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Travel time and trajectory moments of conservative solutes in three dimensional heterogeneous porous media under mean uniform flow

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Abstract

We present expressions satisfied by the first statistical moments (mean and variance–covariance) of travel time and trajectory of conservative solute particles advected in a three-dimensional heterogeneous aquifer under uniform in the mean flow conditions. Closure of the model is obtained by means of a consistent second-order expansion in σ_Y (standard deviation of the log hydraulic conductivity) of (statistical) moments of quantities of interest. As such, the results obtained are nominally limited to mildly non-uniform fields, with $\sigma_Y < 1$. Resulting mean and variance of particles travel time and trajectory are functions of first and second moments and cross-moments of trajectory and velocity components. Our solution is applicable to infinite domains and is free of distributional assumptions. As an important application of the methodology we obtain closed-form expressions for the unconditional mean and variance of travel time and particle trajectory for isotropic log-conductivity domain characterized by an exponential variogram. This allows us to recover the non linear behavior of mean travel time versus distance, in agreement with numerical results published in the literature, as well as a non-linear effect in the mean trajectory. The analysis of trajectory variance allows recovering some known results regarding transverse macro-dispersion, evidencing some limitations typical of perturbation theory.

Keywords: Heterogeneous media; Travel time; Particle trajectory; Stochastic analysis; Three-dimensional media

1. Introduction

While the physics of groundwater flow and solute transport are known and describable by relatively simple equations, the parameters involved in such equations are extremely variable in space. Thus, the prediction of solute movement in groundwater is highly uncertain. The field of stochastic hydrogeology abandons the idea (typical of deterministic models) of calculating actual flow and transport state variables (hydraulic heads, flow rates, travel times, trajectories,...) and is oriented toward rendering ensemble moments of such quantities. Most of the studies in stochastic hydrogeology have been devoted to find low-order moments. First-order moments constitute unbiased predictors of the variables under study. Second-order moments (variances–covariances) can be interpreted as measures of predictive uncertainty.

There are two main categories of approaches aiming at evaluating the (ensemble) moments of solute trajectories and travel times in random media. The first one aims at obtaining the statistics of particle location at a

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(deterministically) given time, t. The second, which we pursue in this work, allows computing the travel time statistics for a particle starting from a given point in space and reaching a given discharge location. In this second approach both the travel time and the particle trajectory are viewed as random variables [5,8].

A summary of the main results available in the literature for the statistical moments of solute travel time and/or trajectory can be found in [15,16]. In these works the authors derived a fully non-linear suite of expressions to calculate mean and variance of travel time and trajectory of a conservative solute in two dimensional bounded domains under non-uniform mean flow conditions. In this Technical Note we provide an extension of this work to the three dimensional case, focusing on uniform in the mean flow conditions in unbounded domains. This simplified flow regime allows us presenting closed-form expressions for the mean and variance of travel time and the variance of transverse particle location. The resulting moments are checked against numerical simulations and to the body of analytical solutions already available in the literature.

2. Ensemble moments of solute travel time

We consider steady-state groundwater in a randomly heterogeneous aquifer. At the local scale the velocity, $\mathbf{V}(\mathbf{x})$ at vector location $\mathbf{x}(x,y,z)$, is related to hydraulic conductivity, $K(\mathbf{x})$ (considered a scalar at the local scale), and hydraulic head, $h(\mathbf{x})$ through Darcy's law:

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

where $q(\mathbf{x})$ is the specific flux and n is the effective porosity, here taken as constant. The trajectory of a conservative solute in three-dimensional domains is rendered by the kinematic equation:

$$\begin{aligned} \mathrm{d}\mathbf{x} &= (\mathrm{d}x,\ \mathrm{d}y,\ \mathrm{d}z) \\ &= (V_x(x,y,z)\,\mathrm{d}t, V_y(x,y,z)\,\mathrm{d}t, V_z(x,y,z)\,\mathrm{d}t) \\ &= \mathbf{V}(\mathbf{x})\,\mathrm{d}t \end{aligned} \tag{2}$$

Here we only consider the advective component of transport and disregard local dispersion. Therefore, all particles injected at a given point within a steady-state flow field follow the same trajectory.

The solution of the coupled system given by (2) renders 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 parametric form by

$$x = x(t,t_0); \quad y = y(t,t_0); \quad z = z(t,t_0) \tag{3}$$

From this point on we will assume that the x-coordinate is oriented along the mean flow direction, while y and z are two orthogonal coordinates, transverse to x. Upon obtaining t as a function of x from the first of (3), with the assumption that $x = x(t,t_0)$ is invertible, and substituting it into the remaining two equations, we are in a position to write the explicit equation for the trajectory:

$$\begin{cases} y = \eta(x,\mathbf{x}_0) \\ z = \zeta(x,\mathbf{x}_0) \end{cases} \tag{4}$$

Combining (4) and (2) we can write a differential equation for the projection of the trajectory along the x-coordinate in terms of the Lagrangian velocity, $V_x(x,\eta(x,\mathbf{x}_0),\zeta(x,\mathbf{x}_0))$ (in short $V_x(x,\eta,\zeta)$), leading to

$$\mathrm{d}t = \frac{\mathrm{d}x}{V_x(x,\eta,\zeta)} \tag{5}$$

The time required for a particle injected (at $t = t_0 = 0$) at $\mathbf{x} = \mathbf{x}_0$ and traveling along the trajectory to reach a point with coordinate X_1 (which is the definition of residence or *travel time*) can be expressed upon integration of (5):

$$t(X_1,\mathbf{x}_0) = \int_{x_0}^{X_1} \frac{1}{V_x(x,\eta,\zeta)}\,\mathrm{d}x \tag{6}$$

Note that, while we are fixing $x = X_1$, in general $\eta(X_1,\mathbf{x}_0)$ and $\zeta(X_1,\mathbf{x}_0)$ would be undetermined (random).

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:

$$\langle t(X_1,\mathbf{x}_0)\rangle = \int_{x_0}^{X_1} \left\langle \frac{1}{V_x(x,\eta,\zeta)}\right\rangle \mathrm{d}x \tag{7}$$

Following a procedure similar to [16] the travel time variance, σ_t^2, is given by

$$\begin{aligned} \sigma_t^2(X_1,\mathbf{x}_0) &= \langle [t'(X_1,\mathbf{x}_0)]^2\rangle \\ &= \left\langle \left[\int_{x_0}^{X_1} \left(\frac{1}{V_x(x,\eta,\zeta)} - \left\langle \frac{1}{V_x(x,\eta,\zeta)}\right\rangle\right)\mathrm{d}x\right]^2\right\rangle \end{aligned} \tag{8}$$

Eqs. (7) and (8) are expressed in terms of (the heterogeneous functions) $\langle 1/V_x\rangle$ and $1/V_x$, evaluated along the (random) particle trajectory. They offer the mean and variance of travel time that an ideal solute particle released at $\mathbf{x}_0$ takes to reach a given coordinate X_1, corresponding to (generally random) coordinates Y_1 and Z_1 (some exceptions would be, e.g., the case of flow to a single point, where Y_1 and Z_1 are deterministically known, or to a vertical draining well of negligible radius, where Y_1 is deterministic while Z_1 is random).

To render these expressions workable we applied Reynolds' decomposition to velocity V_x and particle transverse displacements, $\eta = \eta(x,\mathbf{x}_0)$ and $\zeta = \zeta(x,\mathbf{x}_0)$, and write them as the sum of their ensemble means,

$\langle V_x \rangle$, $\langle \eta \rangle$, and $\langle \zeta \rangle$, and zero-mean fluctuations, V'_x, η', ζ', respectively. This leads to

$$\frac{1}{V_x(x,\eta,\zeta)} = \frac{1}{\langle V_x(x,\eta,\zeta)\rangle + V'_x(x,\eta,\zeta)} = \frac{1}{\langle V_x(x,\eta,\zeta)\rangle}\left[1 + \frac{V'_x(x,\eta,\zeta)}{\langle V_x(x,\eta,\zeta)\rangle}\right]^{-1} \quad (9)$$

Expanding the second factor of (9) in power series, with the assumption that $|V'_x(x,\eta,\zeta)|/|\langle V_x(x,\eta,\zeta)\rangle| < 1$, and disregarding terms with powers of fluctuations larger than 2, yields

$$\frac{1}{V_x(x,\eta,\zeta)} \approx \frac{1}{\langle V_x(x,\eta,\zeta)\rangle}\left[1 - \frac{V'_x(x,\eta,\zeta)}{\langle V_x(x,\eta,\zeta)\rangle} + \frac{V'^2_x(x,\eta,\zeta)}{\langle V_x(x,\eta,\zeta)\rangle^2}\right] \quad (10)$$

Expanding $V_x(x,\eta,\zeta)$ around its mean trajectory, $[\langle \eta \rangle = \overline{\eta}; \langle \zeta \rangle = \overline{\zeta}]$, in Taylor's series and disregarding terms with powers of fluctuations larger than two leads to the following expression for the component of velocity fluctuation along x-direction (see Appendix A for details about the derivation):

$$V'_x(x,\eta,\zeta) \approx V'_x(x,\overline{\eta},\overline{\zeta}) + \eta' D'_{1\eta x}(x) + \zeta' D'_{1\zeta x}(x) - \langle \eta' D'_{1\eta x}(x)\rangle - \langle \zeta' D'_{1\zeta x}(x)\rangle \quad (11)$$

where $D'_{1nx}(x) = \frac{\partial V'_x(x,\eta,\zeta)}{\partial n}|_{\overline{\eta},\overline{\zeta}}$ $(n = \eta, \zeta)$; $\langle \eta' D'_{1\eta x}(x)\rangle$ is the cross-covariance between the transverse displacement evaluated at point x and the transverse derivative of V_x, evaluated at x along the mean trajectory $[\overline{\eta}, \overline{\zeta}]$; and, finally, $\langle \zeta' D'_{1\zeta x}(x)\rangle$ is the cross-covariance between the vertical displacement evaluated at point x and the vertical derivative of V_x, evaluated at x along the mean trajectory $[\overline{\eta}, \overline{\zeta}]$.

On the other hand, from (11) and dropping higher order terms

$$V'^2_x(x,\eta,\zeta) \approx V'^2_x(x,\overline{\eta},\overline{\zeta}) \quad (12)$$

From (10)–(12), the results presented in Appendix A, and after some expansions, we can write the final expression for the inverse of velocity:

$$\frac{1}{V_x(x,\eta,\zeta)} \approx \frac{1}{\langle V_x(x,\overline{\eta},\overline{\zeta})\rangle}[1 - N_1(x) + N_2(x)] \quad (13)$$

where

$$N_1(x) = \frac{V'_x(x,\overline{\eta},\overline{\zeta}) + \eta' D'_{1\eta x}(x) + \zeta' D'_{1\zeta x}(x)}{\langle V_x(x,\overline{\eta},\overline{\zeta})\rangle}, \qquad N_2(x) = \frac{V'^2_x(x,\overline{\eta},\overline{\zeta})}{\langle V_x(x,\overline{\eta},\overline{\zeta})\rangle^2} \quad (14)$$

Substituting (13) into (6) and disregarding powers of fluctuations larger than 2 leads to an expression for the (random) travel time. Finally, ensemble averaging yields the following expression for the mean travel time:

$$\langle t(X_1,\mathbf{x}_0)\rangle = \int_{x_0}^{X_1} \frac{1}{\langle V_x(x,\overline{\eta},\overline{\zeta})\rangle}\left[1 - \frac{\langle \eta' D'_{1\eta x}(x)\rangle}{\langle V_x(x,\overline{\eta},\overline{\zeta})\rangle} - \frac{\langle \zeta' D'_{1\zeta x}(x)\rangle}{\langle V_x(x,\overline{\eta},\overline{\zeta})\rangle} + \frac{\langle V'^2_x(x,\overline{\eta},\overline{\zeta})\rangle}{\langle V_x(x,\overline{\eta},\overline{\zeta})\rangle^2}\right] \mathrm{d}x \quad (15)$$

where $\langle V'^2_x(x,\overline{\eta},\overline{\zeta})\rangle$ is the variance of the velocity V_x, evaluated at x along the mean trajectory, $[\overline{\eta}(x,\mathbf{x}_0); \overline{\zeta}(x,\mathbf{x}_0)]$, of a tracer particle released at $\mathbf{x}_0$.

We are now in the position to write the expression of the travel time variance for a particle injected at a location of abscissa x_0 and ending at a point with abscissa X_1. After some manipulations and disregarding moments of third-order (and higher), we obtain

$$\sigma_t^2(X_1,\mathbf{x}_0) = \int_{x_0}^{X_1}\int_{x_0}^{X_1} \frac{C_{V_x}(x,\overline{\eta},\overline{\zeta},x^*,\overline{\eta}^*,\overline{\zeta}^*)}{\langle V_x(x,\overline{\eta},\overline{\zeta})\rangle^2 \langle V_x(x^*,\overline{\eta}^*,\overline{\zeta}^*)\rangle^2} \mathrm{d}x\,\mathrm{d}x^* \quad (16)$$

3. Ensemble moments of particles trajectory

From (2) and (4) the trajectory of a fluid particle in a three-dimensional steady-state flow is the solution of the following set of stochastic differential equations:

$$\frac{\mathrm{d}\eta}{\mathrm{d}x} = \frac{V_y(x,\eta,\zeta)}{V_x(x,\eta,\zeta)}; \quad \frac{\mathrm{d}\zeta}{\mathrm{d}x} = \frac{V_z(x,\eta,\zeta)}{V_x(x,\eta,\zeta)} \quad (17)$$

Eq. (17) render the transverse displacements at the generic abscissa x of the particle passing through the point $\mathbf{x}_0 \equiv (x_0, y_0, z_0)$. Taking expectation of (17) leads to the following differential equations for the mean trajectory

$$\frac{\mathrm{d}\langle \eta \rangle}{\mathrm{d}x} = \left\langle \frac{V_y(x,\eta,\zeta)}{V_x(x,\eta,\zeta)} \right\rangle; \quad \frac{\mathrm{d}\langle \zeta \rangle}{\mathrm{d}x} = \left\langle \frac{V_z(x,\eta,\zeta)}{V_x(x,\eta,\zeta)} \right\rangle, \quad (18a)$$

subject to the boundary condition

$$\langle \eta(x,\mathbf{x}_0), \zeta(x,\mathbf{x}_0)\rangle = \langle y_0, z_0\rangle; \quad x \equiv x_0, \quad (18b)$$

One should note that in some cases y_0 and z_0 are deterministically known and therefore $\langle y_0 \rangle = y_0$ and $\langle z_0 \rangle = z_0$. The general expression for the ratio between the velocity components is developed in Appendix D at second-order (in powers of fluctuations). Identifying $j = y$ in (D.4) and taking expectations, we can write the second-order approximation of the equation satisfied by the particle mean transverse displacement, $\langle \eta(x,\mathbf{x}_0)\rangle$, being

$$\frac{\mathrm{d}\langle \eta(x,\mathbf{x}_0)\rangle}{\mathrm{d}x} = \frac{\langle \eta' D'_{1\eta y}\rangle + \langle \zeta' D'_{1\zeta y}\rangle}{\langle V_x(x,\overline{\eta},\overline{\zeta})\rangle} \quad (19)$$

where $D'_{1ny} = \frac{\partial V'_y(x,\eta,\zeta)}{\partial n}|_{\overline{\eta},\overline{\zeta}}$ $(n = \eta, \zeta)$. The equation satisfied by $\frac{\mathrm{d}\langle \zeta \rangle}{\mathrm{d}x}$ is formally similar to the right-hand side of (19), just replacing $V'_y(x,\overline{\eta},\overline{\zeta})$ by $V'_z(x,\overline{\eta},\overline{\zeta})$.

Next, we develop an expression for the variance–covariance of the particle trajectory. First, we multiply (17) by the fluctuations of the trajectory at the abscissa x^*, $\eta^{*'} = \eta'(x^*, \mathbf{x}_0)$, and $\zeta^{*'} = \zeta'(x^*, \mathbf{x}_0)$, respectively. We then take expectation and obtain the following set of equations:

$$\begin{aligned}
\left\langle \eta^{*\prime} \frac{\mathrm{d}\eta}{\mathrm{d}x} \right\rangle &= \left\langle \eta^{*\prime} \frac{V_y(x,\eta,\zeta)}{V_x(x,\eta,\zeta)} \right\rangle \\
\left\langle \zeta^{*\prime} \frac{\mathrm{d}\eta}{\mathrm{d}x} \right\rangle &= \left\langle \zeta^{*\prime} \frac{V_y(x,\eta,\zeta)}{V_x(x,\eta,\zeta)} \right\rangle \\
\left\langle \eta^{*\prime} \frac{\mathrm{d}\zeta}{\mathrm{d}x} \right\rangle &= \left\langle \eta^{*\prime} \frac{V_z(x,\eta,\zeta)}{V_x(x,\eta,\zeta)} \right\rangle \\
\left\langle \zeta^{*\prime} \frac{\mathrm{d}\zeta}{\mathrm{d}x} \right\rangle &= \left\langle \zeta^{*\prime} \frac{V_z(x,\eta,\zeta)}{V_x(x,\eta,\zeta)} \right\rangle
\end{aligned} \tag{20}$$

Writing the trajectory components as the sum of their ensemble mean and fluctuation and noting that $\eta^{*\prime}$ and $\zeta^{*\prime}$ do not depend on x, the equations satisfied by the trajectory covariances, $C_{\eta\eta}(x, x^*, \mathbf{x}_0) = \langle \eta'(x, \mathbf{x}_0)\eta'(x^*, \mathbf{x}_0)\rangle$, $C_{\zeta\zeta}(x, x^*, \mathbf{x}_0) = \langle \zeta'(x, \mathbf{x}_0)\zeta'(x^*, \mathbf{x}_0)\rangle$, and $C_{\eta\zeta}(x, x^*, \mathbf{x}_0) = C_{\zeta\eta}(x, x^*, \mathbf{x}_0) = \langle \eta'(x, \mathbf{x}_0)\zeta'(x^*, \mathbf{x}_0)\rangle$, are as follows:

$$\begin{aligned}
\frac{\mathrm{d}C_{\eta\eta}(x,x^*,\mathbf{x}_0)}{\mathrm{d}x} &= \left\langle \eta^{*\prime} \frac{V_y(x,\eta,\zeta)}{V_x(x,\eta,\zeta)} \right\rangle \\
\frac{\mathrm{d}C_{\eta\zeta}(x,x^*,\mathbf{x}_0)}{\mathrm{d}x} &= \left\langle \eta^{*\prime} \frac{V_z(x,\eta,\zeta)}{V_x(x,\eta,\zeta)} \right\rangle \\
\frac{\mathrm{d}C_{\zeta\eta}(x,x^*,\mathbf{x}_0)}{\mathrm{d}x} &= \left\langle \zeta^{*\prime} \frac{V_y(x,\eta,\zeta)}{V_x(x,\eta,\zeta)} \right\rangle \\
\frac{\mathrm{d}C_{\zeta\zeta}(x,x^*,\mathbf{x}_0)}{\mathrm{d}x} &= \left\langle \zeta^{*\prime} \frac{V_z(x,\eta,\zeta)}{V_x(x,\eta,\zeta)} \right\rangle
\end{aligned} \tag{21}$$

with the set of boundary conditions

$$\left.\begin{aligned}
C_{\eta\eta}(x,x^*,\mathbf{x}_0) &= \langle y_0'\eta'(x^*,\mathbf{x}_0)\rangle = C^0_{\eta\eta} \\
C_{\eta\zeta}(x,x^*,\mathbf{x}_0) &= \langle y_0'\zeta'(x^*,\mathbf{x}_0)\rangle = C^0_{\eta\zeta} \\
C_{\zeta\eta}(x,x^*,\mathbf{x}_0) &= \langle z_0'\eta'(x^*,\mathbf{x}_0)\rangle = C^0_{\zeta\eta} \\
C_{\zeta\zeta}(x,x^*,\mathbf{x}_0) &= \langle z_0'\zeta'(x^*,\mathbf{x}_0)\rangle = C^0_{\zeta\zeta}
\end{aligned}\right\}, \quad x \equiv x_0 \tag{22}$$

If the initial location is deterministically known, then $y_0' = z_0' = 0$, and thus $C^0_{\eta\eta} = C^0_{\eta\zeta} = C^0_{\zeta\eta} = C^0_{\zeta\zeta} = 0$.

The next step is to derive analytical expressions for the equations in (21). Discarding terms of third and higher order from (21 top left) and (D.4), we can write, after some manipulations:

$$\frac{\mathrm{d}C_{\eta\eta}(x,x^*,\mathbf{x}_0)}{\mathrm{d}x} = \frac{C_{\eta V_y}(x^*,x,\mathbf{x}_0)}{\langle V_x(x,\overline{\eta},\overline{\zeta})\rangle} \tag{23}$$

where $C_{\eta V_y}(x^*, x, \mathbf{x}_0) = \langle \eta^{*\prime} V_y'(x, \overline{\eta}, \overline{\zeta})$ is the cross-covariance between η^* and $V_y(x, \overline{\eta}, \overline{\zeta})$.

Similarly, the equations satisfied by $C_{\eta\zeta}(x, x^*, \mathbf{x}_0)$, $C_{\zeta\eta}(x, x^*, \mathbf{x}_0)$, and $C_{\zeta\zeta}(x, x^*, \mathbf{x}_0)$ are

$$\frac{\mathrm{d}C_{\eta\zeta}(x,x^*,\mathbf{x}_0)}{\mathrm{d}x} = \frac{C_{\zeta V_y}(x^*,x,\mathbf{x}_0)}{\langle V_x(x,\overline{\eta},\overline{\zeta})\rangle} \tag{24}$$

$$\frac{\mathrm{d}C_{\zeta\eta}(x,x^*,\mathbf{x}_0)}{\mathrm{d}x} = \frac{C_{\eta V_z}(x^*,x,\mathbf{x}_0)}{\langle V_x(x,\overline{\eta},\overline{\zeta})\rangle} \tag{25}$$

$$\frac{\mathrm{d}C_{\zeta\zeta}(x,x^*,\mathbf{x}_0)}{\mathrm{d}x} = \frac{C_{\zeta V_z}(x^*,x,\mathbf{x}_0)}{\langle V_x(x,\overline{\eta},\overline{\zeta})\rangle} \tag{26}$$

with $C_{\zeta V_j}(x^*, x, \mathbf{x}_0) = \langle \zeta^{*\prime} V_j'(x, \overline{\eta}, \overline{\zeta})\rangle$ $(j = x, y, z)$. The corresponding trajectory variances are obtained from the covariances by taking the limit for $x^* \to x$.

These relationships allow predicting the trajectory of a particle starting from a given injection point and reaching a given location of interest, characterized by the abscissa ($x = X_1$) and (generally random) transverse coordinates ($y = Y_1$, $z = Z_1$). They also yield a measure of the uncertainty associated to such a predictor.

4. Discussion and relevance to previous work

The suite of expressions presented allows obtaining the statistics of travel time and trajectory by evaluating simple or double integrals. One should note that up to this point we have not introduced any restriction on the distributional assumptions of the various quantities involved (in particular, the equations are not restricted to multi-Gaussian log conductivity fields). This is so because they essentially rely on (cross-)moments of velocity which can be easily computed via an extension to three-dimensional space of the method proposed by [13,14,17]. Moreover, our approach can be completely integrated with the composite medium approach which allows assessing validity of perturbation approximations when dealing with highly heterogeneous material distributions [24,25]. It is also compatible with models treating aquifers as multi-modal heterogeneous formations [18].

In this section we review some of the results that can be found in the literature, while in the next one we particularize the problem to the case of a multi-log Gaussian distribution of $Y = \ln K$, with a given variogram, where analytical closed-form solutions can be obtained.

Finding the moments of travel time and/or particle trajectory in a three dimensional heterogeneous medium has been the subject of the work by several authors. In almost all cases moments are computed for given predefined mean flow conditions. The statistical moments of solute travel time in an infinite domain under uniform mean flow were initially studied by [23] and then extended by [5,10]. The simplifying hypothesis used by these authors is to substitute the actual velocity at a given point by its projection along the mean trajectory. A direct application of small perturbations for this problem leads to mean travel time becoming linear with travel distance. Numerical simulations in two-dimensions carried out by [6] show that there is a correction term close to the source that leads to a non-linear effect. In order to tackle this non-linearity at short distances, these authors provide an empirical relationship for the transition from near the source to far from the source behaviors. It was then shown [11] that the empirical expression proposed by [6] predicts the mean arrival time in three-dimensional simulations as well when particles are injected evenly in space. When, contrariwise, particles' injection is proportional to flow, mean travel time becomes linear with distance.

The impact of a finite flow domain size on solute travel time statistics for a non-reactive solute in a three-dimensional statistically isotropic porous medium under uniform mean flow conditions has been analyzed by [4] within a first-order framework.

The only works we are aware in which the authors do not project the velocity along the mean trajectory are those of [21] and [26]. In [21], the author provides an integral solution for the mean travel time as a function of distance in a three dimensional isotropic domain, under mean uniform flow conditions and for multi-Gaussian log-conductivity fields. The solution includes an integral of the velocity covariance term, obtained from a Taylor's expansion of the velocity along the mean trajectory. While [26] provides a solution of the travel time variance that formally coincides with our (16), their expression for mean travel time contains only the first term of our (15), since in their expansion for the velocity they drop second-order terms (see also Appendix A for a comment on this point).

With regard to the analysis of trajectories in heterogeneous media, Dagan [7–9] considers a mean uniform flow in an infinite domain of stationary log-conductivity and notes that the trajectory has a normal probability density function (pdf) distribution. For this flow configuration Dagan [7,9] derived closed-form expressions for longitudinal and transverse displacement variance within the classical Lagrangian framework relying upon spectral techniques for representation of velocity (cross-)moments. The assumption of stationarity is basic to the spectral analysis of random flows [3,12], since, in general, it is required for Fourier representation of random fields, such as hydraulic conductivity and hydraulic head. Furthermore, since the presence of boundary conditions renders hydraulic head statistically inhomogeneous, the spectral approach is strictly limited to infinite domains and homogeneous initial conditions. This limitation can be relaxed in some special cases by employing the so-called local stationarity hypothesis [19].

Comparison between the expression of the mean trajectory as obtained by [26] and our solution (19) evidences that both coincide at first-order. The obvious result is that the mean trajectory of a particle starting from (x_0, y_0, z_0), is always (x, y_0, z_0). If, at a given time, the particle is (randomly) located at $(y, z) \neq (y_0, z_0)$, it will eventually tend to revert (in the mean) towards $(y, z) = (y_0, z_0)$. This important feature cannot be grasped by a first-order analysis, while is highlighted by our Eq. (19).

5. Closed-form solution for multi-Gaussian log-*k* field with isotropic exponential variogram

In this section we present a direct application of our procedure. This will be used to check the validity of the approach by recovering some results from the literature and to present some new, closed-form, analytical solutions.

We consider mean uniform flow within an infinite stationary field with simple exponential variogram of the natural logarithm of hydraulic conductivity, $Y = \ln K$, with integral scale I. Without losing generality we consider injection at $\mathbf{x}_0 = 0$, while the discharge surface is a plane located perpendicular to the mean flow direction (x), and located at $X_1 = L$. Changing the notation and setting $U = \langle V_x \rangle$ (a constant value under such flow conditions), we can write (15) as:

$$\langle t(L) \rangle = \int_0^L \frac{1}{U}\left[1 - \frac{\langle \eta' D'_{1\eta x}(x)\rangle}{U} - \frac{\langle \zeta' D'_{1\zeta x}(x)\rangle}{U} + \frac{\langle V_x'^2\rangle}{U^2}\right] \mathrm{d}x \tag{27}$$

In a three dimensional infinite isotropic medium the mean velocity, U, is given by [9]

$$U = \frac{K_G \exp(\sigma_Y^2/6) J}{n} \tag{28}$$

K_G being the geometric mean of hydraulic conductivity, and J the mean gradient. The expression for the velocity variance, $\langle V_x'^2 \rangle$, that appears in (27) is constant throughout the aquifer and can be obtained from [22]. Expressions for the cross-moments between trajectory fluctuations and derivatives of velocities appearing in (27) are obtained on the basis of the expressions of velocity cross-covariances provided by [22].

After performing the corresponding integration, (27) becomes (up to second-order in σ_Y):

$$\langle t(L) \rangle = \frac{1}{U}\left[L + \sigma_Y^2 I\left(1 + \frac{24}{L_1^4}(1 - \exp(-L_1)) - \frac{24}{L_1^3}\exp(-L_1) - \frac{8}{L_1^2}\exp(-L_1) - \frac{4}{L_1^2}\right)\right] \tag{29}$$

with $L_1 = \frac{L}{I}$. Fig. 1 depicts the dependence of mean travel time on distance for different values of σ_Y^2. The following

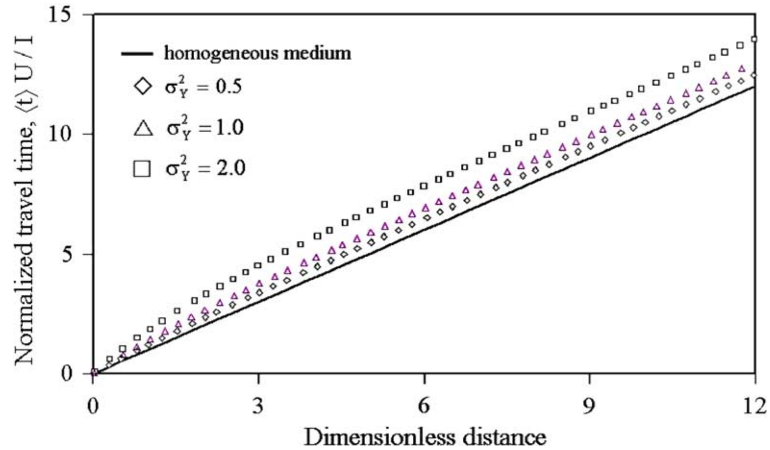

Fig. 1. Normalized mean travel time as a function of dimensionless travel distance for three values of log-conductivity variance σ_Y^2 (from Eq. 29).

expression for the mean travel time is obtained at the limit $L \to 0$:

$$\langle t(L)\rangle = \frac{L}{U}\left[1 + \frac{8}{15}\sigma_Y^2\right] = \frac{L}{U}\left[1 + \frac{\langle V_x'^2\rangle}{U^2}\right] \tag{30}$$

Therefore, for short distances $\langle t\rangle = L/U_H$, as it can be shown that up to a second-order expansion in σ_Y, $\frac{1}{U_H} = \langle\frac{1}{V}\rangle = \langle\frac{1}{U+V'(x,y,z)}\rangle = \frac{1}{U}[1+\frac{\langle V_x'^2\rangle}{U^2}]$. On the other hand, at the limit $L \to \infty$ we obtain

$$\langle t(L)\rangle = \frac{1}{U}[L + \sigma_Y^2 I] \tag{31}$$

where the leading term is inversely proportional to the arithmetic mean of velocity. Previous results in the literature [6,10,11] obtained the leading term in (31), but not the offset term, which includes the effect of heterogeneity at large distance. There is a clear physical explanation for this behavior. At short distances travel time is inversely proportional to local velocity at the injection point. Therefore, the expected value is proportional to the inverse of the harmonic mean of velocity. On the other hand, for large distances the particles locations are not correlated with the velocity at the initial location. Thus, particles tend to find the fastest paths and transport is speeded. This effect is more important as the degree of heterogeneity increases. We emphasize that the closed-form expression (29) describing the nonlinear dependence of mean travel time on distance is an original result which cannot be obtained on the basis of a first-order formalism of the kind proposed by [1] and [26], where only a linear dependence on distance can be recovered.

Now we analyze the variance of travel time. From (16), we can write

$$\sigma_t^2(L,\mathbf{x}_0) = \int_{x_0}^{L}\int_{x_0}^{L} \frac{\langle V_x'(x,0,0)V_x'(x^*,0,0)\rangle}{\langle V_x(x,0,0)\rangle^2\langle V_x(x^*,0,0)\rangle^2}\,\mathrm{d}x\,\mathrm{d}x^* = \frac{1}{U^4}\int_{x_0}^{L}\int_{x_0}^{L} C_{V_X}(x-x^*,0,0)\,\mathrm{d}x\,\mathrm{d}x^* \tag{32}$$

which is the format already provided by [5] (their equation 15). Performing the integration leads to

$$\sigma_t^2(L,\mathbf{x}_0) = \frac{\sigma_Y^2 I^2}{U^2}\left[2L_1 - \frac{16}{3} - \frac{16}{L_1^3}(1-\exp(-L_1)) + \frac{16}{L_1^2}\exp(-L_1) + \frac{8}{L_1}\right] \tag{33}$$

with the corresponding limits

$$\sigma_t^2(L,\mathbf{x}_0) = \frac{\sigma_Y^2 I}{U^2}\left(2L - \frac{16I}{3}\right) \quad \text{for } L \to \infty \tag{34}$$

$$\sigma_t^2(L,\mathbf{x}_0) = \frac{8L^2}{15U^2}\sigma_Y^2 \quad \text{for } L \to 0 \tag{35}$$

Expression (35) and the leading term in (34) were already found by [23].

As an important application, we note that solute flux statistics (mean and variance) can be expressed in terms of the probability density functions of particle travel time and transverse displacement [1]. Thus, contemplating the effect of the nonlinear dependence evidenced by (29) and making use of the closed-form solution (33) for travel time variance could be employed within the context of the work of [1] to lead to a higher order correction of solute flux moments.

In Fig. 2 we plot travel time variance as a function of travel distance. After a travel distance of 15 integral scales, the error induced by using the asymptotic value (34) rather than the actual value (33) is less than 2%. On the other hand, disregarding the offset term in (34) would entail an error close to 18% for the same travel distance (the relative error would also decrease with travel distance, but it would need over 130 integral scales to get down to 2%).

With reference to the trajectory moments, under uniform mean flow conditions in an infinite domain, equation (19) leads to the obvious result $\langle\eta(x,\mathbf{x}_0)\rangle = y_0$,

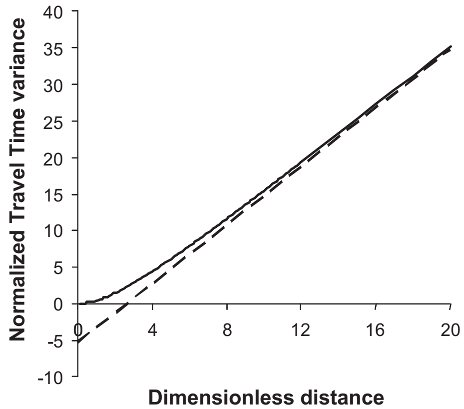

Fig. 2. Normalized travel time variance (defined as $\sigma_t^2 U^2/\sigma_Y^2 I^2$) as a function of dimensionless travel distance (L/I) (from Eq. 33) and the corresponding asymptote.

$\langle \zeta(x, \mathbf{x}_0) \rangle = z_0$, when at a given time a certain particle lies on the mean trajectory. Otherwise, if at some given time the particle has left the mean trajectory, there is a component in (19) which would force the particle to revert (in the mean) to (y_0, z_0).

The equations for the variance–covariance of the trajectory (four terms) are the following:

$$\frac{\mathrm{d}C_{\eta\eta}(x, x^*, \mathbf{x}_0)}{\mathrm{d}x} = \frac{1}{U} C_{\eta V_y}(x^*, x, \mathbf{x}_0) \tag{36}$$

where

$$\begin{aligned} C_{\eta V_y}(x^*, x, \mathbf{x}_0) &= \langle \eta *' V'_y(x_1, \overline{\eta}, \overline{\zeta}) \rangle \\ &= \frac{1}{U} \int_0^x \langle V'_y(x_1, \overline{\eta}(x_1), \overline{\zeta}(x_1)) \\ &\quad \times V'_y(x, \overline{\eta}(x), \overline{\zeta}(x)) \rangle \, \mathrm{d}x_1 \end{aligned} \tag{37}$$

Thus

$$\begin{aligned} C_{\eta\eta}(x^*, x, \mathbf{x}_0) = \frac{1}{U^2} \int_0^x \int_0^{x^*} & \langle V'_y(x_1, \overline{\eta}(x_1), \overline{\zeta}(x_1)) \\ & \times V'_y(x_2, \overline{\eta}(x_2), \overline{\zeta}(x_2)) \rangle \, \mathrm{d}x_1 \, \mathrm{d}x_2 \end{aligned} \tag{38}$$

and

$$\begin{aligned} \sigma^2_{\eta\eta}(x, \mathbf{x}_0) = \frac{1}{U^2} \int_0^x \int_0^x & \langle V'_y(x_1, \overline{\eta}(x_1), \overline{\zeta}(x_1)) \\ & \times V'_y(x_2, \overline{\eta}(x_2), \overline{\zeta}(x_2)) \rangle \, \mathrm{d}x_1 \, \mathrm{d}x_2 \end{aligned} \tag{39}$$

where $\overline{\eta}(x_1) \equiv \overline{\eta}(x_2)$ and $\overline{\zeta}(x_1) \equiv \overline{\zeta}(x_2)$. Integration of (39) leads to

$$\sigma^2_{\eta\eta}(L, \mathbf{x}_0) = 2\sigma_Y^2 I^2 \left[\frac{1}{3} - \frac{1}{L_1} + \frac{4}{L_1^3} - \exp(-L_1) \left(\frac{4}{L_1^3} + \frac{4}{L_1^2} + \frac{1}{L_1} \right) \right] \tag{40}$$

which is equal to (4.6.15) of [9], obtained by means of spectral analysis. Limiting values are recovered as

$$\sigma^2_{\eta\eta}(L, \mathbf{x}_0) = \frac{1}{15} \sigma_Y^2 L^2 \quad \text{for } L \to 0 \tag{41}$$

$$\sigma^2_{\eta\eta}(L, \mathbf{x}_0) = \frac{2}{3} \sigma_Y^2 I^2 \quad \text{for } L \to \infty \tag{42}$$

Fig. 3 is a plot of the variance of the transverse component of the trajectory. Notice that, while it reaches a plateau for large travel distance, the particle needs to travel over 60 integral scales to reach 95% of this limiting value. Fig. 4 depicts the derivative of the variance of transverse particle displacement with respect to distance. This value is usually related to the concept of macrodispersion [9]. The limiting values for the derivative of the transverse component are zero for both $L \to 0$ and $L \to \infty$, thus suggesting that transverse dispersion in three-dimensions tends to vanish for large travel distances. However, one should be aware that this specific result suffers from limitations typical of the perturbation theory used. As was first suggested by Neuman and Zhang [20,27] and recently demonstrated analytically

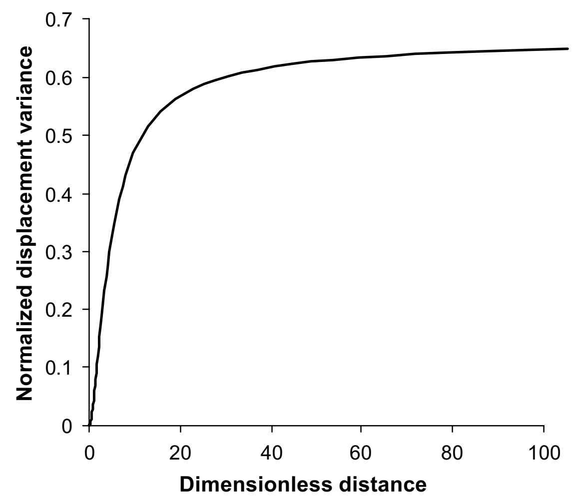

Fig. 3. Variance of the normalized transversal component of the trajectory ($\sigma^2_{\eta\eta}/\sigma_Y^2 I^2$) as a function of dimensionless distance.

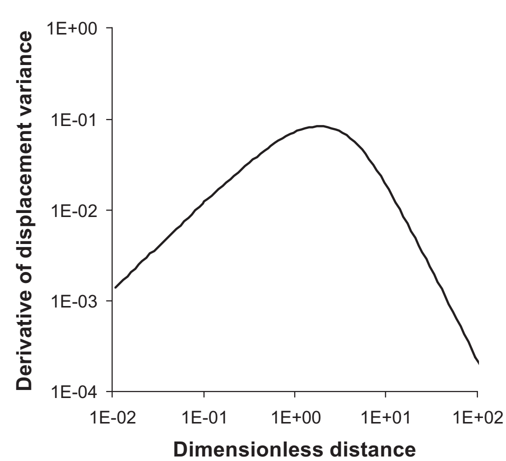

Fig. 4. Derivative of the variance of the normalized transversal component of the trajectory ($\frac{1}{\sigma_Y^2 I}\frac{\mathrm{d}\sigma^2_{\eta\eta}}{\mathrm{d}L}$) as a function of dimensionless distance.

[2], higher order contributions do not cancel out, yielding finite transverse macrodispersion coefficients in three dimensions.

The cross-variance $C_{\eta\zeta}(x, x^*, \mathbf{x}_0) = C_{\zeta\eta}(x, x^*, \mathbf{x}_0)$ is then given by

$$C_{\eta\zeta}(x^*, x, \mathbf{x}_0) = \frac{1}{U^2}\int_0^x \int_0^{x^*} \langle V'_z(x_1, \overline{\eta}(x_1), \overline{\zeta}(x_1)) \times V'_y(x_2, \overline{\eta}(x_2), \overline{\zeta}(x_2))\rangle \, \mathrm{d}x_1 \, \mathrm{d}x_2 \quad (43)$$

From [22] the cross-covariance of transversal velocities is 0 along any given line, so $C_{\eta\zeta}(x^*, x, \mathbf{x}_0) = 0$. Finally, for isotropic correlation $C_{\zeta\zeta}(x, x^*, \mathbf{x}_0) = C_{\eta\eta}(x, x^*, \mathbf{x}_0)$.

6. Conclusions

Our work leads to the following major conclusions.

1. We have presented second-order expressions for the predictor of travel time and trajectory of conservative solute particles advected in randomly heterogeneous three-dimensional infinite aquifers under uniform in the mean flow conditions. These are complemented by expressions yielding the associated prediction errors. Our solutions rely on a methodology which is free of distributional assumptions, and thus applicable to either Gaussian or non-Gaussian log hydraulic conductivity fields.
2. Direct application of the resulting expressions to a multi-Gaussian log hydraulic conductivity field with an exponential isotropic variogram allows recovering some results obtained in the literature and to present some new closed-form analytical solutions. In particular, it is possible to recover the non-linear dependence of the mean travel time on distance that has been observed in numerical simulations. Mean travel time is inversely proportional to the harmonic mean of velocity for short travel distances. For very large travel distances, mean travel time is given by the sum of (a) a term which increases with travel distance and is proportional to the inverse of the arithmetic mean of velocity, and (b) a constant term (offset) which is a function of the parameters characterizing the heterogeneity.
3. A closed-form expression for the travel time variance is also presented. The expression recovers the limiting value for short travel distances already available in the literature, and provides an additional constant term to the linear limiting value published previously. The closed-form solutions provided for travel time moments could be used to obtain higher order approximations to the solute flux approach methodology developed by [1].
4. The equations satisfied by the mean and covariance of particle trajectories are presented. The former allows us to highlight a non-linear feature of the mean trajectory conditioned to the initial position of the particle. Regarding the latter, when applied to the particular case of a multi-Gaussian log-conductivity field, the resulting expressions agree with those already available in the literature. When interpreting the large scale behavior of second-order trajectory moment and attempting to link it to the concept of transverse macro-dispersion coefficients, one should be aware that this specific result suffers from limitations typical of the perturbation theory.

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Appendix A. Ensemble mean and fluctuation of the velocity components

We decompose the j component of the velocity, $V_j(x, \eta, \zeta)$, as a sum of its ensemble mean and a zero-mean fluctuation

$$V_j(x, \eta, \zeta) = \langle V_j(x, \eta, \zeta)\rangle + V'_j(x, \eta, \zeta) \quad \text{with } \langle V'_j(x, \eta, \zeta)\rangle = 0 \quad (A.1)$$

Expanding $V_j(x, \eta, \zeta)$ in a Taylor series around the mean trajectory, $[\overline{\eta}, \overline{\zeta}]$, and disregarding the terms with power of trajectory fluctuations larger than 2, yields

$$\begin{aligned} V_j(x, \eta, \zeta) \cong{}& V_j(x, \overline{\eta}, \overline{\zeta}) + \eta' \left.\frac{\partial V_j(x, \eta, \zeta)}{\partial \eta}\right|_{\substack{\eta=\overline{\eta}\\ \zeta=\overline{\zeta}}} \\ &+ \zeta' \left.\frac{\partial V_j(x, \eta, \zeta)}{\partial \zeta}\right|_{\substack{\eta=\overline{\eta}\\ \zeta=\overline{\zeta}}} + \frac{\eta'^2}{2} \left.\frac{\partial^2 V_j(x, \eta, \zeta)}{\partial \eta^2}\right|_{\substack{\eta=\overline{\eta}\\ \zeta=\overline{\zeta}}} \\ &+ \frac{\zeta'^2}{2} \left.\frac{\partial^2 V_j(x, \eta, \zeta)}{\partial \zeta^2}\right|_{\substack{\eta=\overline{\eta}\\ \zeta=\overline{\zeta}}} + \eta'\zeta' \left.\frac{\partial^2 V_j(x, \eta, \zeta)}{\partial \eta \partial \zeta}\right|_{\substack{\eta=\overline{\eta}\\ \zeta=\overline{\zeta}}} \end{aligned} \quad (A.2)$$

Combining (A.1) and (A.2), disregarding terms with powers of velocity and trajectory fluctuations larger than 2, and setting for brevity of notation $|_{\overline{\eta},\overline{\zeta}}$ instead of $|_{\substack{\eta=\overline{\eta}\\ \zeta=\overline{\zeta}}}$, we obtain:

$$V_j(x,\eta,\zeta) \cong \langle V_j(x,\overline{\eta},\overline{\zeta})\rangle + V'_j(x,\overline{\eta},\overline{\zeta}) + \eta'\left[\left.\frac{\partial\langle V_j(x,\eta,\zeta)\rangle}{\partial\eta}\right|_{\overline{\eta},\overline{\zeta}} + \left.\frac{\partial V'_j(x,\eta,\zeta)}{\partial\eta}\right|_{\overline{\eta},\overline{\zeta}}\right] + \zeta'\left[\left.\frac{\partial\langle V_j(x,\eta,\zeta)\rangle}{\partial\zeta}\right|_{\overline{\eta},\overline{\zeta}} + \left.\frac{\partial V'_j(x,\eta,\zeta)}{\partial\zeta}\right|_{\overline{\eta},\overline{\zeta}}\right] + \frac{\eta'^2}{2}\left.\frac{\partial^2\langle V_j(x,\eta,\zeta)\rangle}{\partial\eta^2}\right|_{\overline{\eta},\overline{\zeta}} + \frac{\zeta'^2}{2}\left.\frac{\partial^2\langle V_j(x,\eta,\zeta)\rangle}{\partial\zeta^2}\right|_{\overline{\eta},\overline{\zeta}} + \eta'\zeta'\left.\frac{\partial^2\langle V_j(x,\eta,\zeta)\rangle}{\partial\eta\partial\zeta}\right|_{\overline{\eta},\overline{\zeta}} \quad (A.3)$$

It is important to notice that our (A.3) includes terms of higher order when compared to Eq. (8) of [26]. This is crucial to capture the non-linear behavior of mean travel time, as demonstrated in Section 5. Under mean uniform flow (A.3) reduces to:

$$V_j(x,\eta,\zeta) \cong \langle V_j(x,\overline{\eta},\overline{\zeta})\rangle + V'_j(x,\overline{\eta},\overline{\zeta}) + \eta'\left.\frac{\partial V'_j(x,\eta,\zeta)}{\partial\eta}\right|_{\overline{\eta},\overline{\zeta}} + \zeta'\left.\frac{\partial V'_j(x,\eta,\zeta)}{\partial\zeta}\right|_{\overline{\eta},\overline{\zeta}} \quad (A.4)$$

Taking ensemble average of (A.3), the second-order approximation of the j component of the mean Lagrangian velocity is given by

$$\langle V_j(x,\eta,\zeta)\rangle \cong \langle V_j(x,\overline{\eta},\overline{\zeta})\rangle + \langle\eta' D'_{1\eta j}(x)\rangle + \langle\zeta' D'_{1\zeta j}(x)\rangle + \frac{\langle\eta'^2\rangle}{2}\overline{D}_{2\eta j}(x) + \frac{\langle\zeta'^2\rangle}{2}\overline{D}_{2\zeta j}(x) + \langle\eta'\zeta'\rangle\overline{D}_{2\eta\zeta j}(x) \quad (A.5)$$

with

$$D'_{1nj}(x) = \left.\frac{\partial V'_j(x,\eta,\zeta)}{\partial n}\right|_{\overline{\eta},\overline{\zeta}} \quad (n=\eta,\zeta) \quad (A.6)$$

and

$$\overline{D}_{2nj}(x) = \left.\frac{\partial^2\langle V_j(x,\eta,\zeta)\rangle}{\partial n^2}\right|_{\overline{\eta},\overline{\zeta}}; \quad (n=\eta,\zeta) \quad (A.7)$$

$$\overline{D}_{2\eta\zeta j}(x) = \left.\frac{\partial^2\langle V_j(x,\eta,\zeta)\rangle}{\partial\eta\partial\zeta}\right|_{\overline{\eta},\overline{\zeta}} \quad (A.8)$$

In the case of uniform flow in the mean, (A.5) reduces to:

$$\langle V_j(x,\eta,\zeta)\rangle \cong \langle V_j(x,\overline{\eta},\overline{\zeta})\rangle + \langle\eta' D'_{1\eta j}(x)\rangle + \langle\zeta' D'_{1\zeta j}(x)\rangle \quad (A.9)$$

Substituting (A.3) and (A.5) into (A.1) yields the fluctuation component, $V'_j(x,\eta,\zeta)$:

$$V'_j(x,\eta,\zeta) \cong V'_j(x,\overline{\eta},\overline{\zeta}) + \eta'[\overline{D}_{1\eta j}(x) + D'_{1\eta j}(x)] + \zeta'[\overline{D}_{1\zeta j}(x) + D'_{1\zeta j}(x)] + \frac{\overline{D}_{2\eta j}(x)}{2} \times (\eta'^2 - \langle\eta'^2\rangle) + \frac{\overline{D}_{2\zeta j}(x)}{2}(\zeta'^2 - \langle\zeta'^2\rangle) + \overline{D}_{2\eta\zeta j}(x)(\eta'\zeta' - \langle\eta'\zeta'\rangle) - \langle\eta' D'_{1\eta j}(x)\rangle - \langle\zeta' D'_{1\zeta j}(x)\rangle \quad (A.10)$$

which, in the case of mean uniform flow, reduces to (11).

Appendix B. Velocity and trajectory cross-moments

In this Appendix we derive the equations satisfied by the cross-moment between the trajectory and the j-component of the velocity (with $j = x, y, z$), i.e. $\langle V'_j(x^*,\overline{\eta}^*,\overline{\zeta}^*)\eta'\rangle$ and $\langle V'_j(x^*,\overline{\eta}^*,\overline{\zeta}^*)\zeta'\rangle$, where $V_j(x^*,\overline{\eta}^*,\overline{\zeta}^*)$ is the j-component of the velocity evaluated along the mean trajectory at the abscissa x^*. Knowledge of these cross-moments is needed to compute the mean and variance of travel time and trajectory. Multiplying the first of (17) by the random velocity fluctuation $V'_j(x^*,\overline{\eta}^*,\overline{\zeta}^*)$ and taking ensemble average, yields:

$$\left\langle V'_j(x^*,\overline{\eta}^*,\overline{\zeta}^*)\frac{d\eta}{dx}\right\rangle = \left\langle V'_j(x^*,\overline{\eta}^*,\overline{\zeta}^*)\frac{V_y(x,\eta,\zeta)}{V_x(x,\eta,\zeta)}\right\rangle \quad (B.1)$$

Since $V'_j(x^*,\overline{\eta}^*,\overline{\zeta}^*)$ is independent from the abscissa x, the cross covariance, $C_{\eta V_j}(x,x^*,\mathbf{x}_0) = \langle\eta' V'_j(x^*,\overline{\eta}^*,\overline{\zeta}^*)\rangle$, between the transverse component of trajectory evaluated at the abscissa x and the j-component of the velocity evaluated at the abscissa x^* along the mean trajectory, satisfies the following equation:

$$\frac{dC_{\eta V_j}(x,x^*,\mathbf{x}_0)}{dx} = \left\langle V'_j(x^*,\overline{\eta}^*,\overline{\zeta}^*)\frac{V_y(x,\eta,\zeta)}{V_x(x,\eta,\zeta)}\right\rangle \quad (B.2)$$

subject to the boundary condition

$$C_{\eta V_j}(x,x^*,\mathbf{x}_0) = C^0_{\eta V_j} \quad x \equiv x_0 \quad (B.3)$$

where $C^0_{\eta V_j} = \langle y'_0 V'_j(x^*,\overline{\eta}^*)\rangle$ ($C^0_{\eta V_j} = 0$ would be zero if the position $\mathbf{x}_0$ were deterministically known (i.e.$y'_0 = z'_0 = 0$)). Substituting (D.4) into (B.2) and disregarding moments of third-and higher order, the cross-moment between transverse component of trajectory and velocity is the solution of the following differential equation:

$$\frac{dC_{\eta V_j}(x,x^*,\mathbf{x}_0)}{dx} = \frac{\langle V'_j(x^*,\overline{\eta}^*,\overline{\zeta}^*)V'_y(x,\overline{\eta},\overline{\zeta})\rangle}{\langle V_x(x,\overline{\eta},\overline{\zeta})\rangle} \quad (B.4)$$

which can be rewritten as

$$\frac{dC_{\eta V_j}(x,x^*,\mathbf{x}_0)}{dx} = \frac{C_{V_jV_y}(x^*,x,\overline{\eta}^*,\overline{\eta},\overline{\zeta}^*,\overline{\zeta})}{\langle V_x(x,\overline{\eta},\overline{\zeta})\rangle} \quad (B.5)$$

with boundary condition (B.3). Here $C_{V_jV_i}(x^*,x,\overline{\eta}^*,\overline{\eta},\overline{\zeta}^*,\overline{\zeta}) = \langle V'_j(x^*,\overline{\eta}^*,\overline{\zeta}^*)V'_i(x,\overline{\eta},\overline{\zeta})\rangle$ is the cross-covariance between the components of the velocity along j-and

i-directions, evaluated along the mean trajectory at the abscissa x^* and x, respectively.

The equation satisfied by $C_{\zeta V_j}(x, x^*, \mathbf{x}_0) = \langle \zeta' V_j'(x^*, \overline{\eta}^*, \overline{\zeta}^*) \rangle$ can be obtained upon following a similar procedure as:

$$\frac{\mathrm{d}C_{\zeta V_j}(x, x^*, \mathbf{x}_0)}{\mathrm{d}x} = \frac{C_{V_j V_z}(x^*, x, \overline{\eta}^*, \overline{\eta}, \overline{\zeta}^*, \overline{\zeta})}{\langle V_x(x, \overline{\eta}, \overline{\zeta}) \rangle} \tag{B.6}$$

subject to the boundary condition

$$C_{\zeta V_j}(x, x^*, \mathbf{x}_0) = C^0_{\zeta V_j} \quad x \equiv x_0 \tag{B.7}$$

The cross-moments at zero lag are obtained upon solving the above system and then taking the limit for $x^* \to x$, as:

$$\begin{aligned} \sigma^2_{\eta V_j}(x, \mathbf{x}_0) &= C_{\eta V_j}(x, x^* \to x, \mathbf{x}_0); \\ \sigma^2_{\zeta V_j}(x, \mathbf{x}_0) &= C_{\zeta V_j}(x, x^* \to x, \mathbf{x}_0) \end{aligned} \tag{B.8}$$

Appendix C. Cross-moment between transverse derivative of velocity and trajectory fluctuations

Here we derive the equations satisfied by the cross-moment between the trajectory and the transverse derivatives of the component of the velocity along j-direction (with $j = x,y,z$). These moments can be written in compact notation as $\langle \eta' D'_{1nj}(x^*) \rangle = \langle \eta' \frac{\partial V_j'(x^*, \eta^*, \zeta^*)}{\partial n^*} |_{\overline{\eta}^*, \overline{\zeta}^*} \rangle$, and $\langle \zeta' D'_{1nj}(x^*) \rangle = \langle \zeta' \frac{\partial V_j'(x^*, \eta^*, \zeta^*)}{\partial n^*} |_{\overline{\eta}^*, \overline{\zeta}^*} \rangle$, where $j = x,y,z$; and $n = \eta, \zeta$.

The knowledge of such quantities is crucial to calculate the predictors of travel time and trajectory. Multiplying (17) by the derivative along direction n of the random velocity fluctuation, and taking expectation yields:

$$\left\langle D'_{1nj}(x^*) \frac{\mathrm{d}\eta}{\mathrm{d}x} \right\rangle = \left\langle D'_{1nj}(x^*) \frac{V_y(x, \eta, \zeta)}{V_x(x, \eta, \zeta)} \right\rangle \tag{C.1}$$

Upon observing that $D'_{1nj}(x^*)$ is independent from the abscissa x and modeling the trajectory as the sum of a mean and a zero-mean random fluctuation, the cross-covariance $C_{\eta D_{1nj}}(x, x^*, \mathbf{x}_0) = \langle \eta' D'_{1nj}(x^*) \rangle$, between the transverse component of trajectory evaluated at the abscissa x and the derivative of the j-component of the velocity along direction n evaluated at the abscissa x^* along the mean trajectory, satisfies the following equation:

$$\frac{\mathrm{d}C_{\eta D_{1nj}}(x, x^*, \mathbf{x}_0)}{\mathrm{d}x} = \left\langle D'_{1nj}(x^*) \frac{V_y(x, \eta, \zeta)}{V_x(x, \eta, \zeta)} \right\rangle \tag{C.2}$$

with the boundary condition

$$C_{\eta D_{1nj}}(x, x^*, \mathbf{x}_0) = C^0_{\eta D_{1nj}} \quad x \equiv x_0 \tag{C.3}$$

where $C^0_{\eta D_{1nj}} = \langle y_0' D'_{1nj}(x^*) \rangle$. Again, $C^0_{\eta D_{1nj}} = 0$ if the position $\mathbf{x}_0$ is deterministically known (i.e.$y_0' = z_0' = 0$). Substituting (D.4) into (C.2) and disregarding moments of third- and higher order yields

$$\frac{\mathrm{d}C_{\eta D_{1nj}}(x, x^*, \mathbf{x}_0)}{\mathrm{d}x} = \frac{1}{\langle V_x(x, \overline{\eta}, \overline{\zeta}) \rangle} \frac{\partial C_{V_j V_y}(x^*, x, \eta^*, \eta, \zeta^*, \zeta)}{\partial n^*} \bigg|_{\overline{\eta}^*, \overline{\zeta}^*} \tag{C.4}$$

where $C_{V_j V_k}$ is the cross-covariance between j- and i-components of velocity.

The equation satisfied by $C_{\zeta D_{1nj}}(x, x^*, \mathbf{x}_0) = \langle \zeta' D'_{1nj}(x^*) \rangle = \langle \zeta' \frac{\partial V_j'(x^*, \eta^*, \zeta^*)}{\partial n^*} |_{\overline{\eta}^*, \overline{\zeta}^*} \rangle$ can be derived following a similar procedure.

Appendix D. Ratio between velocity vector components

In this Appendix we develop the expression of the ratio between the $j - (j = y, z)$ and x-component of the velocity vector. The j-component of the velocity vector is given by (A.1)

$$\begin{aligned} &V_j(x, \eta, \zeta) = \langle V_j(x, \eta, \zeta) \rangle + V_j'(x, \eta, \zeta) \\ &\quad \text{with } \langle V_j'(x, \eta, \zeta) \rangle = 0 \end{aligned} \tag{D.1}$$

From (D.1) and (13), the ratio between V_j and V_x is approximated by

$$\frac{V_j(x, \eta, \zeta)}{V_x(x, \eta, \zeta)} \approx \frac{\langle V_j(x, \eta, \zeta) \rangle + V_j'(x, \eta, \zeta)}{\langle V_x(x, \overline{\eta}, \overline{\zeta}) \rangle} [1 - N_1(x) + N_2(x)] \tag{D.2}$$

Further disregarding in (D.2) fluctuations of order larger than 2, yields:

$$\begin{aligned} \frac{V_j(x, \eta, \zeta)}{V_x(x, \eta, \zeta)} &\cong \frac{\langle V_j(x, \eta, \zeta) \rangle}{\langle V_x(x, \overline{\eta}, \overline{\zeta}) \rangle} [1 - N_1(x) + N_2(x)] \\ &\quad + \frac{V_j'(x, \eta, \zeta)}{\langle V_x(x, \overline{\eta}, \overline{\zeta}) \rangle} \left[1 - \frac{V_x'(x, \overline{\eta}, \overline{\zeta})}{\langle V_x(x, \overline{\eta}, \overline{\zeta}) \rangle} \right] \end{aligned} \tag{D.3}$$

where $N_1(x)$ and $N_2(x)$ are defined in (14).

Writing the expected value and fluctuation of V_j as in (A.4) and (A.6) respectively, and disregarding power of fluctuations larger than 2, (D.3) becomes

$$\begin{aligned} \frac{V_j(x, \eta, \zeta)}{V_x(x, \eta, \zeta)} &\cong \frac{\langle V_j(x, \overline{\eta}, \overline{\zeta}) \rangle}{\langle V_x(x, \overline{\eta}, \overline{\zeta}) \rangle} [1 - N_1(x) + N_2(x)] \\ &\quad - \frac{V_j'(x, \overline{\eta}, \overline{\zeta}) V_x'(x, \overline{\eta}, \overline{\zeta})}{\langle V_x(x, \overline{\eta}, \overline{\zeta}) \rangle^2} \\ &\quad + \left[\frac{V_j'(x, \overline{\eta}, \overline{\zeta}) + \eta' D'_{1\eta j}(x) + \zeta' D'_{1\zeta j}(x)}{\langle V_x(x, \overline{\eta}, \overline{\zeta}) \rangle} \right] \end{aligned} \tag{D.4}$$

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