substitute the head perturbation into the perturbed form of the Darcy equation in developing the spectrum of the flow velocity in the following section.

The random fields in (1), head and $\ln T$, are decomposed into ensemble means and small perturbations around the mean, i.e.,

$$\phi(X_1, X_2) = <\phi(X_1, X_2)> + h(X_1, X_2) = HX_1) + h(X_1, X_2)$$
$$\ln T(X_1, X_2) = <\ln T(X_1, X_2)> + f(X_1, X_2) = F + f(X_1, X_2)$$
$$\qquad (2)$$

The H in (2) is only a function of the X_1 direction, implying unidirectional mean flow.

Expanding these terms and taking expectation of (1) yields the mean head gradient equation

$$\frac{\partial^2 H}{\partial X_1^2} + \frac{Q_R}{e^F} = 0 \qquad (3)$$

The general solution for the ensemble mean head gradient is

$$J(X_1) = -\frac{\partial H}{\partial X_1} = \frac{Q_R}{e^F}(x - x_0) + J_0 \qquad (4)$$

where J_0 is the known value of J at $X_1 = X_0$. As in the previous studies (Rubin and Bellin, 1994; Butera and Tanda, 1999), the parameter $\beta = Q_R\lambda/(e^F J_0)$ is defined to quantify the degree of flow nonuniformity due to the groundwater recharge, in which λ is the integral scale of $\ln T$. Thus, Eq. (4) can be rewritten as

$$J(X_1) = J_0[1 + \beta(X_1 - X_0)/\lambda] \qquad (5)$$

After subtracting the mean of the resulting Eq. (3) from (1), the result is the following first-order equation describing the hydraulic head perturbation

$$\frac{\partial^2 h}{\partial X_i^2} = \frac{\partial f}{\partial X_1}J(X_1) + \frac{Q_R}{e^F}f \qquad (6)$$

Eq. (6) represents the spatial variability in head induced by aquifer heterogeneity and the groundwater recharge. It is clear from (5) that the mean hydraulic head gradient is dependent of X. This spatially variant mean head gradient leads the head random perturbation in (6) to be nonstationary.

The solution of (6) for the head perturbation h in terms of f and β can be developed using a nonstationary spectral approach (Li and McLaughlin, 1991, 1995) based on Fourier-Stieltjes representations for the perturbed quantities in wave number space. By using this approach, the random perturbations are represented by the following two-dimensional wave number integrals:

$$h(X) = \int_{-\infty}^{\infty} \Phi(X, K)\,dZ_f(K) \qquad (7)$$

$$f(X) = \int_{-\infty}^{\infty} \exp[iK \cdot X]\,dZ_f(K) \qquad (8)$$

where $\Phi(X, K)$ is a transfer function to be given, $dZ_f(K)$ is the complex Fourier amplitude of $\ln T$, and $K = K_1, K_2$ is the wave number vector. Substituting (7) and (8) into (6) and recalling that $\beta = Q_R\lambda/(e^F J_0)$ results in

$$\frac{\partial^2 \Phi}{\partial X_i^2} = [iK_1 J(X_1) + \beta J_0/\lambda]\exp[iK \cdot X] \qquad (9)$$

The solution to (9) is found to be

$$\Phi(X, K) = -\frac{iK_1 K^2 J(X_1) - (K_1^2 - K_1^2)\beta J_0/\lambda}{K^4}\exp[iK \cdot X] \qquad (10)$$

in which $K = (K_1^2 + K_2^2)^{1/2}$ represents the magnitude of the wave number vector K. The nonstationary representation for the head perturbation is then obtained by substituting (10) into (7)

$$h(X) = -\int_{-\infty}^{\infty}\frac{iK_1 K^2 J(X_1) - (K_1^2 - K_2^2)\beta J_0/\lambda}{K^4}\exp[iK \cdot X]\,dZ_f(K) \qquad (11)$$

where $J(X_1)$ is defined by (5).

Flow perturbation

In this section, we develop the spectrum of the flow velocity from the perturbed form of the Darcy equation, which relates the velocity variation to the $\ln T$ perturbations. The spectrum of the flow velocity, the key analytical development presented in this paper, is necessary for the determination of closed-form solutions for the field-scale coefficients of transport using the formalism proposed by Gelhar and Axness (1983).

Using Darcy's equation, the first-order equation for the velocity perturbation takes the form (e.g., Gelhar, 1993; Rubin and Bellin, 1994; Butera and Tanda, 1999) a

$$u_i' = T_G\left[\delta_{i1}J(X_1)f - \frac{\partial h}{\partial}X_i\right] \qquad (12)$$

where $T_G = \exp[F]$, $u_i' = u(X) - U(X)$, $u(X)$ is the groundwater flow velocity vector and $U(X) = (U, 0)$ is the mean flow velocity vector. Note that the zero-order approximation for the mean velocity is in the form (Rubin and Bellin, 1994; Butera and Tanda, 1999)

$$U = T_G J = T_G J_0[1 + \beta(X_1 - X_0)/\lambda]$$
$$= U_0[1 + \beta(X_1 - X_0)/\lambda] \qquad (13)$$

where U_0 is the known mean velocity at $X_1 = X_0$.

The last term on the right-hand side of (12) in the X_1 direction is found using (11)

$$\frac{\partial h}{\partial X_1} = \int_{-\infty}^{\infty}\frac{K_1^2 K^2 J(X_1) - i2K_1 K_2^2\beta J_0/\lambda}{K^4}\exp[iK \cdot X]\,dZ_f(K) \qquad (14)$$

Similarly, in the X_2 direction

$$\frac{\partial h}{\partial X_2} = \int_{-\infty}^{\infty}\frac{K_1 K_2 K^2 J(X_1) + iK_2(K_1^2 - K_2^2)\beta J_0/\lambda}{K^4}\exp[iK \cdot X]\,dZ_f(K) \qquad (15)$$

Substituting (8), (14), (15) and the Fourier-Stieltjes representations of velocity perturbations, i.e.,

$$u_i' = \int_{-\infty}^{\infty}\exp[iK \cdot X]\,dZ_{u_i}(K)$$

into the velocity perturbation Eq. (12) gives the complex Fourier amplitudes of the longitudinal and transverse velocities, respectively

$$dZ_{u_1}(K) = U_0\left\{(1 - \frac{K_1^2}{K^2})\left[1 + \beta\frac{X_1 - X_0}{\lambda}\right] + i2\frac{\beta}{\lambda}\frac{K_1 K_2^2}{K^4}\right\}dZ_f(K) \qquad (16)$$

$$dZ_{u_2}(K) = -U_0\left\{\frac{K_1 K_2}{K^2}\left[1 + \beta\frac{X_1 - X_0}{\lambda}\right] + i\frac{\beta}{\lambda}\frac{K_2(K_1^2 - K_2^2)}{K^4}\right\}dZ_f(K) \qquad (17)$$

The spectra of the longitudinal and transverse velocities in terms of the $\ln T$ spectrum are obtained by multiplying each side of (16) and (17), respectively, by its complex conjugate and taking the expected value

$$S_{u_1}u_1(K) = U_0^2\left\{(1 - \frac{K_1^2}{K^2})^2\left[1 + \beta\frac{X_1 - X_0}{\lambda}\right]^2 + 4\frac{\beta^2}{\lambda^2}\frac{K_1^2 K_2^4}{K^8}\right\}S_{ff}(K) \qquad (18)$$

$$S_{u_2}u_2(K) = U_0^2\left\{\frac{K_1^2 K_2^2}{K^4}\left[1 + \beta\frac{X_1 - X_0}{\lambda}\right]^2 + \frac{\beta^2}{\lambda^2}\frac{K_2^2(K_1^2 - K_2^2)^2}{K^8}\right\}S_{ff}(K) \qquad (19)$$

where $S_{ff}(K)$ is the spectrum of $\ln T$. Eqs. (18) and (19) allow for the development of macrodispersion coefficients at large times.

Velocity variances

To verify indirectly our results in (18) and (19), we compare the velocity variances, obtained using (18) and (19), with existing theoretical results of Li and Graham (1998). In order to evaluate the velocity variation explicitly the spectrum $S_{ff}(K)$ in (18) and (19) must be specified. For this analysis the random $\ln T$ perturbation field under consideration is characterized by the following spectral density function (e.g., Mizell et al., 1982; Li and Graham, 1998)

$$S_{ff}(K) = \frac{3\sigma_f^2 \alpha^2 K^4}{\pi(K^2 + \alpha^2)^4} \tag{20}$$

where σ_f^2 is the variance of $\ln T$, $\alpha = 3\pi/16\lambda$, K is a two-dimensional wave number vector, and $K^2 = K_1^2 + K_2^2$.

With $S_{ff}(K)$ given in (20), integration of (18) and (19) over the wave number domain yields the longitudinal and transverse velocity variances, respectively

$$\sigma_{u_1}^2 = \int_{-\infty}^{\infty} S_{u_1 u_1}(K)\,dK = \sigma_f^2 U_0^2 \left[\frac{3}{8}\left(1 + \beta\frac{X_1 - X_0}{\lambda}\right)^2 + \frac{32}{9\pi^2}\beta^2 \right] \tag{21}$$

$$\sigma_{u_2}^2 = \int_{-\infty}^{\infty} S_{u_2 u_2}(K)\,dK$$
$$= \sigma_f{}^2 U_0{}^2 \left[\frac{1}{8}\left(1 + \beta\frac{X_1 - X_0}{\lambda}\right)^2 + \frac{32}{9\pi^2}\beta^2 \right] \tag{22}$$

These are precisely equivalent to the results found by Li and Graham (1998) (their (22) and (24)) using a first-order perturbation technique under the assumption of spatially invariant recharge. This agreement between two disparate methods is important because it justifies the application of the nonstationary spectral approach to problems involved in nonstationary velocity fields.
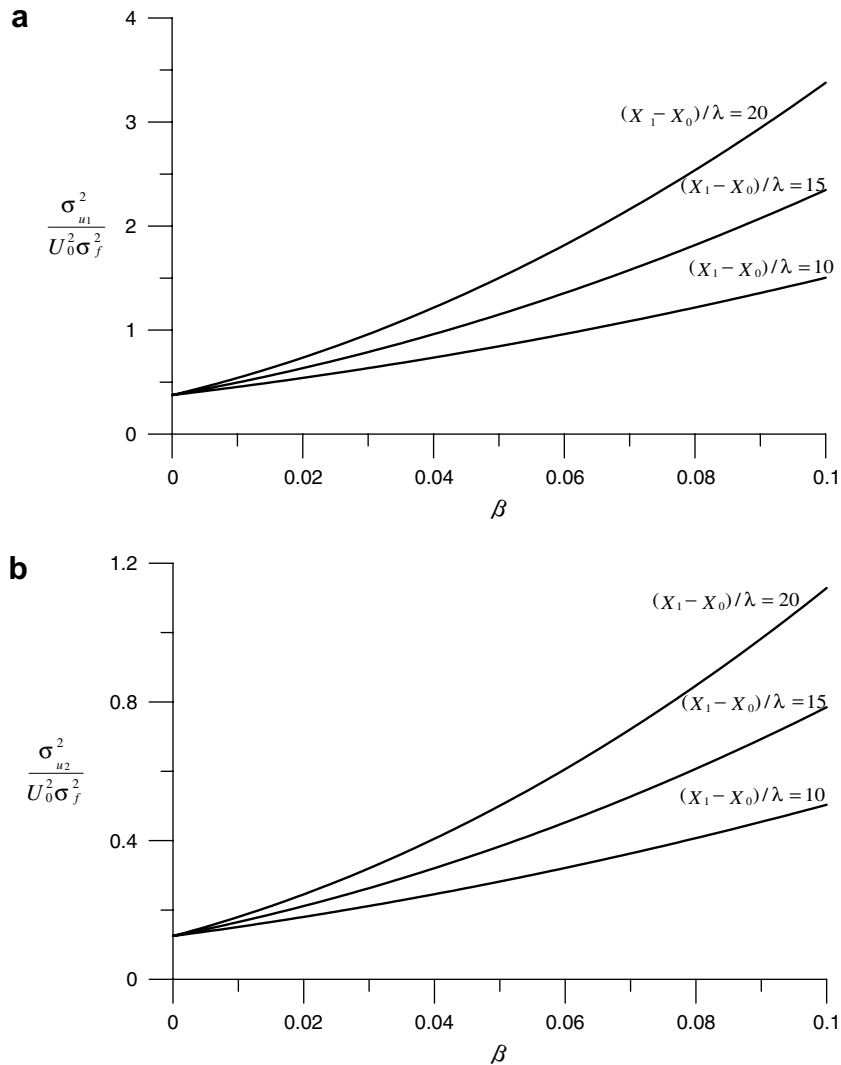

Figure 1 Dimensionless variance of the (a) longitudinal and of the (b) transverse velocity versus dimensionless recharge parameter β for various values of $(X_1 - X_0)/\lambda$.

It is clear that in the case of no recharge ($\beta \to 0$), Eqs. (21) and (22) reduce to

$$\sigma_{u_1}^2 = \frac{3}{8}\sigma_{f^2}U_0^2 \tag{23}$$

$$\sigma_{u_2}^2 = \frac{1}{8}\sigma_{f^2}U_0^2 \tag{24}$$

which are well-known expressions for two-dimensional flow reported in the literature.

Fig. 1a and b depict the longitudinal and transverse velocity variances, respectively, as a function of β based on (21) and (22) for various values of $(X_1 - X_0)/\lambda$. These results show that an introduction of groundwater recharge leads to an increase in the velocity variance. This can be attributed to larger recharge resulting in shorter correlation distance of hydraulic head and hence larger variability of the flow velocity.

Approximate solutions for the macroscopic dispersion coefficients

Once the relationship between the spectrum of the flow velocity and that of the local $\ln T$ field is obtained, we are in a position to develop the approximate solutions for the asymptotic macrodispersion coefficients. The goal here is to show the influence of the recharge on the asymptotic behavior of field-scale solute transport. Following Gelhar and Axness (1983), under the unidirectional mean flow condition, the macrodispersion coefficient tensor, D_{ij}, at large times is given by:

$$D_{ij} = \int_{-\infty}^{\infty} \frac{\alpha_L K_1^2 + \alpha_T K_2^2}{[K_1^2 + (\alpha_L K_1^2 + \alpha_T K_2^2)^2]U} S_{u_j u_i}(\mathbf{K})(\mathbf{K})d\mathbf{K} \tag{25}$$

where α_L and α_T are the local longitudinal and transverse dispersivities and U is the mean flow velocity. The longitudinal and transverse macrodispersion coefficients from (25),
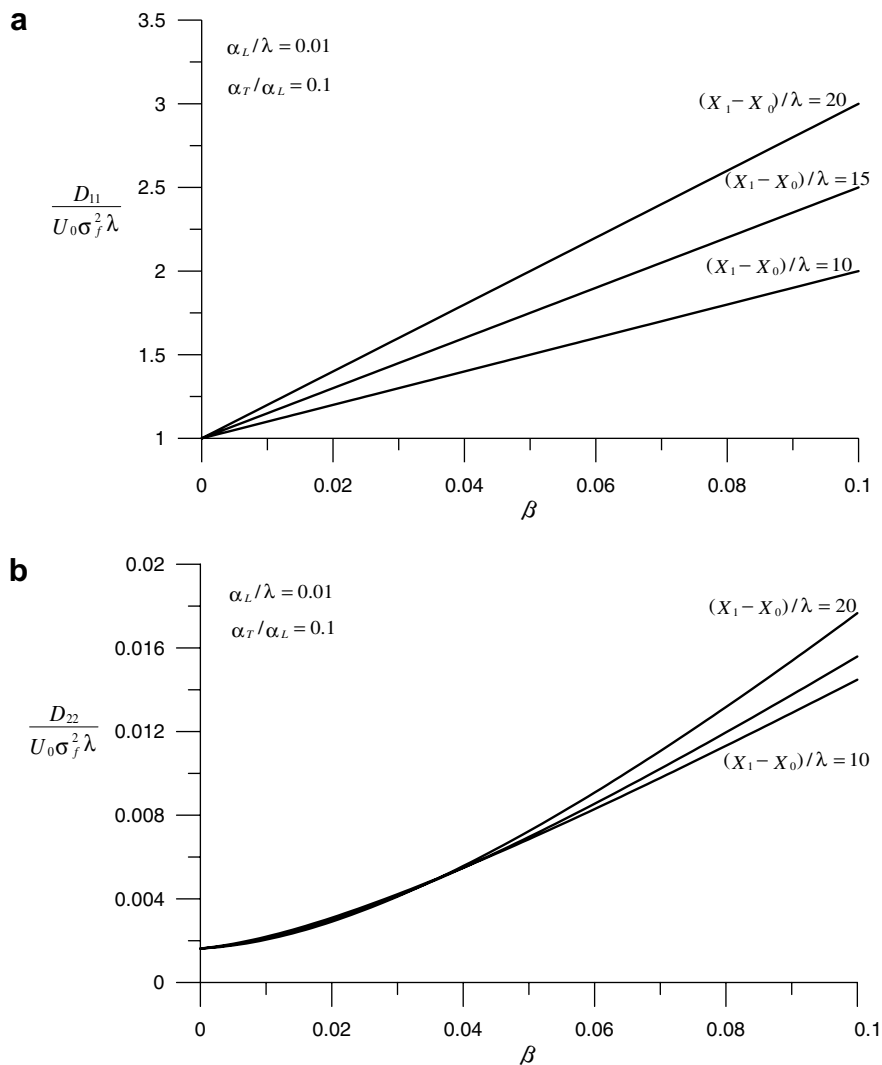

Figure 2 Dimensionless (a) longitudinal and (b) transverse asymptotic macrodispersion coefficients versus dimensionless recharge parameter β for various values of $(X_1 - X_0)/\lambda$ and the indicated values of α_L/λ and α_T/α_L.

D_{11} and D_{22}, can be written by substituting (18) and (19) into (25), respectively, as

$$D_{11} = \frac{3\sigma_f^2\mu^2 U_0}{\pi}\left\{[1 + \beta(X_1 - X_0)/\lambda]\right.$$

$$\times \int_{-\infty}^{\infty}\int \frac{\lambda(\varepsilon^2 v^2 + \eta R_2^2)(1 - \varepsilon^2 v^2/R^2)^2}{[v^2 + (\varepsilon^2 v^2 + \eta R_2^2)^2]}\frac{R^4}{(R^2 + \mu^2)^4}\,dv\,dR_2$$

$$+ \frac{4\beta^2\alpha_L}{[1 + \beta(X_1 - X_0)/\lambda]}$$

$$\left.\times \int_{-\infty}^{\infty}\int \frac{(R_{1^2} + \eta R_2^2)}{[R_1^2 + \varepsilon^2(R_1^2 + \eta R_2^2)^2]}\frac{R_1^2 R_2^4}{R^4(R^4 + \mu^2)^4}\,dR_1\,dR_2\right\}$$

$$(26)$$

$$D_{22} = \frac{3\sigma_f^2\mu^2 U_0}{\pi}\left\{[1 + \beta(X_1 - X_0)/\lambda]\right.$$

$$\times \int_{-\infty}^{\infty}\int \frac{\alpha_L(R_1^2 + \eta R_2^2)}{[R_1^2 + \varepsilon^2(R_1^2 + \eta R_2^2)^2]}\frac{R_1^2 R_2^2}{(R^2 + \mu^2)^4}\,dR_1\,dR_2$$

$$+ \frac{\beta^2\lambda}{[1 + \beta(X_1 - X_0)/\lambda]}$$

$$\left.\times \int_{-\infty}^{\infty}\int \frac{(\varepsilon^2 v^2 + \eta R_2^2)}{[v^2 + (\varepsilon^2 v^2 + \eta R_2^2)^2]}\frac{R_2^2(\varepsilon^2 v^2 - R_2^2)^2}{R^4(R^4 + \mu^2)^4}\,dv\,dR_2\right\}$$

$$(27)$$

where $R_i = \lambda K_i, R^2 = R_1^2 + R_2^2 = \lambda^2 K^2, \varepsilon = \alpha_L/\lambda, v = R_1/\varepsilon, \eta = \alpha_T/\alpha_L$, and $\mu = 3\pi/16$.

The integrals of the forms of (26) and (27), for the general case, cannot be integrated analytically. Because of the form of the denominator in (26) or (27), the main contribution to the integral comes from $v \cong 0$ as $\varepsilon \to 0$ (Gelhar and Axness, 1983). Therefore, for the physically reasonable case of relative small local dispersion ($\varepsilon = \alpha_L/\lambda \ll 1$), approximate analytical expressions can be developed by taking the limit $\varepsilon \to 0$, as illustrated by Gelhar and Axness (1983). Note that for field conditions the ratio α_L/λ is typically 10^{-2} or small (Gelhar and Axness, 1983).

The integrals in (26) and (27) are approximated by taking the limit $\varepsilon \to 0$ in the integrands and integrating separately over each variable, to get

$$D_{11} = U_0\sigma_f^2\lambda\left\{[1 + \beta(X_1 - X_0)/\lambda] + \frac{32}{9\pi^2}\frac{\varepsilon\beta^2(1 + 5\eta)}{[1 + \beta(X_1 - X_0)/\lambda]}\right\}$$

$$(28)$$

$$D_{22} = U_0\sigma_f^2\lambda\left\{\frac{1}{8}\varepsilon(1 + 3\eta)[1 + \beta(X_1 - X_0)/\lambda]\right.$$

$$\left.+ \frac{256}{9\pi^2}\frac{\beta}{[1 + \beta(X_1 - X_0)/\lambda]}\right\}$$

$$(29)$$

It is evident from (28) and (29) that for the case of advection-dominated transport ($\alpha_L \to 0$ and $\alpha_T \to 0$), the longitudinal and transverse macrodispersion coefficients in (28) and (29), respectively, reduce to

$$D_{11} = U_0\sigma_f^2\lambda[1 + \beta(X_1 - X_0)/\lambda]$$

$$(30)$$

$$D_{22} = \frac{256}{9\pi^2}\frac{U_0\sigma_f^2\beta^2}{[1 + \beta(X_1 - X_0)/\lambda]}$$

$$(31)$$

Fig. 2a and b shows how the longitudinal and transverse macrodispersion coefficients, respectively, vary with β, according to (28) and (29). The increase of macrodispersion coefficient with β is related to the fact that larger recharge results in increases in the variation of flow velocity (Fig. 1a or b) and, consequently, results in more spreading of the solute plume. In the limit as $\beta \to 0$ (the no-recharge case), the longitudinal and transverse macrodispersion coefficients tend to

$$D_{11} = U_0\sigma_f^2\lambda$$

$$(32)$$

$$D_{22} = \frac{U_0\sigma_f^2\lambda\varepsilon}{8}(1 + 3\eta) = \frac{U_0\sigma_f^2\alpha_L}{8}(1 + 3\eta)$$

$$(33)$$

which recover the results of Gelhar and Axness (1983) in the case of the two-dimensional flow.

Conclusions

The problem of solute transport in two-dimensional uniformly recharged heterogeneous aquifers has been investigated from a stochastic point of view. Results here have been developed to quantify the influence of groundwater recharge on the spectrum and the variation of flow velocity and asymptotic macrodispersion, in terms of the statistical properties and the integral scale of ln$T$, local transport parameters and a parameter β (Rubin and Bellin, 1994) characterizing the degree of flow nonuniformity due to recharge. The stochastic methodology employed to develop the results of this work is based on the nonstationary spectral approach (Li and McLaughlin, 1991, 1995). In particular, the introduction of this approach allows for quantifying the nonstationarity of head perturbation, and in turn developing the spectrum of the flow velocity, which is the key analytical development in the prediction of the field-scale transport coefficients in random nonstationary velocity fields. Our results indicate that the increase of the variation of the groundwater flow velocity caused by the recharge leads to more spreading of the solute plume. This implies that ignoring the influence of the recharge in field applications leads to the erroneous conclusion in the predicted spreading of solute plume. Our presented formulation for velocity variances compares well with the solutions obtained by Li and Graham (1998) using a first-order perturbation technique.

Acknowledgements

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