A simple closed-form solution for assessing concentration uncertainty

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[1] We propose closed-form approximate solutions for the moments of a nonreactive tracer that can be used in applications, such as risk analysis. This is in line with the tenet that analytical solutions provide useful information, with minimum cost, during initial site characterization efforts and can serve as a preliminary screening tool when used with prior knowledge. We show that with the help of a few assumptions, the first-order solutions of the concentration moments proposed by Fiori and Dagan (2000) can be further simplified to assume a form similar to well-known deterministic solutions, therefore facilitating their use in applications. A highly anisotropic formation is assumed, and we neglect the transverse components of the two-particle correlation trajectory. The proposed solution compares well with the work of Fiori and Dagan while presenting the same simplicity of use of existing solutions for homogeneous porous media.

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1. Introduction

[2] Despite the fact that stochastic hydrogeology is well consolidated in the literature [e.g., *Rubin*, 2003], its acceptance among practitioners is still limited. In part, this is due to the limited amount of data typically available in applications, which in most cases are insufficient to infer the model of spatial variability. Some of the difficulties hindering the application of stochastic models have been alleviated by recent technological breakthroughs, which allow to acquire, at an affordable cost, much more data than in the past, for aquifer characterization and inference of the stochastic model of spatial variability at a variety of scales [e.g., *Hubbard and Rubin*, 2000]. However, in order to facilitate the use of stochastic methods, simple-to-use protocols for risk analysis should be devised, possibly based on simple analytical solutions [e.g., *Andricevic and Cvetkovic*, 1996].

[3] In this work, we provide a simple expression to quantify uncertainty in concentration of a nonreactive tracer, which is based on closed-form solutions for the concentration ensemble mean and variance. The latter depends on the interplay between macroscale advection and local scale dispersion, and it is representative of the dilution processes occurring in porous formations [e.g., *Kapoor and Kitanidis*, 1998]. In particular, we show that with a few assumptions the expressions available in literature for the concentration distribution in a homogeneous media [e.g., *van Genuchten and Alves*, 1982] can be used to obtain the ensemble mean concentration, while similar expressions can be obtained for the coefficient of variation. The only parameters required are those characterizing the model of spatial variability, which can be obtained through field tests. This approach is appealing because it allows to evaluate uncertainty in the concentration and its effect on risk analysis with a minimized additional effort with respect to solving flow and transport within a deterministic framework.

2. Problem Formulation

[4] A passive tracer is instantaneously released within a source volume $\mathcal{V}_o$ of dimensions L_1, L_2, and L_3 in a 3-D heterogeneous formation. We assume that the inlet concentration is constant, C_0, within $\mathcal{V}_o$, while the initial concentration in the porous systems is zero. The quantity of interest here is the concentration $C(\mathbf{x}, t)$, where $\mathbf{x}(x_1, x_2, x_3)$ is the Cartesian coordinate vector and t is time. In addition, we introduce the following assumptions:

[5] 1. Flow is at steady state in an unbounded domain and uniform in the average with the mean velocity $\mathbf{U}(U, 0, 0)$.

[6] 2. The hydraulic logconductivity $Y = \ln K$, where K is the hydraulic conductivity, is represented as a statistically stationary Random Space Function and the porosity is constant. Y is normally distributed and statistically stationary with constant mean $\langle Y \rangle$ and variance σ_Y^2. Its covariance function C_Y is given by a Gaussian model with $I_{Y,h}$ and $I_{Y,v}$ denoting the horizontal and vertical integral scales of Y, respectively.

[7] 3. Hydrodynamic local dispersion is given by a constant and isotropic diagonal dispersion tensor $\mathbf{D} = \mathrm{diag}[D_d]$.

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[8] Because of the randomness of K, C is also random. In this study we consider the following expressions for the ensemble mean concentration $\langle C \rangle$ and variance σ_C^2:

$$\frac{\langle C \rangle}{C_0} = \prod_{i=1}^{3} \eta(x_i - U_i t), \tag{1}$$

$$\frac{\sigma_C^2}{C_0^2} = \prod_{i=1}^{3} \int_{-L_i/2}^{L_i/2} \Theta_i(x_i; a_i) da_i - \langle C \rangle^2, \tag{2}$$

where $\mathbf{a}(a_1, a_2, a_3)$ is the initial location of a solute particle within $\mathcal{V}_o$ and the functions η and Θ_i are given by *Fiori and Dagan* [2000]

$$\eta(x_i - U_i t) = \frac{1}{2}\mathrm{erf}\left(\frac{x_i - U_i t + L_i/2}{\sqrt{2X_{t,ii}}}\right) - \frac{1}{2}\mathrm{erf}\left(\frac{x_i - U_i t - L_i/2}{\sqrt{2X_{t,ii}}}\right) \tag{3}$$

$$\Theta_i(x_i; a_i) = \frac{1}{2\sqrt{2\pi X_{t,ii}}} \exp\left[\frac{-(x_i - a_i - U_i t)^2}{2X_{t,ii}}\right] (\mathrm{erf}[\mathcal{A}] - \mathrm{erf}[\mathcal{B}]), \tag{4}$$

where $\mathcal{A}$ and $\mathcal{B}$ assume the following expressions:

$$\mathcal{A} = \frac{L_i + (x_i - U_i t)(1 - \rho_{ii} + a_i \rho_{ii})}{\sqrt{2X_{t,ii}(1 - \rho_{ii}^2)}}$$
$$\mathcal{B} = \frac{-L_i + (x_i - U_i t)(1 - \rho_{ii} + a_i \rho_{ii})}{\sqrt{2X_{t,ii}(1 - \rho_{ii}^2)}}, \tag{5}$$

with $\rho_{ii} = Z_{ii}/X_{t,ii}$ denoting the trajectory autocorrelation function. $X_{t,ii}$ and Z_{ii} are the one- and two-particle covariances and are assumed to be multi-Gaussian [*Fiori and Dagan*, 2000, equations (14) and (15)]. In the following we develop an analytical solution for σ_C^2 under the hypothesis of small source (i.e., $L_1 \ll I_{Y,h}$, $L_2 \ll I_{Y,h}$ and $L_3 \ll I_{Y,v}$) and $\sigma_Y^2 < 1$, which builds on the semianalytical solution by *Fiori and Dagan* [2000].

3. Approximation for σ_C^2

[9] The integrals contained in (2) cannot be solved analytically and therefore numerical quadratures are needed or, as an alternative, suitable simplifications should be introduced such that an analytical expression can be obtained. We decide for the second option since resorting to several numerical quadrature hampers the use of (2) in applications. As shown by *Fiori and Dagan* [2000], the computation of the trajectory autocorrelation function, ρ_{ii}, also requires three numerical quadratures [*Fiori and Dagan*, 2000, equations (14) and (15)]. We start by observing that it is more convenient (and robust) to develop an approximate solution of the coefficient of variation $\mathrm{CV}_C = \sigma_C / \langle C \rangle$ instead of σ_C^2:

$$\mathrm{CV}_C^2 = \frac{\prod_{i=1}^{3} \int_{-L_i/2}^{L_i/2} \Theta_i(x_i; a_i) da_i}{\left[\prod_{i=1}^{3} \eta(x_i - U_i t)\right]^2} - 1. \tag{6}$$

The three integrals over a_i in (6) can be carried out after assuming that a_i varies slightly in (5), given the small source assumption, such that the following approximation can be introduced into equation (5): $(1 - \rho_{ii} + \rho_{ii} a_i) \cong (1 - \rho_{ii})$. This is consistent with the assumption of small source ($L_i/I_Y \ll 1$) introduced by *Fiori and Dagan* [2000] in order to compute Z_{ii}. With this approximation, equation (6) reduces to

$$\mathrm{CV}_C^2 = \frac{\prod_{i=1}^{3} \zeta(x_i - U_i t)}{\prod_{i=1}^{3} \eta(x_i - U_i t)} - 1, \tag{7}$$

where the function ζ assumes the following expression

$$\zeta(x_i - U_i t) = \frac{1}{2}\mathrm{erf}\left[\frac{(x_i - U_i t)(1 - \rho_{ii}) + L_i/2}{\sqrt{2X_{t,ii}(1 - \rho_{ii})}}\right] - \frac{1}{2}\mathrm{erf}\left[\frac{(x_i - U_i t)(1 - \rho_{ii}) - L_i/2}{\sqrt{2X_{t,ii}(1 - \rho_{ii})}}\right]. \tag{8}$$

Equation (8) is very simple, as it coincides with the function η (3) used in the expression (1) after replacing $(x_i - U_i t)$ with $(x_i - U_i t)$ $(1 - \rho_{ii})$ and $X_{t,ii}$ with $X_{t,ii}$ $(1 - \rho_{ii})$. When $\rho_{ii} \to 0$ such that $\zeta \to \eta$, CV_C (7) tends to 0. Hence, σ_C^2 can be approximated by a simple transformation of the classic deterministic solution for $\langle C \rangle$.

[10] The above simplifications eliminated three numerical quadratures, but this does not suffice for an analytical expression for ρ_{ii} and σ_C^2. However, as discussed by *Fiori and Dagan* [2000], the main contribution to σ_C^2 stems from longitudinal spreading, with the longitudinal autocorrelation function ρ_{11} that overwhelms both ρ_{22} and ρ_{33}. Longitudinal spreading increases the interfacial area of the plume with the surrounding fluid thus enhancing the effect of local scale dispersion. Therefore, we may further simplify the analysis and assume $\rho_{22} \simeq 0$ and $\rho_{33} \simeq 0$, such that (7) reduces to

$$\mathrm{CV}_C^2 = \frac{\zeta(x_1 - Ut)}{\eta(x_1 - Ut)} - 1 \tag{9}$$

Equation (9) is the core of the present contribution since it provides CV_C in a simple and convenient form for applications. Once CV_C is known, σ_C^2 can be computed through the following expression: $\sigma_C^2 = \langle C \rangle^2 \mathrm{CV}_C^2$ with $\langle C \rangle$ given by (1).

[11] Despite its simplicity, (9) still requires a few numerical quadratures in order to compute ρ_{11}. This term is crucial as it accounts for the interactions between large scale advection and local scale dispersion, which control dilution, and therefore it is expected to exert a large impact on σ_C^2.

[12] To further simplify the computation of ρ_{11}, we consider that most sedimentary formations are characterized by a strong anisotropy in the integral scales, i.e., $e = I_{Y,v}/I_{Y,h} \ll 1$ [see *Rubin*, 2003, Table 2.1]. *Indelman and Dagan* [1999] showed that for $e \ll 1$, the longitudinal velocity covariance function u_{11} is well approximated by $\sigma_u^2 C_Y / \sigma_Y^2$, where σ_u^2 is the longitudinal velocity variance. This approximation leads to the suppression of the term k_i^2/k^2 (where k_i

is the wave number) in the expression of Z_{ii} [see *Fiori and Dagan*, 2000]. Furthermore, in agreement with a common assumption adopted in applications, we assume the Fickian limit (i.e., $X_{t,ii} = 2UA_{ii}t$, with A_{ii} denoting the macrodispersivity tensor) when computing ρ_{11}. For a Gaussian C_Y and with the above simplifications, an analytical form for ρ_{11} can be obtained as follows:

$$\rho_{11}(t') = \frac{ePe}{2\pi t'} \ln\left[1 + \frac{4\pi t' + 2\sqrt{(Pe + 2\pi t')(e^2 Pe + 2\pi t')}}{Pe(1+e)^2}\right], \tag{10}$$

where $t' = tU/I_{Y,h}$ and $Pe = UI_{Y,h}/D_d$. Expression (10) assumes the following limiting values:

$$\begin{aligned} &\rho_{11} \to 1 \qquad (t' \to 0) \\ &\rho_{11} \to e\ Pe \ln(t'/Pe)/t' \qquad (t' \to \infty). \end{aligned} \tag{11}$$

The large time limit (11) is the same as that obtained for the exponential C_Y model by the first-order exact solution proposed by *Fiori and Dagan* [2000], and is independent of the particular model adopted for C_Y. Summarizing, equation (9), together with equations (8), (3), and (10), allows the computation of CV_C, which after multiplication with (1), leads to σ_C. As opposed to other approaches, where the probability density function (pdf) of C is analytically derived from governing equations [e.g., *Tartakovsky et al.*, 2009; *Sanchez-Vila et al.*, 2009], a complete characterization of C in terms of its pdf can be achieved after adopting the Beta distribution model which depends on $\langle C \rangle$ and σ_C only [see, e.g., *Fiorotto and Caroni*, 2002; *Bellin and Tonina*, 2007].

4. Comparison With the Work of *Fiori and Dagan* [2000]

[13] We test here the approximation developed against the complete solution provided by *Fiori and Dagan* [2000]. For the *Fiori and Dagan* [2000] solution, $X_{t,ii}$ and Z_{ii} are calculated through numerical quadratures. The comparison is performed in terms of concentration statistics evaluated along the ensemble mean plume trajectory at the following two positions: $\bar{\mathbf{x}} = (2.5I_{Y,h}, 0, 0)$ and $\bar{\mathbf{x}} = (10I_{Y,h}, 0, 0)$. Simulation input data are included in the figure captions.

[14] Figures 1a and 1b depict CV_C as a function of dimensionless time for $Pe = 1000$ at $x_1/I_{Y,h} = 2.5$ and 10, respectively. The proposed approximated solution (AP) is smaller than CV_C provided by *Fiori and Dagan* [2000] (FD2000). We also note that the difference between AP and FD2000 reduces with increasing distance from the source. At a given position, larger differences are observed along the leading and trailing fringes of the plume where uncertainty is the highest [*Rubin*, 1991]. At short distances from the source, these differences are mainly due to neglecting ρ_{22} and ρ_{33} in (9). Nevertheless, the approximate solution is able to capture the main features of the full solution, with reasonable tolerance.

[15] Similar results, but for $Pe = 100$, are depicted in Figures 2a and 2b. Comparing Figure 1 with Figure 2, we note that at the centroid location of the ensemble mean plume the agreement between AP and FD2000 improves

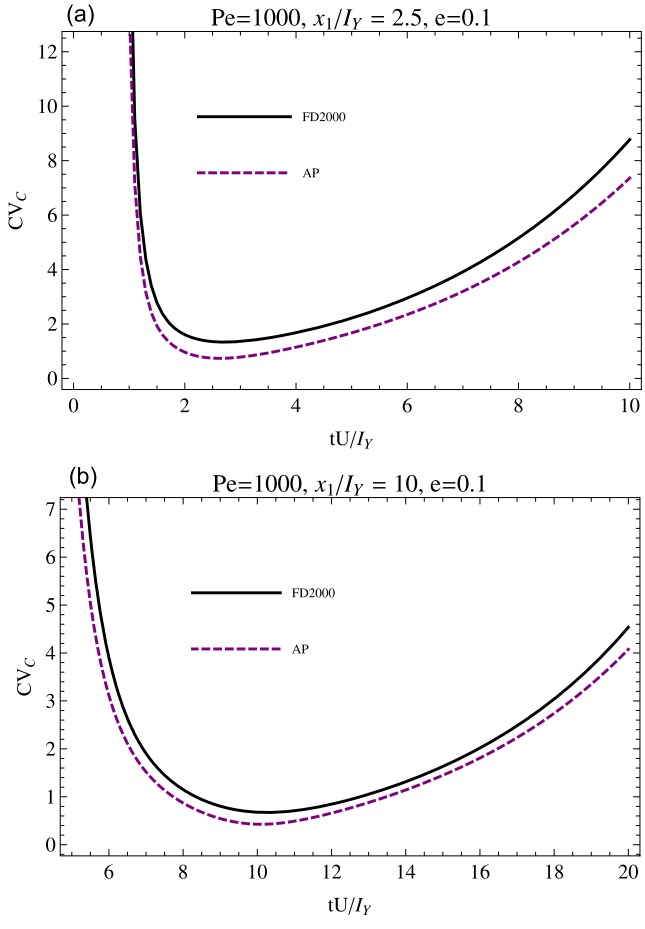

Figure 1. Coefficient of variation of the concentration CV_C versus dimensionless time at the distances (a) $x_1/I_Y = 2.5$ and (b) $x_1/I_Y = 10$ along the mean plume trajectory ($x_2 = x_3 = 0$). The solid line indicates the exact first-order solution by *Fiori and Dagan* [2000] (FD2000), while the dashed line indicates our approximation (AP). Results are for $Pe = 1000$, $L_1 = L_2 = 0.1I_{Y,h}$, $L_3 = 0.1I_{Y,v}$, $e = 0.1$, and $\sigma_Y^2 = 0.3$.

when decreasing Pe. Similarly to the case with $Pe = 1000$, the main differences are observed at the trailing fringe of the plume. These differences are slightly larger for $Pe = 100$ (compare Figures 1 and 2). Again, this is an outcome of neglecting ρ_{22} and ρ_{33} in the model for CV_C, given that their impact on dilution is enhanced for smaller Pe.

[16] In Figure 3, we evaluate CV_C at the mean plume centroid, for $Pe = 100$ and 1000. As expected, CV_C decreases with travel distance. Figure 3 also illustrates that uncertainty is larger at higher Pe. Although AP underestimate CV_C, and thus the uncertainty, when compared to FD2000, the overall comparison is good. Note that this underestimation may be a positive outcome of our approximation because the solution of FD2000 generally overestimates σ_C^2 since it neglects the dependence of ρ_{ii} on the separation vector between particle positions at the source. This has also been shown numerically by *Tonina and Bellin* [2008]. Furthermore, the performance of AP (relative to

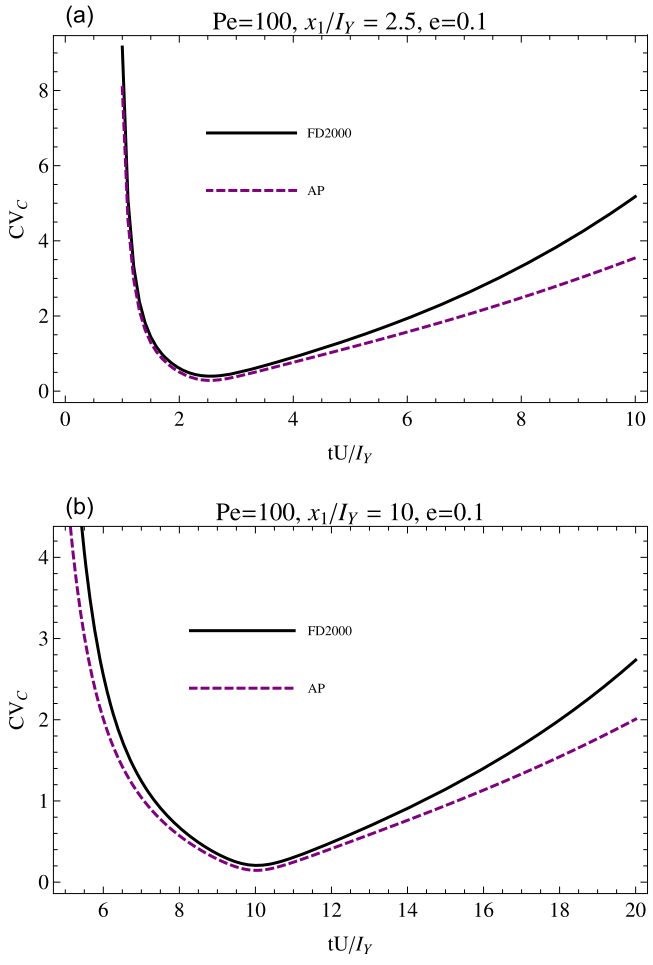

Figure 2. Same as Figure 1, but for $Pe = 100$.

FD2000) improves with decreasing *Pe* and the differences between AP and FD2000 are due to the assumptions listed in section 3.

5. Summary and Final Remarks

[17] The importance of quantifying uncertainty in contaminant transport has been emphasized in the hydrogeological community over the past years [*Rubin*, 2003]. Several field evidences and theoretical developments illustrated the significance of concentration fluctuations and our inability to model in detail the concentration field. As pointed out by *Fitts* [1996] and *Kapoor and Kitanidis* [1998], peak concentrations found in the field can be larger than the maximum mean concentration modeled through the common approach used in most applications (the standard deterministic approach). The uncertainty in the concentration is generally very large (especially for nonergodic cases) and therefore cannot be ignored. Accounting for σ_C^2 in practical applications is of interest since it allows one to evaluate an upper bound on exceedance probabilities. Moreover, σ_C^2 is an indicator of the proximity of the mean concentration to the actual, erratic concentration. The challenge is that most expressions for σ_C^2 require numerical quadratures and are provided in a rather complex mathematical

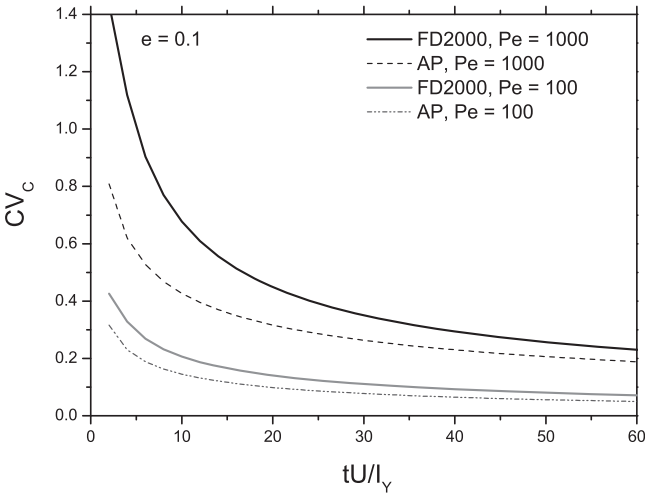

Figure 3. Coefficient of variation of the plume's centroid motion versus dimensionless time. Results for $Pe = 100$ and 1000 using FD2000 and AP. In all cases, $L_1 = L_2 = 0.1I_{Y,h}$, $L_3 = 0.1I_{Y,v}$, $e = 0.1$, and $\sigma_Y^2 = 0.3$.

form to be used in conjunction with the available deterministic solution.

[18] In this work, we report a simple-to-use expression to estimate concentration uncertainty. The solution for CV_C developed here relies on the first-order approximation of *Fiori and Dagan* [2000] and consequently inherits its assumptions (e.g., steady state uniform-in-the-average flow, small σ_Y^2), while introducing the following further approximations: (1) ρ_{22} and ρ_{33} are neglected, (2) highly anisotropic formation ($e \ll 0.1$), and (3) small source, such that a_i varies slightly in equation (6). Despite these assumptions, the limits of applicability of the *Fiori and Dagan* [2000] solution goes beyond expected, as shown by *Tonina and Bellin* [2008] (e.g., source dimensions as large as $10I_Y$). As pointed out by *Bellin et al.* [1994], if CV_C is used as a measure of uncertainty, then point concentrations can be operationally equivalent as the concentration within a sampling device of dimensions smaller than $0.2I_Y$. Our approximation performs well against the first-order solution of *Fiori and Dagan* [2000] at the mean plume's centroid. At the plume's fringe, where uncertainty is highest, the quality of the approximation deteriorates but it is still acceptable in applications.

[19] As a final remark, we highlight that our approximation, when used with prior knowledge, could provide useful information toward allocation of resources and data acquisition, which in turn could be used for model refinement and conditioning. This is particularly important in health risk assessment where multiple sources of uncertainty exists and characterization efforts should be prioritized [e.g., *de Barros et al.*, 2009]. Within this context, our approximate solution may serve as a preliminary tool of analysis. We favored simplicity in the mathematical expressions without compromising accuracy in the solutions for the concentration moments. We argue that in applications, the amount of uncertainty is so large that it becomes difficult to justify the use of complex models (especially in the presence of scarce data and early stages of analysis) and also to predict in great detail the concentration field.

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References

Andricevic, R., and V. Cvetkovic (1996), Evaluation of risk from contaminants migrating by groundwater, *Water Resour. Res.*, *32*(3), 611–621, doi:10.1029/95WR03530.

Bellin, A., and D. Tonina (2007), Probability density function of non-reactive solute concentration in heterogeneous porous formations, *J. Contam. Hydrol.*, *94*(1–2), 109–125, doi:10.1016/j.jconhyd.2007.05.005.

Bellin, A., Y. Rubin, and A. Rinaldo (1994), Eulerian-Lagrangian approach for modeling of flow and transport in heterogeneous geological formations, *Water Resour. Res.*, *30*(11), 2913–2924, doi:10.1029/94WR01489.

de Barros, F. P. J., Y. Rubin, and R. M. Maxwell (2009), The concept of comparative information yield curves and its application to risk-based site characterization, *Water Resour. Res.*, *45*, W06401, doi:10.1029/2008WR007324.

Fiori, A., and G. Dagan (2000), Concentration fluctuations in aquifer transport: A rigorous first-order solution and applications, *J. Contam. Hydrol.*, *45*(1–2), 139–163.

Fiorotto, V., and E. Caroni (2002), Solute concentration statistics in heterogeneous aquifers for finite Peclet values, *Transp. Porous Media*, *48*(3), 331–351.

Fitts, C. (1996), Uncertainty in deterministic groundwater transport models due to the assumption of macrodispersive mixing: Evidence from the Cape Cod (Massachusetts, USA) and Borden (Ontario, Canada) tracer tests, *J. Contam. Hydrol.*, *23*(1–2), 69–84.

Hubbard, S., and Y. Rubin (2000), Hydrogeological parameter estimation using geophysical data: A review of selected techniques, *J. Contam. Hydrol.*, *45*(1–2), 3–34.

Indelman, P., and G. Dagan (1999), Solute transport in divergent radial flow through heterogeneous porous media, *J. Fluid. Mech.*, *384*, 159–182.

Kapoor, V., and P. Kitanidis (1998), Concentration fluctuations and dilution in aquifers, *Water Resour. Res.*, *34*(5), 1181–1193, doi:10.1029/97WR03608.

Rubin, Y. (1991), Transport in heterogeneous porous media: Prediction and uncertainty, *Water Resour. Res.*, *27*(7), 1723–1738, doi:10.1029/91WR00589.

Rubin, Y. (2003), *Applied Stochastic Hydrogeology*, Oxford Univ. Press, Oxford, U. K.

Sanchez-Vila, X., A. Guadagnini, and D. Fernandez-Garcia (2009), Conditional probability density functions of concentrations for mixing-controlled reactive transport in heterogeneous aquifers, *Math. Geosci.*, *41*(3), 323–351, doi:10.1007/s11004-008-9204-2.

Tartakovsky, D., M. Dentz, and P. Lichtner (2009), Probability density functions for advective-reactive transport with uncertain reaction rates, *Water Resour. Res.*, *45*, W07414, doi:10.1029/2008WR007383.

Tonina, D., and A. Bellin (2008), Effects of pore-scale dispersion, degree of heterogeneity, sampling size, and source volume on the concentration moments of conservative solutes in heterogeneous formations, *Adv. Water Resour.*, *31*(2), 339–354, doi:10.1016/j.advwatres.2007.08.009.

van Genuchten, M., and W. Alves (1982), Analytical solutions of the one-dimensional convective-dispersive solute transport equation, *Tech. Bull. 1661*, Agric. Res. Serv., U.S. Dep. of Agric., Washington, D. C.

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