# Higher-Order Stochastic Models for Flow and Transport in Geologic Media

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## Abstract

Recursive perturbation solutions are provided for the steady flow problem and the eulerian transport problem for chemicals undergoing deterministic, nonequilibrium, first-order reactions. The mean flux of the solvent is obtained up to $O(\sigma_f^4)$ where $\sigma_f^2$ is the variance in fluctuating conductivity. The stochastic concentration is found to arbitrary order in $\sigma_v$, where $\sigma_v^2$ is the variance in fluctuation solvent velocity. The stochastic concentration is obtained as a perturbation to the deterministic concentration associated with the constant mean velocity. The solutions do not suffer from the common closure problems encountered with earlier eulerian methods.

## 1 Introduction

Over the last several decades stochastic aproaches have been extensively applied to study solute evolution in random porous media (Dagan, 1989; Gelhar, 1993; Cushman, 1997). Studies have suggested that natural heterogeneity plays a large role in mixing processes in the subsurface. Much of this heterogeneity is manifest in the spatial variability of hydraulic conductivity which induces fluctuating velocities that enhance spreading and contribute to the uncertainty in solute transport. Recently, Deng and Cushman (1995) have provided a second order in $\sigma_f^2$ ($\sigma_f^2$ being the variance in fluctuating conductivity) solution to the steady flow problem. We summarize that result here and then go on to summarize a $k^{th}$-order in $\sigma_v$ ($\sigma_v^2$ being the variance in fluctuating velocity) solution to the eulerian transport problem for conservative trancers which was obtained in Cushman and Hu (1997). Finally we extend this latter result to account for linear, nonequilibrium, deterministically-reacting chemicals.

## 2 Second-Order Flow Solution (Deng and Cushman, 1995)

In an unbounded locally isotropic medium under steady flow conditions, the head, $\Phi$, is assumed to satisfy

$$\frac{\partial}{\partial x_i}\left(K\frac{\partial \Phi}{\partial x_i}\right) = 0 \tag{1}$$

where $K(\mathbf{x})$ is the hydraulic conductivity. If we define $Y = \ln K$, assume $\frac{\partial \Phi}{\partial x_i} = -J_i + \frac{\partial h}{\partial x}$ where $\mathbf{J} = (J, 0, 0)$ is the mean head gradient, then with $Y = \overline{Y} + f(\mathbf{x})$, where $\overline{Y}$ is constant, (1) takes the form

$$\frac{\partial^2 h}{\partial x_i \partial x_i} + \frac{\partial f}{\partial x_i}\frac{\partial h}{\partial x_i} - J\frac{\partial f}{\partial x_1} = 0. \tag{2}$$

The Darcy velocity can be decomposed as

$$\begin{aligned} v_i &= -\frac{K}{n}\frac{\partial \Phi}{\partial x_i} \\ &= -\frac{K_g}{n}\left(1 + f + \frac{1}{2}f^2 + \frac{1}{6}f^3 + \ldots\right) \cdot \\ &\quad \cdot \left(-J\delta_{i1} + \frac{\partial h}{\partial x_i}\right) \end{aligned} \tag{3}$$

where $V_i = \overline{V}_i + v_i$. To second order in $\sigma_f^2$ we have

$$\overline{V}_i \approx \frac{K_g}{n}\left[J\delta_{i1}\left(1+\frac{1}{2}\sigma_f^2+\frac{1}{8}\sigma_f^4\right) -\overline{f\frac{\partial h}{\partial x_i}}-\frac{1}{2}\overline{f^2\frac{\partial h}{\partial x_i}}-\frac{1}{6}\overline{f^3\frac{\partial h}{\partial x_i}}\right], \quad (4)$$

$$v_i = v_i^{(1)} + v_i^{(2)}, \quad (5)$$

$$v_i^{(1)} = \frac{K_g}{n}\left(J\delta_{i1}f - \frac{\partial h}{\partial x_i}\right), \quad (6)$$

$$v_i^{(2)} = \frac{K_g}{n}\left[J\delta_{i1}\left(\frac{1}{2}f^2-\frac{1}{2}\sigma_f^2\right) - \left(f\frac{\partial h}{\partial x_i} - \overline{f\frac{\partial h}{\partial x_i}}\right) + J\delta_{i1}\left(\frac{1}{6}f^3+\frac{1}{24}f^4-\frac{1}{8}\sigma_f^4\right) - \frac{1}{2}\left(f^2\frac{\partial h}{\partial x_i} - \overline{f^2\frac{\partial h}{\partial x_i}}\right) - \frac{1}{6}\left(f^3\frac{\partial h}{\partial x_i} - \overline{f^3\frac{\partial h}{\partial x_i}}\right)\right]. \quad (7)$$

Here $v_i^{(1)}$ and $v_i^{(2)}$ are, respectively, the linear component of the fluctuating velocity and its nonlinear correction. Using this latter decomposition the fluctuating-velocity covariance, $R_{ij}$, takes the form

$$R_{ij}(\mathbf{x},\mathbf{y}) = R_{ij}^{(1,1)} + R_{ij}^{(2,2)} + R_{ij}^{(1,2)} + R_{ij}^{(2,1)} \quad (8)$$

where

$$R_{ij}^{(k,\ell)}(\mathbf{x},\mathbf{y}) = \overline{v_i^{(k)} v_j^{(\ell)}(\mathbf{y})}. \quad (9)$$

Using (2) one can relate the covariance for the fluctuating head, $R_{hh}$, to the fluctuating log-conductivity covariance, $R_{ff}$. Setting

$$R_{hh}(\mathbf{x},\mathbf{y}) = \sum_{m=2}^{\infty} R_{hh,m}(\mathbf{x},\mathbf{y}) \quad (10)$$

with

$$R_{hh,m}(\mathbf{x},\mathbf{y}) = \overline{h_i(\mathbf{x})h_j(\mathbf{y})},\ m = i+j \quad (11)$$

and assuming $f$ is a stationary Gaussian process gives

$$R_{hh}(\mathbf{u}) = R_{hh,2}(\mathbf{u}) + R_{hh,4}(\mathbf{u}),\ O(\sigma_f^4) \quad (12)$$

where $\mathbf{u} = \mathbf{x} - \mathbf{y}$ and

$$R_{hh,2} = -J^2 A_1 *_\mathbf{u} A_1 *_\mathbf{u} R_{ff},\ O(\sigma_f^2) \quad (13)$$

$$R_{hh,4} = -J^2 A *_\mathbf{u} A *_\mathbf{u}\left[(A_1 * P_{ij})^2 + P_{ij}(A_1 *_\mathbf{u} A_1 *_\mathbf{u} P_{ij})\right] - 2J^2 A *_\mathbf{u} A_1 *_\mathbf{u} P_j *_\mathbf{u}\left[A_i(A_1 *_\mathbf{u} P_{ij}) - A_1 *_\mathbf{u}(A_i P_{ij})\right] \quad (14)$$

with

$$P_{ij}(\mathbf{u}) = \frac{\partial^2 R_{ff}}{\partial u_i \partial u_j}, \quad (15)$$

$$P_j(\mathbf{u}) = \frac{\partial R_{ff}}{\partial u_j}, \quad (16)$$

$$\hat{A}(\mathbf{k}) = -k^2, \quad (17)$$

$$A_1(\mathbf{x}) = \frac{\partial A}{\partial x_1}. \quad (18)$$

Here $\mathbf{k}$ is dual under $FT$ to $\mathbf{x}$.

Using (6) and (7) we find

$$R_{ij}^{(1,1)}(\mathbf{x},\mathbf{y}) = R_{ij}^{(1,1)}(\mathbf{x}-\mathbf{y}) = R_{ij,1}^{(1,1)}(\mathbf{u}) + R_{ij,2}^{(1,1)}(\mathbf{u}), \quad (19)$$

where

$$R_{ij,1}^{(1,1)} = \frac{K_g^2 J^2}{n^2}\left\{\delta_{i1}\delta_{j1}R_{ff} + A_1 *_\mathbf{u}(\delta_{j1}P_i + \delta_{i1}P_j) + A_1 *_\mathbf{u} A_1 *_\mathbf{u} P_{ij}\right\}, \quad (20)$$

$$R_{ij,2}^{(1,1)} = \frac{K_g^2 J^2}{n^2}\left\{A_i *_\mathbf{u} A_j *_\mathbf{u} \cdot \right.$$

$$\left. \cdot\left[(A_1 *_\mathbf{u} P_{nm})^2\right.\right.$$

$$+P_{mn}(A_1 *_{\mathbf{u}} A_1 *_{\mathbf{u}} P_{mn})\Big]$$

$$+\Big[\delta_{i1} A_i *_{\mathbf{u}} P_n + \delta_{i1} A_j *_{\mathbf{u}} P_n$$

$$+A_1 *_{\mathbf{u}} A_i *_{\mathbf{u}} P_{jn} + A_1 *_{\mathbf{u}} \cdot$$

$$\cdot A_j *_{\mathbf{u}} P_{in}\Big] *_{\mathbf{u}} \Big[A_m(A_1 *_{\mathbf{u}} P_{mn})$$

$$-A_1 *_{\mathbf{u}} (A_m P_{mn})\Big]\Big\} \quad (21)$$

$$R_{ij}^{(2,2)}(\mathbf{x},\mathbf{y}) = R_{ij}^{(2,2)}(\mathbf{u})$$

$$= \frac{K_g^2 J^2}{n^2}\Big[(\delta_{i1} R_{ff} + A_1 *_{\mathbf{u}} P_i)\cdot$$

$$\cdot(\delta_{i1} R_{ff} + A_1 *_{\mathbf{u}} P_j)$$

$$+R_{ff}\Big(A_1 *_{\mathbf{u}} A_1 *_{\mathbf{u}} P_{ij}$$

$$-\frac{1}{2}\delta_{i1}\delta_{j1} R_{ff}\Big)\Big], \quad (22)$$

$$R_{ij}^{(1,2)}(\mathbf{x},\mathbf{y}) = R_{ij,1}^{(1,2)}(\mathbf{u})$$

$$+R_{ij,2}^{(1,2)}(\mathbf{u}), \quad (23)$$

where

$$R_{ij,1}^{(1,2)}(\mathbf{u}) = \frac{K_g^2 J^2}{n^2}\Big\{\frac{1}{2}\sigma_f^2\Big[\delta_{i1}\delta_{j1} R_{ff}$$

$$+A_1 *_{\mathbf{u}} (\delta_{j1} P_i + \delta_{i1} P_j)$$

$$+A_1 *_{\mathbf{u}} A_1 *_{\mathbf{u}} P_{ij}\Big] + (A_1 *_{\mathbf{u}} P_j \,|_{u=0})\cdot$$

$$\cdot(\delta_{i1} R_{ff} + A_1 *_{\mathbf{u}} P_i)\Big\}, \quad (24)$$

$$R_{ij,2}^{(1,2)}(\mathbf{u}) = \frac{K_g^2 J^2}{n^2}\Big\{\delta_{j1} A_1 *_{\mathbf{u}} \cdot$$

$$\cdot[P_m(A_1 *_{\mathbf{u}} P_m)]$$

$$+[\delta_{i1} P_m + A_1 *_{\mathbf{u}} P_{im}] *_{\mathbf{u}} \cdot$$

$$\cdot\Big[A_j(A_1 *_{\mathbf{u}} P_m) - A_1 *_{\mathbf{u}} (A_j \cdot P_m)\Big]$$

$$+A_i *_{\mathbf{u}} \Big[(A_1 *_{\mathbf{u}} P_{jm})(A_1 *_{\mathbf{u}} P_m)$$

$$+(A_1 *_{\mathbf{u}} A_1 *_{\mathbf{u}} P_{jm})P_m\Big]\Big\}, \quad (25)$$

and

$$R_{ij}^{(2,1)}(\mathbf{u}) = R_{ji,1}^{(1,2)}(\mathbf{u}) + R_{ji,2}^{(1,2)}(\mathbf{u}). \quad (26)$$

It can be shown that $R_{ij,1}^{(1,1)}$ is accurate to $O(\sigma_f^2)$ whereas $R_{ij,1}^{(1,1)} + R_{ij,2}^{(1,1)}$ and $R_{ij}^{(1,1)}$ are accurate to $O(\sigma_f^4)$.

Finally set

$$C_{ij}^{[1]} = \alpha\,\overline{v_i^{(1)} v_j^{(1)}} = \alpha R_{ij,1}^{(1,1)}$$
$$\text{with } \overline{hh} \sim O(\sigma_f^2), \quad (27)$$

$$C_{ij}^{[2]} = \alpha\,\overline{v_i^{(1)} v_j^{(1)}} = C_{ij}^{[1]} + \alpha R_{ij,2}^{(1,1)}$$
$$\text{with } \overline{hh} \sim O(\sigma_f^2 + \sigma_f^4), \quad (28)$$

$$C_{ij}^{[3]} = \alpha\,\overline{(v_i^{(1)} + v_i^{(2)})(v_j^{(1)} + v_j^{(2)})}$$
$$= C_{ij}^{[1]} + \alpha\Big[R_{ij,1}^{(1,2)} + R_{ij,1}^{(2,1)} + R_{ij}^{(2,2)}\Big]$$
$$\text{with } \overline{hh} \sim O(\sigma_f^2), \quad (29)$$

and

$$C_{ij}^{[4]} = \alpha\,\overline{(v_i^{(1)} + v_i^{(2)})(v_j^{(2)} + v_j^{(2)})}$$
$$= C_{ij}^{[3]} + \alpha\Big[R_{ij,2}^{(1,1)} + R_{ij,2}^{(1,2)} + R_{ij,2}^{(2,1)}\Big]$$
$$\text{with } \overline{hh} \sim O(\sigma_f^2 + \sigma_f^4) \quad (30)$$

where $\alpha = \sigma_f^2 K_g^2 J^2/n^2$.

Figures 1-3 illustrate the effects of these various approximations for a Gaussian log-fluctuating conductivity with $e = \lambda_v/\lambda_h$ being the ratio of vertical to horizontal integral scales.

## 3 Solutions to the Stochastic Transport Problem for Conservative Traces Which Are $O(\sigma_v^N)$

We follows Cushman and Hu (1997). For simplicity, suppose we have an infinite domain and steady

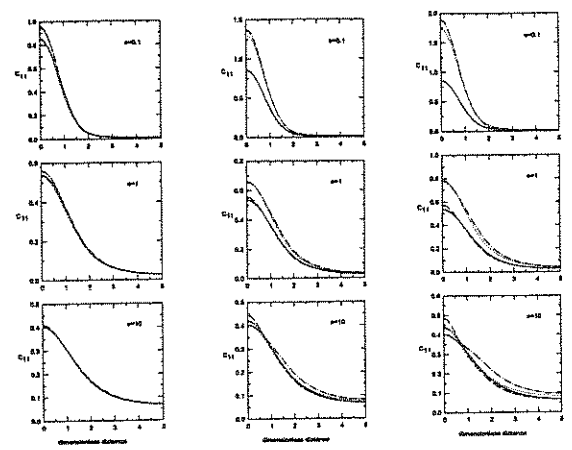

Figure 1: $C_{11}$ as a function of $\rho$ and $u^* = u_1/\lambda_h$ and various $\sigma_f^2$, a) $\sigma_f^2 = 0.1$, b) $\sigma_f^2 = 0.5$, c) $\sigma_f^2 = 1.0$. From Deng and Cushman (1997), Fig. 1

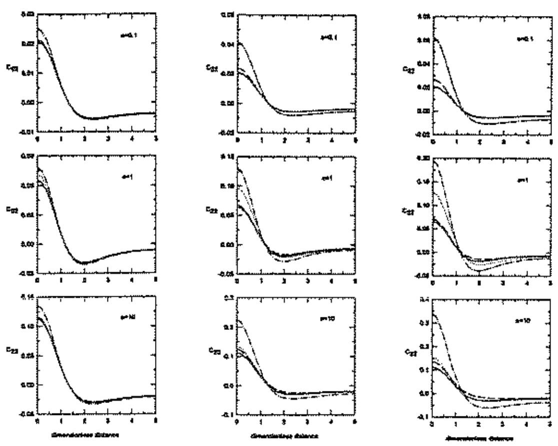

Figure 2: Same as Fig. 1 except $C_{22}$. From Deng and Cushman (1997), Fig. 2

divergence free flow with the concentration satisfying

$$\frac{\partial C}{\partial t} + V_i \frac{\partial C}{\partial x_i} - d_i \frac{\partial^2 C}{\partial x_i^2} = 0 \tag{31}$$

where $\overline{V}_i$ is assumed constant and of order unity. Here $C$ is the stochastic concentration, $V_i = \overline{V}_i + v_i$, and $d_i$ is the assumed deterministic-constant local dispersivity. Let $C^0$ be the solution to the sure problem

$$HC^0 \equiv \frac{\partial C^0}{\partial t} + \overline{V}_i \frac{\partial C^0}{\partial x_i} - d_i \frac{\partial^2 C^0}{\partial x_i^2} = 0 \tag{32}$$

subject to $C^0 = C_0(x)$ where $C_0$ is the deterministic initial concentration for the stochastic problem given in (31). We write the solution to (31) as a sum of perturbations to (32). Let

$$C = \sum_{j=0}^{\infty} C^j \tag{33}$$

with

$$C^j \sim O(\sigma_v^j) \tag{34}$$

where $\sigma_v^2$ is the variance in the fluctuating velocity with

$$\frac{\sigma_v^2}{\|\overline{V}\|^2} < 1. \tag{35}$$

Let $G$ be the fundamental solution for the operator $H$. For the problem here

$$G(x,t) = \prod_{k=1}^{3} \exp\left[ -\frac{(x_k - \overline{V}_k t)^2}{4 d_k t} \right] \cdot \cdot (4\pi d_k t)^{-\frac{1}{2}}. \tag{36}$$

We have

$$C^0(x,t) = \int_{R^3} G(x-y,t) C_0(y) dy. \tag{37}$$

By inserting (33) into (31) and equating like-powers in $\sigma_v$ we obtain the following recursive sequence ($N \geq 0$)

$$HC^N = -v_j(x) \frac{\partial C^{N-1}}{\partial x_j} (1 - \delta_{N0}). \tag{38}$$

It follows that the stochastic concentration to $O(\sigma_v^N)$ is given by

$$C(\mathrm{x},t) = \int_{R^3} G(\mathrm{x}-\mathrm{y},t) C_0(\mathrm{y}) d\mathrm{y} + \sum_{k=1}^{m} (-1)^k \int_0^t \cdots \int_0^{t^{k-1}} \int_{R^{3(k+1)}} \cdot \cdot \Big\{ G(\mathrm{x}-\mathrm{x}', t-t')$$

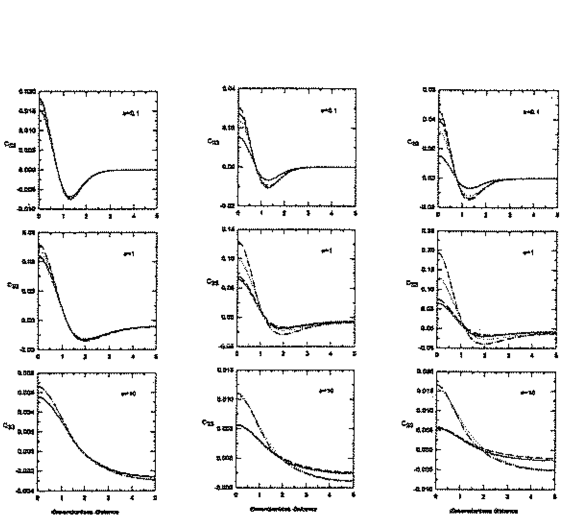

Figure 3: Same as Fig. 1 except $C_{33}$. From Deng and Cushman (1997), Fig. 3

$$\left[\prod_{\ell=1}^{k-1} \frac{\partial G}{\partial x_{j_\ell}^{\ell}}(\mathbf{x}^{\ell} - \mathbf{x}^{\ell+1}, t^{\ell} - t^{\ell+1})\right] \cdot$$

$$\cdot \frac{\partial G}{\partial x_{j_k}^{k}}(\mathbf{x}^{k} - \mathbf{x}^{k+1}, t^{k}) \left[\prod_{\ell=1}^{k} v_{j_\ell}(\mathbf{x}^{\ell})\right] \cdot$$

$$\left. \cdot C_0(\mathbf{x}^{k+1}) \right\} d\mathbf{x}^1 \dots d\mathbf{x}^{k+1} dt^1 \dots dt^{k+1}. \quad (39)$$

From (39) the mean concentration to $O(\sigma_v^N)$ is

$$\begin{aligned} \overline{C}(x,t) &= \int_{R^3} G(\mathbf{x}-\mathbf{y},t) C_0(y) dy \\ &+ \sum_{k=1}^{N} (-1)^k \int_0^t \cdots \int_0^{t^{k-1}} \int_{R^{3(k+1)}} \cdot \\ &\cdot \left\{ G(\mathbf{x}-\mathbf{x}', t-t') \cdot \right. \\ &\cdot \left[\prod_{\ell=1}^{k-1} \frac{\partial G}{\partial x_{j_\ell}^{\ell}}(\mathbf{x}^{\ell} - \mathbf{x}^{\ell+1}, t^{\ell} - t^{\ell+1})\right] \cdot \\ &\cdot \frac{\partial G}{\partial x_{j_k}^{k}}(\mathbf{x}^{k} - \mathbf{x}^{k+1}, t^{k}) \left[\overline{\prod_{\ell=1}^{k} v_{j_\ell}(\mathbf{x}^{\ell})}\right] \cdot \\ &\left. \cdot C_0(\mathbf{x}^{k+1}) \right\} d\mathbf{x}^1 \dots d\mathbf{x}^{k+1} dt^1 \dots dt^{k}. \end{aligned} \quad (40)$$

# 4 The Case of Linear Nonequilibrium Deterministic Reactions

In this case we assume the basic underlying equations are

$$\frac{\partial C}{\partial t} + \frac{\partial S}{\partial t} + V_i \frac{\partial C}{\partial x_i} - d_i \frac{\partial^2 C}{\partial x_i^2} = 0, \quad (41)$$

$$\frac{\partial S}{\partial t} - K_r(K_d C - S) = 0, \quad (42)$$

where again we assume an infinite domain. Here, $K_r$ is the reaction rate, $K_d$ is the partition coefficient, and $S$ is the sorbed phase concentration. As in the previous section we expand $C$ in an infinite series of terms of order $\sigma_v^j$, and write a recursive system of equations

$$PC^N = -v_j(x) \frac{\partial C^{N-1}}{\partial x_j}(1 - \delta_{N0}) \quad (43)$$

where $P$ is defined by

$$\begin{aligned} PC &\equiv \frac{\partial C}{\partial t} + K_r K_d C \\ &- K_r K_d \int_0^t e^{-K_r(t-\tau)} C(x,\tau) d\tau \\ &+ \overline{V}_i \frac{\partial C}{\partial x_i} - d_i \frac{\partial^2 C}{\partial x_i^2}. \end{aligned} \quad (44)$$

The Green's function for $P$ is given by

$$\tilde{\tilde{G}} = \left[\omega + \frac{\omega K_r K_d}{\omega + K_r} + \overline{V}_j i k_j + d_j k_j^2\right]^{-1} \quad (45)$$

where $\tilde{\tilde{\ }}$ indicates Fourier-Laplace transform with $\omega$ dual to $t$ and $\mathbf{k}$ dual to $\mathbf{x}$. Thus $C$ and $\overline{C}$ take the form of (39) and (40) where $G$ is given by (45).

# 5 Discussion

We have provided a closed form perturbation solution to the steady flow problem. The solution is accurate to $O(\sigma_f^4)$ where $\sigma_f^2$ is the variance in fluctuating log-hydraulic conductivity. Numerical computations show second order corrections are important for computing transverse moments.

We have also provided closed form perturbation solutions to the transport problems for conservative chemicals and chemicals experiencing nonequilibrium first-order reversible, deterministic reactions. These solutions are of arbitrary high accuracy in $\sigma_v$ where $\sigma_v^2$ is the variance in fluctuating velocity. These solutions do not suffer from problems associated with truncation in more classical eulerian approaches.


### 5.1 Acknowledgements

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## 6 References


Cushman, J. H., *The Physics of Fluids in Hierarchial Porous Media: Angstroms to Miles,* Kluwer, Amsterdam, 1997.

Cushman, J. H., and B. X. Hu, Solutions to the stochastic transport problem of $O(\sigma_v^N)$ for conservative solutes, *Stoch. Hydrol. Hyd., 11*(3), 1997 (in press).

Dagan, G., *Flow and Transport in Porous Formations,* Springer, New York, 1989.

Deng, F. W., and J. H. Cushman, On higher-order corrections to the flow velocity covariance tensor, *Water Resour. Res.,* 1569-1672, 1995.

Deng, F. W., and J. H. Cushman, Addendum to On higher-order corrections to the flow velocity covariance tensor, *Water Resour. Res.,* 1997 (in press).

Gelhar, L. W., *Stochastic Subsurface Hydrology,* Prentice-Hall, Englewood Cliffs, NJ, 1993.