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Mean travel time of conservative solutes in randomly heterogeneous unbounded domains under mean uniform flow

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[1] We derive a closed-form expression for mean travel time of a conservative solute migrating under uniform in the mean flow conditions within an infinite stationary field with simple exponential correlation of the natural logarithm of hydraulic conductivity. Our expression is developed from a consistent second-order expansion in σ_Y (standard deviation of the log hydraulic conductivity) of the equations for moments of travel time and trajectories of conservative solutes in two-dimensional randomly nonuniform flows of *Guadagnini et al.* [2001]. As such, it is nominally valid for moderately heterogeneous fields, with $\sigma_Y^2 < 1$. Its validity for larger heterogeneity degrees is tested against numerical Monte Carlo simulations. Our results clarify the nonlinear effect in the mean travel time with respect to distance that has been observed numerically (and modeled empirically) in the literature. *INDEX TERMS:* 1829 Hydrology: Groundwater hydrology; 1832 Hydrology: Groundwater transport; 1869 Hydrology: Stochastic processes; *KEYWORDS:* contaminant travel time, solute spreading, stochastic groundwater, moment equations, random media

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1. Introduction

[2] Prediction of solute movement in groundwater is always affected by uncertainty. If, on one hand, the physics of flow and transport are known and describable by relatively simple equations, on the other hand, geologic media are ubiquitously complex and their hydraulic properties are elusive. It is therefore appropriate to think of the subsurface as being randomly heterogeneous and to cast the equations that govern groundwater flow and contaminant transport within a stochastic framework. Stochastic models drop the idea (typical of deterministic models) of calculating flow and transport parameters and state variables (hydraulic heads, flux, travel time, trajectory, etc.) and are oriented toward rendering ensemble moments of such quantities. The moments most commonly computed from such models include (conditional) mean of hydraulic heads and gradients, volumetric water fluxes and seepage velocities, solute concentrations and mass fluxes, solute particle travel time and trajectories, and plume spatial or temporal moments. First-order moments constitute unbiased predictors of system behavior and/or performance under uncertainty, while variance-covariance of the prediction errors constitutes a measure of predictive uncertainty.

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[3] Existing approaches aiming to evaluate the (ensemble) moments of solute trajectories and travel times can be essentially grouped into two categories. One method [e.g., *Matheron and de Marsily*, 1980; *Dagan*, 1984, 1987; *Indelman and Dagan*, 1999] allows evaluating the statistics of the location reached by a particle (i.e., spatial coordinates are random variables) in a (deterministically) given time, *t*. The second approach [e.g., *Cvetkovic et al.*, 1992; *Dagan et al.*, 1992; *Dagan and Indelman*, 1999; *Zhang et al.*, 2000; *Lawrence et al.*, 2002], which we pursue in this work, views both travel time *t* and the particle trajectory η as random variables and allows computing the travel time statistics for a particle starting from a given point in space and reaching a fixed location (either a point or a plane normal to the dominant mean flow direction). The first approach is preferable when one desires to produce predictions (and associated bounds of uncertainty) of contaminant trajectories (and therefore spreading) for a given time of travel, while the second approach allows obtaining important answers to the problem of estimating the time of residence of a solute particle in an aquifer.

[4] Most analytical solutions determine statistical moments of solute travel time and/or trajectory in an infinite domain under uniform mean flow [*Shapiro and Cvetkovic*, 1988; *Dagan et al.*, 1992; *Cvetkovic et al.*, 1992]. These authors assume that the velocity component in the mean flow direction is always positive and the particle does not deviate significantly from the mean flow direction. Thus

velocity and its moments are always calculated along the mean trajectory that coincides with that of a homogeneous medium (zero-order trajectory). A direct application of small perturbations for this problem leads to mean travel time becoming linear with mean travel distance. *Selroos and Cvetkovic* [1992] and *Cvetkovic et al.* [1996] observed in numerical simulations that there is a correction term close to the source that leads to a nonlinear effect. The latter authors provide an empirical relationship for the transition from near the source to far from the source behaviors. *Rajaram* [1997] provides an integral solution for the full mean travel time curve in the three-dimensional (3-D) isotropic case, which includes an integral of the velocity covariance term, obtained from a Taylor's expansion of the velocity along the mean trajectory. Finally, *Demmy et al.* [1999] show that the nonlinear effect described is due to injection as resident concentration; when, on the contrary, particles are injected proportional to flow, mean travel time becomes linear with distance.

[5] Here we start from the approach proposed by *Guadagnini et al.* [2001] for calculating mean and variance of travel time and trajectory of tracer particles in two-dimensional domains under general nonuniform mean flow and apply it to the full evaluation of the mean travel time as a function of travel distance for uniform in the mean flow conditions. The results are presented in closed form, which, to the best of our knowledge, has never before been presented. The quality of the solution is checked against numerical simulations and to the analytical limiting values already available in the literature.

2. Perturbation Solutions for Travel Time and Trajectory Moments of Conservative Solutes in Heterogeneous Media

[6] Equations for moments of travel time and trajectories of conservative solutes in bounded two-dimensional randomly nonuniform flows have been developed by *Guadagnini et al.* [2001]. For completeness, in this section we briefly outline the procedure and the results relevant to this work.

[7] We consider incompressible groundwater steady state flow that takes place in a randomly heterogeneous aquifer; the velocity $\mathbf{V}(\mathbf{x})$ at vector location $\mathbf{x}(x, y)$ is related to the hydraulic conductivity $K(\mathbf{x})$ (considered a scalar at the local scale) and to the hydraulic head $h(\mathbf{x})$ through Darcy's law:

$$\mathbf{V}(\mathbf{x}) = \frac{\mathbf{q}(\mathbf{x})}{n} = -\frac{K(\mathbf{x})}{n}\nabla h(\mathbf{x}), \tag{1}$$

where $\mathbf{q}(\mathbf{x})$ is the specific flux and n is the effective porosity. The latter is taken as a constant since it shows less variability in the space than the hydraulic conductivity [e.g., *Varljen and Shafer*, 1991]. The trajectory of a nonreactive tracer in a two-dimensional domain is given by the kinematic equation:

$$d\mathbf{x} = (dx, dy) = \left(V_x(x,y)dt, V_y(x,y)dt\right), \tag{2}$$

where $V_x(x, y)$ and $V_y(x, y)$ are the components of the velocity vector, $\mathbf{V}(\mathbf{x})$. Here we consider only the advective component of transport and disregard local dispersion.

[8] The solution of the coupled system given by equation (2) gives the position reached at time t by the particle originated from location $\mathbf{x} = \mathbf{x_0}$ at time $t = t_0$ and is given in a parametric form by

$$x = x(t, t_0); \qquad y = y(t, t_0). \tag{3}$$

Upon obtaining t as a function of x from the first of equation (3), with the assumption that $x = x(t, t_0)$ is invertible, and substituting it into the second of equation (3), we are in the position to write the explicit equation of the trajectory with respect to the y coordinate:

$$y = \eta(x, \mathbf{x_0}). \tag{4}$$

Substituting equation (4) into equation (2) we can write a differential equation for the projection of the trajectory along the x-coordinate in terms of the Lagrangian velocity, $V_x\,(x, \eta(x, \mathbf{x_0}))$, leading to

$$dt = \frac{dx}{V_x(x, \eta(x, \mathbf{x_0}))}. \tag{5}$$

Travel time, i.e., the time required for a particle leaving at point $\mathbf{x} = \mathbf{x_0}$ at time $t = t_0 = 0$ and traveling along the trajectory η to reach a point with coordinate X_1, is given by

$$t(X_1, \mathbf{x_0}) = \int_{x_0}^{X_1} \frac{1}{V_x(x,\eta)}\, dx. \tag{6}$$

Next we make use of Reynolds' decomposition and write the travel time as a sum of its (ensemble) mean $\langle t \rangle$ and a zero-mean fluctuation t', i.e., $t = \langle t \rangle + t'$, to obtain the following expression for the mean travel time that an ideal solute particle released at $\mathbf{x_0}$ takes to reach a given coordinate X_1, corresponding to a (generally random) coordinate Y_1:

$$\langle t(X_1, \mathbf{x_0}) \rangle = \int_{x_0}^{X_1} \left\langle \frac{1}{V_x(x,\eta)} \right\rangle dx. \tag{7}$$

Equation (7) is expressed in terms of $\langle 1/V_x \rangle$, evaluated along the (random) trajectory. To render these expressions workable, *Guadagnini et al.* [2001] applied Reynolds' decomposition to velocity V_x and trajectory η, and expanded velocity $V_x(x, \eta)$ around its mean trajectory, $\langle \eta \rangle = \overline{\eta}$, in Taylor's series. Upon neglecting (ensemble) moments of order larger than 2, these authors obtained approximate expressions for $\langle 1/V_x(x, \eta) \rangle$ in terms of velocity and trajectory mean and (cross) covariance. The final expression for second-order mean travel time is [*Guadagnini et al.*, 2001]

$$\begin{aligned}\langle t(X_1, \mathbf{x_0}) \rangle = \int_{x_0}^{X_1} \frac{1}{\langle V_x(x,\overline{\eta}) \rangle} \Bigg[1 - \langle \eta' D'_{1x}(x) \rangle \frac{1}{\langle V_x(x,\overline{\eta}) \rangle} \\ - \frac{\langle \eta'^2 \rangle}{2} \frac{\overline{D}_{2x}(x)}{\langle V_x(x,\overline{\eta}) \rangle} + \frac{\langle V_x'^2(x,\overline{\eta}) \rangle}{\langle V_x(x,\overline{\eta}) \rangle^2} \\ + 2\langle V_x'(x,\overline{\eta})\eta' \rangle \frac{\overline{D}_{1x}(x)}{\langle V_x(x,\overline{\eta}) \rangle^2} + \langle \eta'^2 \rangle \frac{\overline{D}_{1x}^2(x)}{\langle V_x(x,\overline{\eta}) \rangle^2} \Bigg] dx,\end{aligned} \tag{8}$$

where η' is the trajectory fluctuation and the nonlinear terms are defined as follows: $\langle V_x'^2(x, \overline{\eta})\rangle$ is the variance of Lagrangian velocity V_x, evaluated at x along the mean trajectory, $\overline{\eta}(x, \mathbf{x_0})$, followed by a tracer particle released at $\mathbf{x_0}$; $\langle \eta'^2\rangle = \langle \eta'^2(x, \mathbf{x_0})\rangle$ is the trajectory variance evaluated at location x; $\langle \eta' V_x'(x, \overline{\eta})\rangle$ is the cross covariance between V_x evaluated at point x along the mean trajectory and the trajectory evaluated at x; the expression

$$\overline{D}_{mx}(x) = \frac{\partial^m \langle V_x(x, \eta)\rangle}{\partial \eta^m}\bigg|_{\overline{\eta}}$$

($m = 1, 2$) is the mth transversal derivative of $\langle V_x\rangle$, evaluated at x along the mean trajectory $\overline{\eta}$; and the expression

$$\langle \eta' D'_{1x}(x)\rangle = \left\langle \eta' \frac{\partial V_x'(x, \eta)}{\partial \eta}\bigg|_{\overline{\eta}} \right\rangle$$

is the cross covariance between the trajectory evaluated at point x and the transversal derivative of V_x, evaluated at x along the mean trajectory $\overline{\eta}$.

[9] *Guadagnini et al.* [2001] show that all quantities in equation (8) can be expressed in terms of mean and variance-covariance of the groundwater velocity, different to the expressions for travel time moments proposed by *Shapiro and Cvetkovic* [1988] and *Dagan et al.* [1992], which contain moments of the reciprocal of a velocity. As such, the terms in equation (8) can be integrated making full use of the moment equations of steady state groundwater flow of *Guadagnini and Neuman* [1999a, 1999b], which render second-order (in σ_Y) (cross) moments of hydraulic heads and fluxes. As such, equation (8) is applicable to infinite as well as bounded domains [e.g., *Riva et al.*, 2001; *Guadagnini et al.*, 2002], is free of distributional assumptions (and so applies to both Gaussian and non-Gaussian log conductivity fields), and formally includes conditioning [*Hernandez et al.*, 2002]. A detailed derivation of equation (8) and companion expressions for travel time variance and trajectory moments are given by *Guadagnini et al.* [2001].

[10] The dependence of travel time moments on the trajectory moments evidenced in equation (8) is physically justified. The trajectory followed by a particle between two points varies in the ensemble of equally probable realizations. Moreover, since each individual realization trajectory is characterized by its own residence time, the randomness of the trajectory must influence the travel time predictor and associated estimation errors. Such dependence is not evidenced in the studies of *Shapiro and Cvetkovic* [1988], *Cvetkovic et al.* [1992], and *Dagan and Indelman* [1999], since these authors calculate the travel time along the trajectory that the particle would cover in a homogeneous isotropic conductivity field (zero-order approximation).

3. Closed-Form Solution for Mean Travel Time in Infinite Stationary Field Under Mean Uniform Flow

[11] While equation (8) could be applied to different flow configurations, we consider next mean uniform flow conditions in an infinite stationary field. At time $t = 0$, particles are injected at $x_0 = 0$, and they travel toward a crossing plane, normal to the mean flow direction, located at $X_1 = L$. Since the particle, in the mean, would not have transversal displacement, the mean trajectory is given by $\overline{\eta} = y_0$, where y_0 is the transversal initial position of the particle. In an infinite domain it is possible to set $y_0 = 0$ to evaluate the mean travel time without losing the generality of the solution, as it is independent of the particular coordinate y_0 considered. Since for mean uniform flow $\langle V_x\rangle$ is independent of location, it follows that $\bar{D}_{mx}(\boldsymbol{x}) = 0$ ($m = 1, 2$). Setting $U = \langle V_x\rangle$, and recalling that the velocity covariance tensor is stationary [e.g., *Rubin*, 1990], we can write equation (8) as

$$\langle t(X_1, \mathbf{x_0})\rangle = \langle t(L)\rangle = \int_0^L \frac{1}{U}\left[1 - \langle \eta' D'_{1x}(x)\rangle \frac{1}{U} + \frac{\langle V_x'^2(x, 0)\rangle}{U^2}\right] dx. \tag{9}$$

Shapiro and Cvetkovic [1988] provide an expression for equation (9) that does not contain the term $\langle \eta' D'_{1x}(x)\rangle$, representing the (cross) correlation between the trajectory and the derivative of the x-component of the velocity along the transversal direction. The reason is that these authors assume that V_x is independent on the transversal coordinate and therefore do not account for the randomness of the trajectory. *Dagan et al.* [1992] and *Cvetkovic et al.* [1992], using the same assumption, find that the expression of *Shapiro and Cvetkovic* [1988] is only valid for small travel distances, while for large distances a good approximation for $\langle t(L)\rangle$ can be obtained by disregarding also the last term in equation (9). In fact, we show later that what happens is that the second and third terms cancel out mutually for large distances (except for a constant value).

[12] In a 2-D isotropic medium the mean velocity U is given by [e.g., *Matheron*, 1967]

$$U = \frac{K_G J}{n}, \tag{10}$$

with K_G the geometric mean of transmissivity (or hydraulic conductivity) and J the mean gradient. The last term in equation (9) is given, e.g., by *Dagan* [1989]:

$$\frac{\langle V_x'^2(x, 0)\rangle}{U^2} = \frac{3}{8}\sigma_Y^2, \tag{11}$$

with σ_Y^2 the variance of $Y(= \ln K)$. Thus the only term to be integrated in equation (9) is the one involving the cross covariance between trajectory and derivative of velocity. We start by writing the transverse component of the trajectory in terms of velocities [*Guadagnini et al.*, 2001]:

$$\eta'(x) \equiv \eta(x) = \int_0^x \frac{V_y(x_1, \eta_1)}{V_x(x_1, \eta_1)} dx_1 = \int_0^x \frac{V_y'(x_1, \eta_1)}{U} \cdot \left[1 - \frac{V_x'(x_1, \eta_1)}{U} + \ldots\right] dx_1, \tag{12}$$

where $\eta_1 \equiv \eta(x_1)$. Taylor's expansions of the velocity fluctuations around the mean trajectory, $\overline{\eta}(x_1)$, yield

$$V_y'(x_1, \eta_1) = V_y'(x_1, \overline{\eta}_1) + \eta'(x_1) \frac{\partial V_y'(x_1, \eta)}{\partial \eta}\bigg|_{\overline{\eta}_1} + \ldots \tag{13}$$

$$V_x'(x_1, \eta_1) = V_x'(x_1, \overline{\eta}_1) + \eta'(x_1) \frac{\partial V_x'(x_1, \eta)}{\partial \eta}\bigg|_{\overline{\eta}_1} + \ldots \tag{14}$$

Using equations (12)–(14) and keeping only the terms up to second order in the expansion leads to

$$\left\langle \eta' D'_{1x}(x) \right\rangle = \frac{1}{U} \int_0^x \left\langle V'_y(x_1, \overline{\eta}_1) \frac{\partial V'_x(x,\eta)}{\partial \eta}\bigg|_{\overline{\eta}} \right\rangle dx_1$$
$$= \frac{1}{U} \int_0^x \frac{\partial}{\partial \eta} \left\langle V'_y(x_1, \overline{\eta}_1) V'_x(x,\eta) \right\rangle \Big|_{\overline{\eta}} dx_1. \tag{15}$$

The cross covariance of the velocity is given by *Rubin* [1990] for an exponential correlation model for *Y*. Using our notation we can write Rubin's expression for velocity covariance as

$$\left\langle V'_x(x,\eta) V'_y(x_1,\overline{\eta}_1) \right\rangle = U^2 \sigma_Y^2 \left\{ -\frac{r_1 r_2}{r} \left[e^{-r} \left(\frac{1}{r} + \frac{2}{r^2} + \frac{2}{r^3} \right) - \frac{2}{r^3} \right] + \frac{\beta r_1 r_2}{2} \left[\frac{4}{r^4} - \frac{72}{r^6} + e^{-r} \left(\frac{1}{r^2} + \frac{8}{r^3} + \frac{32}{r^4} + \frac{72}{r^5} + \frac{72}{r^6} \right) \right] + \frac{r_1 r_2}{2r^2} \left[e^{-r} \left(\frac{2}{r} + \frac{2}{r^2} + 1 \right) - \frac{2}{r^2} \right] \right\}, \tag{16}$$

with $r_1 = (x_1 - x)/I$, $r_2 = (\overline{\eta}_1 - \eta)/I$, $r = \sqrt{r_1^2 + r_2^2}$, $\beta = (r_1^2 - r_2^2)/r^2$, and I being the integral scale of log-hydraulic conductivity, which is assumed finite [*Rubin*, 1990]. Taking the derivative with respect to η, evaluated at $\eta = \overline{\eta}$, is equivalent to deriving with respect to r_2 and then setting $r_2 = 0$, except for a minus sign and a value of I dividing (chain rule). Therefore we get

$$\frac{\partial}{\partial \eta} \left\langle V'_y(x_1, \overline{\eta}_1) V'_x(x,\eta) \right\rangle \Big|_{\overline{\eta}} = \frac{U^2}{I} \sigma_Y^2 \left\{ e^{-r} \left(\frac{3}{r^2} + \frac{15}{r^3} + \frac{36}{r^4} + \frac{36}{r^5} \right) + \frac{3}{r^3} - \frac{36}{r^5} \right\}. \tag{17}$$

Equation (17) is now used to evaluate equation (15). Changing the integration variable to r in the integral sign, we have

$$\left\langle \eta' D'_{1x}(x) \right\rangle = U\sigma_Y^2 \int_0^{x'} \left\{ e^{-r} \left(\frac{3}{r^2} + \frac{15}{r^3} + \frac{36}{r^4} + \frac{36}{r^5} \right) + \frac{3}{r^3} - \frac{36}{r^5} \right\} dr$$
$$= U\sigma_Y^2 \left(\frac{9}{x'^4} \left(1 - e^{-x'} \right) - \frac{9}{x'^3} e^{-x'} - \frac{3}{x'^2} e^{-x'} - \frac{3}{2x'^2} + \frac{3}{8} \right), \tag{18}$$

where $x' = x/I$. Finally, we use equation (18) to evaluate in closed form one of the integrals in equation (9):

$$-\frac{1}{U^2} \int_0^L \left\langle \eta' D'_{1x}(x) \right\rangle dx = -\frac{\sigma_Y^2}{U} I \left(\frac{3}{x'^3} \left(e^{-x'} - 1 \right) + \frac{3}{x'^2} e^{-x'} + \frac{3}{2x'} - 1 + \frac{3x'}{8} \right), \tag{19}$$

where $x' = L/I$. Now, from equations (11) and (19) we can evaluate in closed form the mean travel time given by equation (9):

$$\frac{\langle t \rangle}{I/U} = x' - \sigma_Y^2 \left[\frac{3}{x'^3} \left(\exp(-x') - 1 \right) + \frac{3}{x'^2} \exp(-x') + \frac{3}{2x'} - 1 \right]. \tag{20}$$

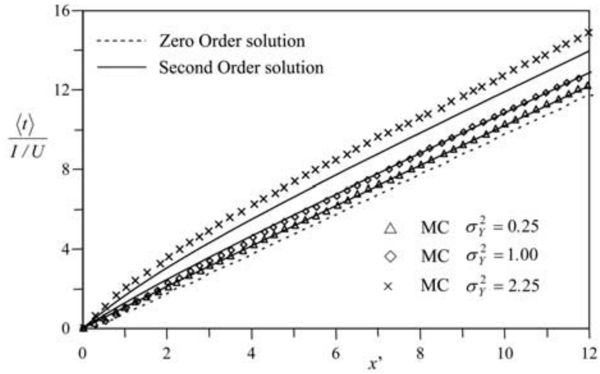

Figure 1. Normalized mean travel time as a function of dimensionless travel distance for three values of variance σ_Y^2. Monte Carlo simulations results are taken from *Cvetkovic et al.* [1996].

To check whether equation (20) is a valid solution for the mean travel time as a function of distance, we first check the limits. In the limit for $L \to 0$, we have

$$\langle t \rangle = \frac{L}{U} \left[\left(1 + \frac{3\sigma_Y^2}{8} \right) \right] + O(L^2). \tag{21}$$

Therefore for short distances, $\langle t \rangle = L/U_H$, as $U_H = U(1 + \frac{3}{8}\sigma_Y^2)^{-1}$ [*Cvetkovic et al.*, 1996].

[13] The other limit is for very long distances ($L \to \infty$). In such a case

$$\langle t \rangle \approx \frac{L}{U} \left[\left(1 + \frac{3\sigma_Y^2}{8} \right) \right] - \frac{\sigma_Y^2 I}{U} \left(\frac{3}{8} \frac{L}{I} - 1 \right) = \frac{L}{U} + \frac{\sigma_Y^2 I}{U}, \tag{22}$$

where the leading term is inversely proportional to the arithmetic mean of velocity. These two limiting cases (for small and large distances) were already found by *Dagan et al.* [1992], with the exception of the offset term we obtained in equation (22). The advantage of our formulation is that it allows obtaining the full curve. To our knowledge neither the full curve expression nor the offset term has been presented previously in the literature.

[14] In order to grasp the effect of the nonlinearity, Figure 1 depicts the normalized mean travel time given by equation (20) as a function of dimensionless travel distance for three values of the variance of log-hydraulic conductivity, $\sigma_Y^2 = 0.25$, 1, and 2.25. The results obtained from equation (20) are compared with the numerical results of *Cvetkovic et al.* [1996]. For ease of reference, the homogeneous case line is also reported. From the figure it can be noticed that equation (20) is capable of reproducing the numerical results up to $\sigma_Y^2 = 1$. The agreement with the numerical data deteriorates for larger degrees of heterogeneity, consistently with the order of approximation of the formalism. However, the maximum percentage differences between our solution and numerical Monte Carlo results are always below 15% for dimensionless distances $L/I < 4–5$ and they reduce to about 6% for $L/I > 7–8$, even for the larger variance case. This is consistent with the findings of *Guadagnini and Neuman* [1999b], who obtained good

agreement between second-order finite elements approximations of two-dimensional moment equations and numerical Monte Carlo results for at least $\sigma_Y^2 = 4$ under superimposed mean uniform and convergent steady state flows in a rectangular aquifer. Furthermore, *Riva et al.* [2001] obtained equally good agreement between second-order analytical solutions of two-dimensional moment equations and numerical Monte Carlo results for at least $\sigma_Y^2 = 1.5$ under convergent steady state flow to a well in a bounded aquifer.

4. Conclusions

[15] Our work leads to the following major conclusions.

[16] 1. We offer a closed-form expression for mean travel time of a conservative solute migrating in a mean uniform flow within an infinite stationary field with an exponential correlation model for the natural logarithm of hydraulic conductivity. Although this scenario has already been addressed in the literature, a complete expression for mean travel time as a function of the travel distance was still lacking.

[17] 2. Our solution relies on the methodology of *Guadagnini et al.* [2001], which provides the predictor and the corresponding prediction errors for the travel time of a particle migrating under (generally) nonuniform flow conditions in bounded domains. As such, it is nominally valid for moderately heterogeneous aquifers. The closed-form expression compares excellently with numerical simulations of *Cvetkovic et al.* [1996] up to unit variance of log-hydraulic conductivity, and quite satisfactorily for $\sigma_Y^2 = 2.25$. These results are in line with the findings of *Guadagnini and Neuman* [1999a, 1999b] and *Riva et al.* [2001] about the validity of moment equations in random media.

[18] 3. Our results allow rigorous demonstration of the nonlinear effect in the mean travel time with respect to distance that has been observed numerically (and modeled empirically) in the literature.

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