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Analysis of Displacement Variances in Stochastic Nonuniform Flows by Means of a First Order Analytical Model and Comparison with Monte-Carlo Simulations

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Abstract. Flow, particle displacement and particle arrival time statistics in 2D nonuniform flows, without microdispersion, are studied both theoretically, in the framework of stochastic modelling, and numerically by means of Monte-Carlo simulations.

Turning, radial convergent and dipolar flow fields are considered. These three types of flow are numerically investigated in heterogeneous media with different levels of heterogeneity. Monte-Carlo simulations show (1) that the scale separation hypothesis, frequently used in fluid mechanics, is justified for one-point flow statistics; and (2) how displacement variances, and consequently the dispersivities defined as their spatial derivatives, depend on the type and the amplitude of flow nonuniformity: in none of the investigated cases does the assumption of scale separation hold for displacement, except in the turning flow when the spatial scale associated to the nonuniformity is much greater than the correlation scale of transmissivity.

The theoretical approach of displacement and arrival time statistics relies on the analysis of particle trajectory. Displacement variances expressions are derived by the perturbation method for each type of flow and for different approximation orders. The proposed expressions of displacement variances are, on the whole, in good agreement with the numerical results. On the other hand, the uniform flow approximation – commonly used for the interpretation of tracer experiments – chosen such as to satisfy the mean arrival time to the pumping well, gives the best prediction of the breakthrough curves.

Key words: displacement variance, dispersivity, nonuniform flow, scale separation, particle, transport, stochastic modelling, heterogeneous media.

1. Introduction

Contaminant transport in heterogeneous aquifers or single fractures is commonly modelled by an advection-diffusion-dispersion equation. In this equation, dispersivities are often implicitly assumed time- and flow-independent. The first assump-

⋆Present address: Institut de Protection et Sureté Nucléaire C.E. Fontenay-aux-Roses, DPRE/SERGD, 92265 Fontenay-aux-Roses, Cedex, France tion means that some kind of asymptotic dispersion is achieved, as it would be expected in uniform flows after a sufficient travel distance (Dagan, 1989); while the second assumption allows one to use, in a given kind of flow, the dispersivity derived from tracer experiments in another type of flow: natural gradient (uniform or non uniform), radial convergent or radial divergent, dipole, ... (Bear, 1975). In other words, these various experiments would equally account for the heterogeneity of the medium, as the obtained dispersivities would be the same.

Within the stochastic approach, different authors, among which G. Dagan and L. Gelhar proposed expressions of dispersivities based on the statistical structure of the transmissivity – or permeability – spatial distribution; see (Dagan, 1989) and (Gelhar, 1993) as general references on the subject. These expressions were derived theoretically for uniform average flows (mean head gradient constant in norm and direction) and have been validated by both field tracer experiments; see for a review (Gelhar, 1993), and Monte-Carlo numerical simulations (see for instance (Bellin *et al.*, 1992) for 2D simulations and (Chin and Wang, 1992) for 3D simulations).

According to Dagan's approach of transport stochastic modelling, based on statistics of fluid particles displacements, the dispersivity tensor of an ergodic plume is related to the statistics of particle displacement, more precisely to its autocovariance matrix. This matrix relies on the knowledge of velocity statistics (mainly its first two moments). If these statistics differ from those prevailing in uniform flow, particle position statistics, and consequently dispersivity, will surely also do. This may happen in various cases: (i) when the boundary conditions generate non-uniform mean flows (see for instance the analysis of 3D turning flows presented by Mouche *et al.* (1995)); (ii) when the plume is transported in the vicinity of deterministic hydraulic boundaries, such as imposed head or flux (Bellin *et al.*, 1992; Maugis and Mouche, 1998a), who also emphasized the influence of the nature of these boundaries); (iii) when the medium is subject to recharge (Rubin and Bellin, 1994a; Butera and Tanda, 1999); (iv) in the presence of well(s) (Maugis and Mouche, 1998b; Dagan and Indelman, 1999; Indelman and Dagan, 1999); (v) when the permeability field is not stationary (due to a linear trend (Rubin and Seong, 1994b; Indelman and Rubin, 1995; Mouche *et al.*, 1995), or to conditioning (Butera and Tanda, 1999)); etc. We have only selected some of the references accounting for velocity statistics.

If the flow-dependency of effective transmissivity has been proved nearly a decade ago by Desbarats (1992; 1993) and calculated theoretically, along with the specific flow variables statistics, by various authors (Rubin and Dagan, 1987; Indelman and Abramovitch, 1994; Indelman and Rubin, 1996; Indelman and Zlotnik, 1997; Sánchez-Vila, 1997), the question of flow-dependency of dispersivity, though object of an increasing interest, has been addressed only recently. It is of great importance as dispersivities are measured in different flow patterns, like dipole, radial convergent or uniform tests, whereas a single flow-independent dispersivity is calibrated by means of the classical advection-dispersion equation. This possibly ill-estimated dispersivity value is then used in a number of applications in water-quality management, pollution prevention, safety assessment of chemical or nuclear waste repositories, and so on. Indelman and Rubin (1996) studied analytically particle transport in a nonuniform flow field generated by a linear trend in the mean log-conductivity, and produced the corresponding modified position covariances. The nonuniformity was here a consequence of the nonstationarity of conductivity. Analytical calculation of transport variables in nonuniform flows, generated by boundary conditions in a stationary permeability field, have been published by Dagan and Indelman for two cases. They produced the position covariance in a radial divergent flow (Indelman and Dagan, 1999) and the first two moments of arrival time in a dipolar flow (a doublet composed of a pumping and a recharging well) along the direct trajectory to the pumping well (Dagan and Indelman, 1999). These results are valid for a 2D transmissivity field, yielding a stationary gaussian two-point correlation, and velocity two-point covariance equal to the one in a uniform flow, and without pore-scale dispersion. A semi-analytical solution is also given for the dipolar case without the last hypothesis and for any launch position around the injection well.

The present study takes part to this research area. It is the result of former studies undertaken a few years ago for the modelling of nuclear waste repositories. Most of the work has been published as internal CEA (Commissariat à l'Energie Atomique) reports or congress proceedings. Among these let us cite Mouche *et al.* (1995) who showed in large single realizations of 3D heterogeneous media, by spatial averaging over surfaces of same mean head gradient, under the ergodic hypothesis, how velocity mean and variances in turning flows are equal to the ones in uniform flow calculated with the local head gradient. In other words, Darcy's velocity, with respect to its mean and its variance, can be considered locally uniform. This is the zeroth order of scale separation between mean and fluctuations as classically formulated in fluid turbulence theory (Tennekes and Lumley, 1972). It suggests to investigate the extendability to two-point velocity correlation, and consequently to dispersivity, in more strongly nonuniform flows such as those created by wells. It has been shown by the authors (Maugis and Mouche, 1998a; Maugis and Mouche, 1998b) that dispersivity strongly depends both on proximity and nature (fixed-head or fixed-flux) of boundaries, and on flow nonuniformity. This latter point is detailed here.

Three types of nonuniform flow are studied: a turning flow – which can be encountered in natural situations –, a radial convergent flow and a dipolar flow – classical experimental flow fields. The heterogeneous media is assumed to be bidimensional. In a first step, the statistics of particle trajectories is analyzed theoretically and displacement variances are proposed for each type of flow. Then the flow and transport statistics are computed by Monte-Carlo simulations and theoretical displacement variances are compared to the simulated ones. Finally, arrival time statistic is computed.

2. Theoretical Framework

We consider here a heterogeneous medium, aquifer or single fracture for instance. Its log-transmissivity Y is assumed to be a stationary, gaussian, random variable, of given mean $\langle Y \rangle$, standard deviation σ_Y, exponential two-point correlation, and correlation length λ.

2.1. GENERATION OF THE NONUNIFORM FLOWS

The three investigated flow types (see Figure 1) are obtained by imposing adequate boundary conditions. Dirichlet conditions (imposed head) are applied on the outer boundaries whereas either Dirichlet or Neuman (imposed flux) conditions are applied on the inner boundaries modelling the wells. In the following, (x_1, x_2) denote the cartesian coordinates.

The turning flow is derived from a quadratic head field such that the mean velocity varies linearly with space, and its divergence is zero (there is no recharge):

$$\langle H(x_1, x_2) \rangle = H_0 - J_0 x_2 - \frac{J_0}{2L}(x_1^2 - x_2^2) + \delta x_1 x_2 \, . \tag{1}$$

Taking the non-diagonal term δ null, and under the first-order approximation detailed later, Darcy's law allows to write

$$\langle \vec{U}(x_1, x_2) \rangle = U_0 \left| \begin{array}{c} x_1/L, \\ 1 - x_2/L. \end{array} \right. \tag{2}$$

H_0, J_0 and U_0 are the values at the origin (0,0) of the mean head, the mean head gradient and the mean velocity respectively. $U_0 = -T_G J_0$ where T_G is the geometrical mean of the transmissivity. In this case, L is immediately eligible as the characteristical length of flow nonuniformity.

The radial convergent velocity field has the following expression, assuming a fully penetrating well located at the origin, of null radius, and without natural gradient:

$$\langle \vec{U}(\vec{X}) \rangle = -C \frac{\vec{X}}{X^2}, \tag{3}$$

where C is the pumping rate divided by 2π.

The dipolar velocity field is the sum of two single-well velocity fields:

$$\langle \vec{U}(\vec{X}) \rangle = C \left[\frac{\vec{X} + \vec{a}}{\| \vec{X} + \vec{a} \|^2} - \frac{\vec{X} - \vec{a}}{\| \vec{X} - \vec{a} \|^2} \right]. \tag{4}$$

The origin has been located half-way between the wells. The injection well is located at $(-a, 0)$ and the pumping well, at $(+a, 0)$. In those two latter cases: radial convergent and dipolar velocity fields, there is no characteristical length associated to flow nonuniformity, as nonuniformity increases in the vicinity of the wells.

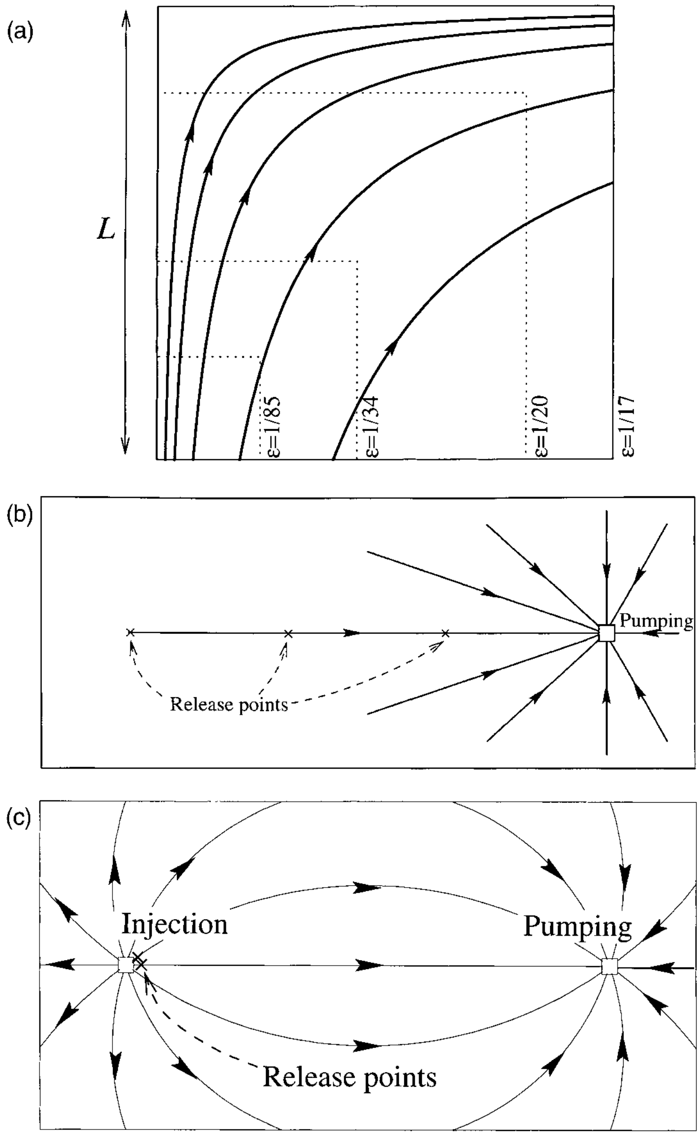

Figure 1. Sketch of the three types of flow considered in this study with the release points. (a) Turning flow, the inner windows show the studied areas according to separation scale coefficient ε; (b) single pumping; (c) dipolar pumping.

So that, if a scale was to be defined, it would depend on time as particles move away from a well or come closer to another.

2.2. DERIVATION OF PARTICLE POSITION

For each type of flow, Darcy's velocity $\vec{U}$ is expressed as the sum of its mean $\langle\vec{U}\rangle$ and its fluctuation $\vec{u}$. Similarly, the particle trajectory is described by the particle position $\vec{X}(t)$, split into its mean $\langle\vec{X}\rangle$ and its fluctuation $\vec{x}$. It is solution of the following stochastic equation:

$$\frac{\mathrm{d}\langle\vec{X}\rangle + \vec{x}}{\mathrm{d}t} = \langle\vec{U}\rangle(\langle\vec{X}\rangle + \vec{x}) + \vec{u}(\langle\vec{X}\rangle + \vec{x}). \tag{5}$$

According to Indelman and Rubin (1996), followed by Maugis, and Mouche (1998b), and under the preceding assumptions, position mean and fluctuation, at the first order in σ_Y, satisfy the following stochastic equations:

$$\frac{\mathrm{d}\langle\vec{X}\rangle}{\mathrm{d}t} = \langle\vec{U}(\langle\vec{X}(t)\rangle)\rangle, \tag{6}$$

$$\frac{\mathrm{d}\vec{x}}{\mathrm{d}t} = \vec{u}(\langle\vec{X}(t)\rangle) + [\vec{\nabla} \otimes \langle\vec{U}(\langle\vec{X}(t)\rangle)\rangle] \times \vec{x}(t), \tag{7}$$

where $\otimes$ denotes tensorial product. To obtain these expressions, Taylor expansion of $\langle\vec{U}\rangle$ and $\vec{u}$ have been processed up to order one in $\vec{x}$, but limited to the first order in fluctuations. This is why the term $[\vec{\nabla} \otimes \langle\vec{u}(\langle\vec{X}(t)\rangle)\rangle] \times \vec{x}(t)$, that should have normally appeared in both Equations (6) and (7), has been neglected in (6). Mean and fluctuation of $\vec{X}$ have then been identified.

Let us consider the spatial scales in Equations (6) and (7): $\vec{x}$ is scaled by λ, and the gradient by $1/L$, where L would be the local flow characteristical length. The Taylor expansion of mean Darcy's velocity is consequently limited to the first order of scale separation, with the scale separation gauge $\varepsilon = \lambda/L$. This second term, $\vec{\nabla}\otimes\langle\vec{U}(\langle\vec{X}(t)\rangle)\rangle$ describes the influence on the particle position fluctuation of the mean velocity variation along the mean trajectory. It vanishes under the zeroth order of scale separation approximation. The first order development may or may not be sufficient to account for highly nonuniform flow such as those generated by wells.

This ε expansion is classical in problems with two scales such as those encountered classically in fluid mechanics or other fields (Cole and Kevorkian, 1981).

In the following, velocity mean $\langle\vec{U}\rangle$ and fluctuations $\vec{u}$ are approximated to their first order terms in their expansion in powers of σ_Y (see Appendix A for a detailed derivation of velocity mean and fluctuation in uniform flows):

$$\begin{aligned}\langle\vec{U}\rangle &\simeq -T_G\vec{\nabla}\langle H\rangle,\\ \vec{u} &\simeq -T_G(y\vec{\nabla}\langle H\rangle + \vec{\nabla}h),\end{aligned} \tag{8}$$

where H, $\langle H\rangle$ and h are respectively the hydraulic head, its mean and its fluctuation. $\langle\vec{U}\rangle$ is therefore equal to the velocity that would prevail if the aquifer was homogeneous. This assumption is justified in a 2D uniform flow, for which it has been shown that the first-and second-order terms in the expansion of $\langle\vec{U}\rangle$ in powers of σ_Y are null (Grenier, 1996). The approximation materialized by Equation (8) degenerates to order zero in nonuniform flows, because the non-zeroth-order terms are not null anymore (see Appendix A). Nevertheless, it will prove itself sufficient in the frame of this paper.

Equations (6) and (7) can be solved analytically for the three aforementioned types of flow (see Appendix B). The displacement variances are found to be:

$$\langle x_i(s)x_j(s)\rangle = \iint_{s',s''=0}^{s} u^*_{ij}(s',s'')f_{ij}(s,s',s'')\,\mathrm{d}s'\,\mathrm{d}s'', \tag{9}$$

where the dimensionless velocity fluctuation covariance reads

$$u^*_{ij}(s',s'') = \frac{\langle u_i(s')u_j(s'')\rangle}{\|\langle\vec{U}(s')\rangle\|\|\langle\vec{U}(s'')\rangle\|}, \tag{10}$$

where the curvilinear abscissa along the mean trajectory s is equivalent to time with the convention $f(s(t)) = f(\langle\vec{X}(t)\rangle)$, and

$$f_{11} = \frac{g(s')}{g(s)}\frac{g(s'')}{g(s)}, \qquad f_{22} = \frac{g(s)}{g(s')}\frac{g(s)}{g(s'')}, \qquad f_{12} = \frac{g(s')}{g(s'')}, \tag{11}$$

where the function g is defined as follows:

$$\begin{aligned} g(s) &= 1, && \text{for the uniform flow,}\\ g(s) &= \exp(U_0 t(s)/L), && \text{for the quadratic turning flow,}\\ g(s) &= R_0 - s, && \text{for the radial convergent flow,}\\ g(s) &= (s+r_w)(D-s-r_w), && \text{for the dipolar flow.} \end{aligned} \tag{12}$$

R_0 is the distance between the pumping well, located at the origin, and the initial position of the particle, D is the distance between the pumping well and the injection well, with the origin located at the center of the dipole, and r_w is the well radius. In the two cases involving wells, the axis X_1 is aligned with the mean trajectory. In the dipolar flow case, only the mean trajectory along the dipole axis is considered. The function g accounts for the second term on the right hand side of Equation (7), that is for the flow nonuniformity on the position fluctuation. These expressions complete those given by Dagan and Indelman (Dagan and Indelman, 1999; Indelman and Dagan, 1999) who focused on the longitudinal spreading in radial divergent and dipolar flows.

In order to compute the displacement variances for each type of flow the normalized velocity covariance u^*_{ij} (10) must be known. We shall assume, as previous studies suggest (Mouche *et al.*, 1995; Fiori *et al.*, 1998) that the velocity fluctuation is the product of mean Darcy's velocity by a second order stationary random function. The normalized velocity covariances may then be taken equal to the ones in uniform flow (Rubin, 1990). Thus, the normalized covariance does not depend on the flow and is a function of the absolute distance $|s' - s''|$ only. This assumption has been shown to be wrong (Indelman and Dagan, 1999; Butera and Tanda, 1999), but does not necessarily introduce great error. Nevertheless, Equation (9) shows that the flow-dependence of dispersivity does not come solely from the variation in velocity statistics due to discrepancies of the flow from uniformity, but also from the shape of the mean trajectory through the f_{ij} functions.

2.3. DISPERSIVITY IN NONUNIFORM FLOWS

The definition of dispersivity is problematic in nonuniform flows. From a general point of view, it accounts, at a given scale, for the influence of lower scale variability on plume spreading. Macrodispersivity – (Indelman and Dagan, 1999) call it *equivalent dispersivity* – is practically used in an eulerian transport equation (written here without microdispersion nor diffusion, and with porosity equal to unity):

$$\frac{\partial C}{\partial t} + \operatorname{div}(C\vec{U} + (\overline{\overline{\alpha}}_{\text{eq.}}|\vec{U}|)\vec{\nabla}C) = 0. \tag{13}$$

This dispersivity describes the spatial spreading of a plume, and any discrepancy from a diffusive spreading is ignored. Backward spreading, as (De Marsily, 1981) pointed out, is one of the artifacts that might arise. Moreover, even if $\alpha_{\text{eq.}}$ is allowed to vary with the plume position, it is not obvious why dispersion at short times, near boundaries and near wells should be equivalent to diffusion. Another definition of dispersivity if used, based on the stochastic approach. The *apparent dispersivity* (named after (Indelman and Dagan, 1999)) is derived from the ensemble position variances by the relationship

$$\overline{\overline{\alpha}}_{\text{app.}}(s) = \frac{1}{2}\frac{\partial\langle\vec{x}\otimes\vec{x}\rangle}{\partial s}(s). \tag{14}$$

Only gaussian position statistics are completely described by apparent dispersivity. As soon as the plume is not gaussian, and this is the case at short times and near boundaries, the knowledge of higher order moments is necessary to describe properly the position statistics (CEA internal report 1997). Let us emphasize that the gaussianity of a plume may never be reached, or reached hypothetically at ranges too long to be of interest, as it may be the case in unsaturated media (Padilla *et al.*, 1999). Non-ergodicity in transport results in inequality between equivalent and apparent dispersivities. Therefore, to avoid mis-definitions in dispersivity, calculations and results presented here will rather focus on particle position variance.

3. Monte-Carlo Simulations

The Monte-Carlo simulations have been performed with the multi-purpose finite element code CASTEM2000, currently developed at the CEA (CASTEM2000, 1997). Darcy's velocity fields are computed using a mixed hybrid finite element method (Chavent and Jaffré, 1986). This method, which solves simultaneously

Darcy and mass balance equations, respects local mass conservation; see Mosé *et al.* (1993) for the application of this formulation to hydrogeology. The Log-transmissivity fields are generated either with the matrix decomposition method or with the turning band method (Christakos, 1992). The mesh size is $\delta x = \lambda/4$ or $\delta x = \lambda/5$, depending on the studied case. The number of realizations depends on σ_Y: 800, 1000, 1500, 2000 for $\sigma_Y = 0.1, 0.5, 1.0, 1.5$ respectively. Trajectories are computed by particle tracking. The computed quantities are the one-point flow statistics, the mean trajectory and the displacement variances, and, finally, the arrival time probability density function. For each flow condition, three transport models have been tested: (i) 'uniform flow model' describing transport in a mean uniform flow where Darcy's velocity honors the mean arrival time and position (Lenda and Zuber, 1970): the trajectory is approximated by a straight line traveled at a constant velocity; (ii) 'order zero model' describing transport in a locally uniform mean flow: the trajectory is the zeroth-order mean trajectory, and $\langle \vec{U} \rangle$ is assumed to be constant in the neighborhood of any point of the mean trajectory. This is the zeroth order of the scale separation hypothesis: the ε expansion of Equation (6) is limited to its first term and the $g(s)$ function in Equation (12) is equal to unity; (iii) 'order one model' or the model proposed above: the trajectory is the zeroth-order mean trajectory, and $\langle \vec{U} \rangle$ is assumed to vary linearly with space in the vicinity of any given point of the trajectory.

Simulations of the turning flow have been performed on a 17λ square domain by imposing the trace of the quadratic head field along the domain border. Different particle starting positions have been considered and three degrees of nonuniformity have been studied: $\varepsilon = \lambda/L = 1/85$, $1/34$, $1/20$. Figure 2 shows realizations of particle trajectories for a given starting position, and the three values of ε. Simulations of the radial convergent flow have been performed on a rectangular domain of $40\lambda \times 16\lambda$ extent by imposing the trace of the radial head field, associated to the homogeneous media, on the domain border. Three starting particle positions have been considered, $R_0 = 10\lambda$, 20λ, 30λ, and the flow is imposed either by a fixed draw-down or a fixed flow rate. Simulations of the dipolar flow are performed in identical conditions. Distance between pumping and injection wells is 30λ.

It must be said that the domain extent have been chosen wide enough so that the plumes remain at a certain distance from the borders. However, it has been proved that the head boundary conditions influence transport whatever their distance from the plume (Maugis and Mouche, 1998a). Keeping in mind our computer resources, the dimensions of the mesh have been optimized with respect to this problem.

3.1. FLOW STATISTICS

Monte-Carlo simulations show that, for the three considered types of flow, means and variances of head and Darcy's velocity verify the zeroth order scale separation

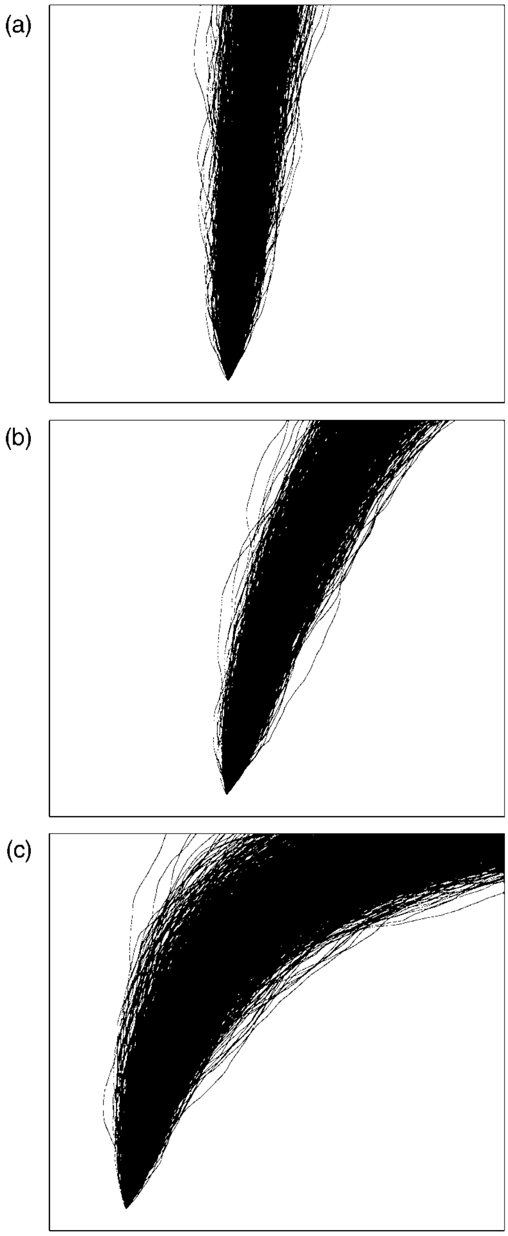

Figure 2. Plumes generated by Monte-Carlo simulations in the turning flow fields. (a) $\varepsilon = 1/85$; (b) $\varepsilon = 1/34$; (c) $\varepsilon = 1/20$.

assumption: they can be calculated with the uniform flow theory by use of the local head gradient, neglecting the spatial variation of this gradient. For instance, velocity variances may be written as:

$$u_{11}(\vec{x}) \;=\; \tfrac{3}{8}\sigma_y^2\langle\vec{U}(\vec{x})\rangle^2, \tag{15}$$

$$u_{22}(\vec{x}) = \frac{1}{8}\sigma_y^2 \langle \vec{U}(\vec{x}) \rangle^2, \tag{16}$$

$$u_{12}(\vec{x}) = 0. \tag{17}$$

Velocity means and variances along the two axis are shown in the radial convergent case on Figures 3 and 4 and in the dipolar case on Figures 5 and 6. The influence of the type of boundary condition imposed at the wells is clear: An imposed head at the well boundary increases the longitudinal velocity variance much more than in the case where flux is imposed (Figures 3(c) and 5(c)). Moreover, it is a long range increase. This is in agreement with the fact that an imposed head boundary condition has much more effect on the flow statistics than an imposed flux (Maugis and Mouche, 1998a). A similar influence of the boundary type on the head field has been previously described by (Rubin and Dagan, 1988, 1989).

3.2. POSITION STATISTICS

The variation of mean position with time appears to be perfectly predicted by Equation (6), whatever the flow field and the values of σ_Y, thus validating the zeroth-order approximation of mean velocity used for the establishment of Equation (8). This result is not surprising and is therefore not figured. As a consequence, the calculated variances will not be biased by erroneous means.

Figure 2 gives an idea of the level of nonuniformity pertaining to the different values of ε. There are no major differences between the three flow models (uniform flow, zeroth and first order of scale separation) in the estimate of the displacement variances in the turning flow when $\varepsilon = 1/85$. All models are good because the flow nonuniformity is very weak. These results are therefore not represented here. At higher nonuniformity ($\varepsilon = 1/34$), both uniform flow assumption and order zero model fail to predict the particle positions moments X_{ij} (Figures 7(a) and (b)), save for X_{12} where the order 0 model is enough to correctly predicts its spatial evolution (Figure 7(c)). In all of these three cases, the order one model gives a fair fit. If the nonuniformity increases again to reach $\varepsilon = 1/20$ (see Figures 7(d) and 7(e)), the order one model – though it gives the best predictions – is not valid anymore. This suggests that higher order terms must be taken into account to properly estimate X_{11} and X_{22}. It is however surprising how the position cross-covariance X_{12} seems not to depend upon these optional terms (see Figure 7(f)).

In the radial convergent flow, the first order model gives a remarkable fit to the simulated position variance, whatever the distance of the release point (see Figures 8(a) and 8(b)). It accounts both for the lengthening of the plume and for the annulation of its lateral extension at the pumping well; although the validity of the simulations fails too early – in terms of the number of particles remaining in the domain – to assess it with certainty. This is of tremendous importance because the assumption of velocity correlation being equal to the one in uniform flows – and, consequently being stationary – is confirmed; at least for the studied values of σ_y (0.2, 0.5 and 1). In this case as in the next one, the uniform flow model and

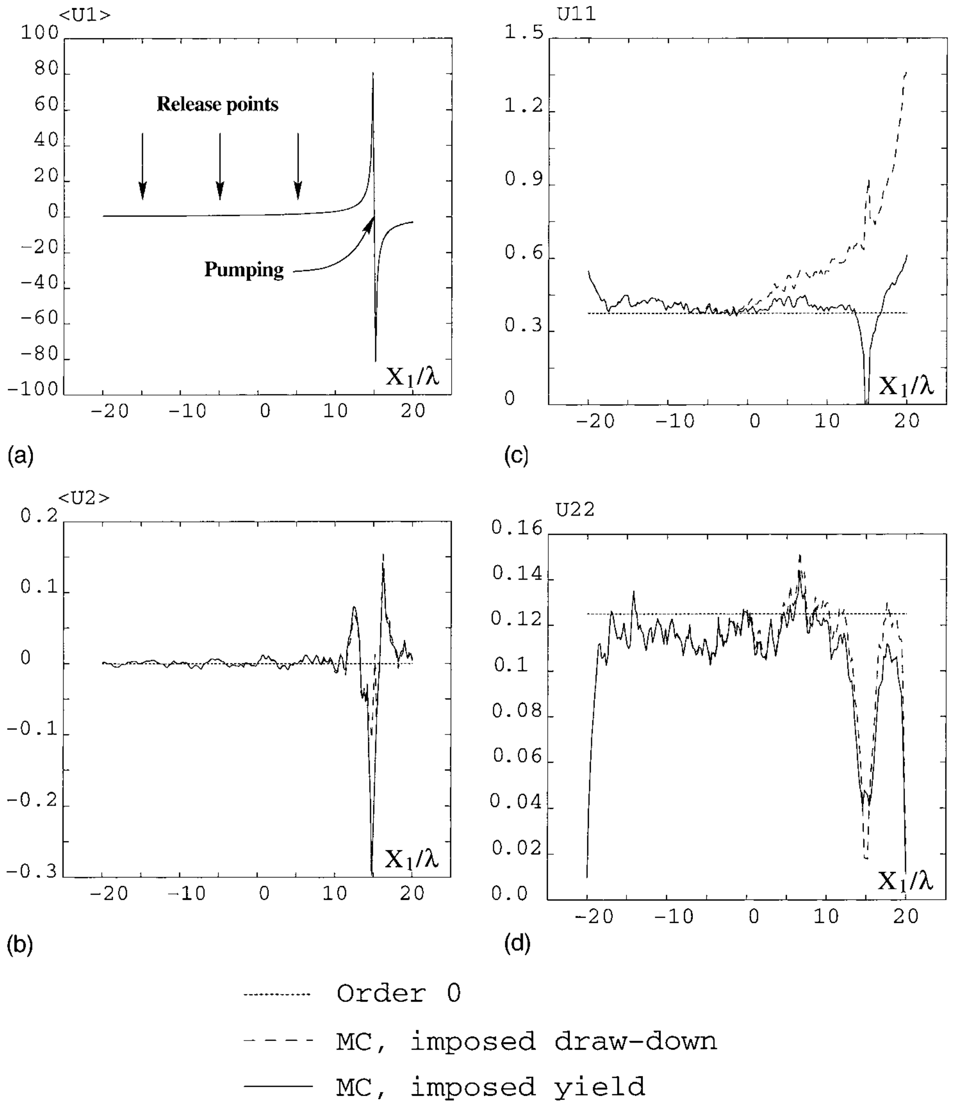

Figure 3. Radial convergent flow: First and second normalized moments of Darcy's velocity along axis one ($x_2 = 0$). Notation: $U = \| \langle \vec{U} \rangle \|$, $\langle U_i \rangle \equiv \langle U_i \rangle / U$ and $u_{ii} \equiv u_{ii}/U^2\sigma_y^2$. The release points are situated on the axis 1, at the coordinates shown by the arrows on Figure (a). (a) Mean longitudinal velocity; (b) mean transverse velocity; (c) longitudinal velocity variance; (d) transverse velocity variance.

the order zero model give identical results along the axis because the order zero model takes into account the variation in velocity orientation only. The simulated longitudinal dispersivity, given by Equation (14), is approximatively three times greater than the value given by the uniform flow model after a 15 λ mean travel. Moreover, the nature of the boundary condition at the pumping well has no visible influence on dispersion.

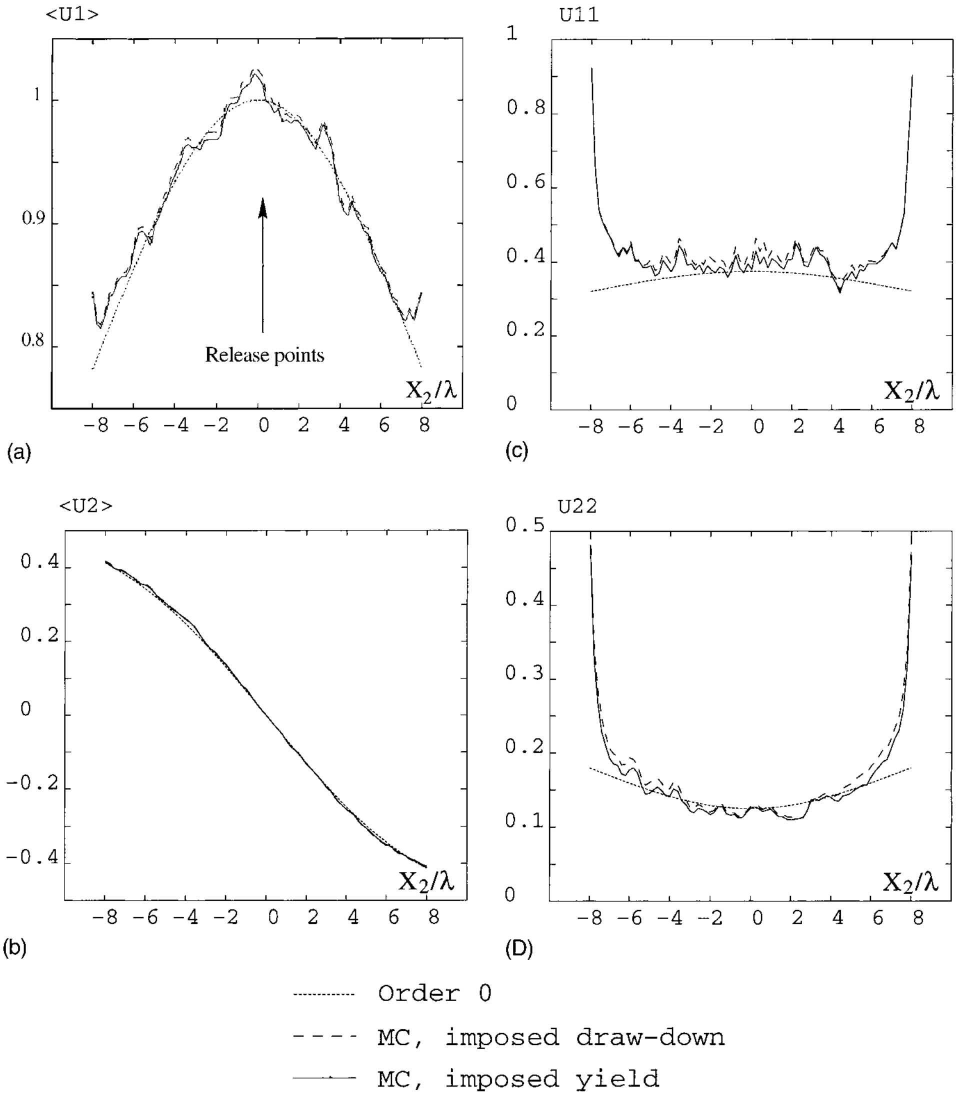

Figure 4. Radial convergent flow: First and second normalized moments of Darcy's velocity along axis two ($x_1 = 0$). Notation : $U = \| \langle \vec{U} \rangle \|$, $\langle U_i \rangle \equiv \langle U_i \rangle / U$ and $u_{ii} \equiv u_{ii}/U^2\sigma_y^2$. Contrary to what Figure (a) might suggest, the release points are situated at different abscissa upstream of the axis 2. (a) Mean longitudinal velocity; (b) mean transverse velocity; (c) longitudinal velocity variance; (d) transverse velocity variance.

The release of a tracer on the closest point of the axis to the injection well in the dipolar flow field yields a longitudinal position variance significantly lower than with the pumping well alone, by a factor of about 2 (Figure 8(c)). On the other hand, transverse dispersion is nearly one order of magnitude higher (Figure 8(d)). This latter point is easily explained by the diverging nature of the flow in the injection half-plane. The former is probably a compensation of the latter: particles

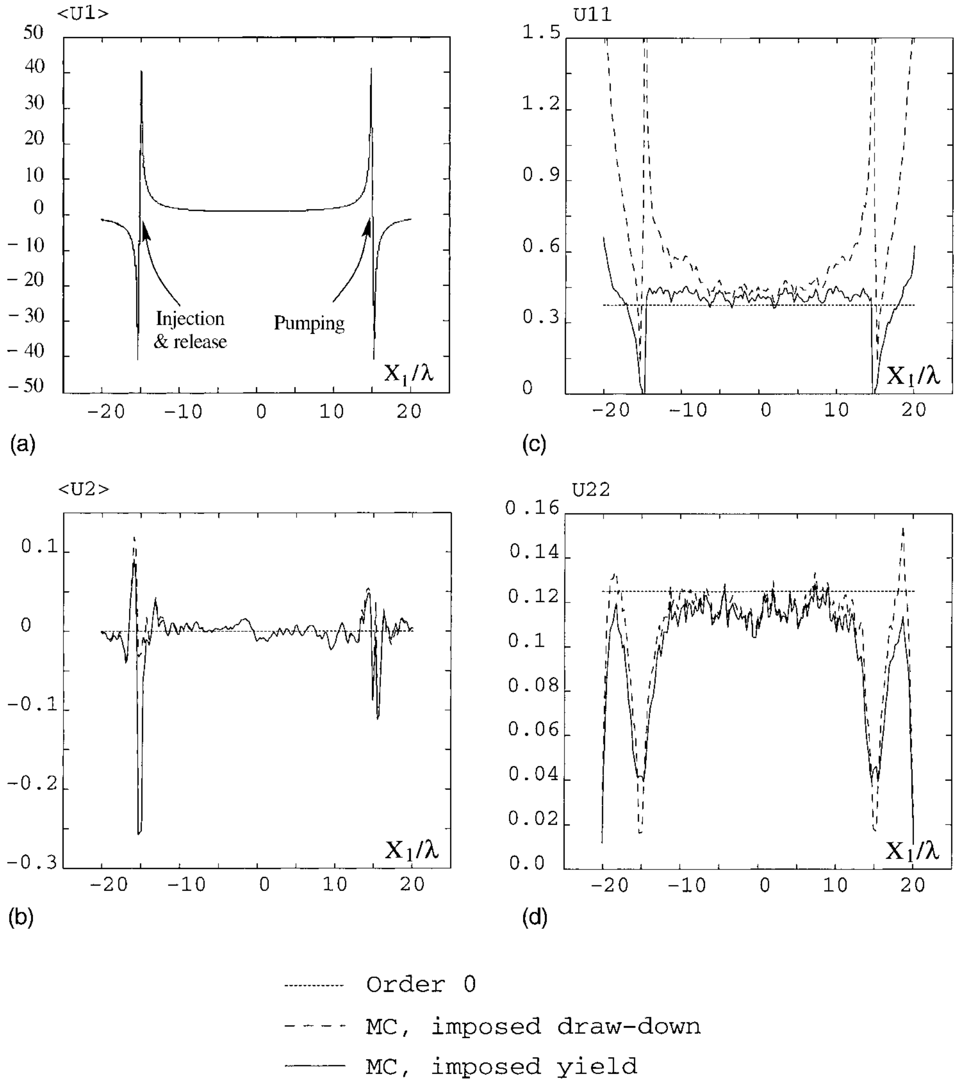

Figure 5. Dipolar flow: First and second normalized moments of Darcy's velocity along axis one ($x_2 = 0$). Notation : $U = \| \langle \vec{U} \rangle \|$, $\langle U_i \rangle \equiv \langle U_i \rangle / U$ and $u_{ii} \equiv u_{ii}/U^2\sigma_y^2$. The release point is situated on the axis 1, on the direct line to the pumping well, as illustrated by the arrow on Figure (a). (a) Mean longitudinal velocity; (b) mean transverse velocity; (c) longitudinal velocity variance; (d) transverse velocity variance.

spreading laterally encounter slower velocities oriented more transversally than along the mean trajectory. Displacement along axis 1 is thus partially lowered by displacement along the other axis. In the second half of the flow field, pumping flow field, flow becomes converging again, and, as in the single well situation, transverse position variance shows a clear tendency to tend to zero, although the quality of the simulation vanishes before. The order one model fits well the variance of the

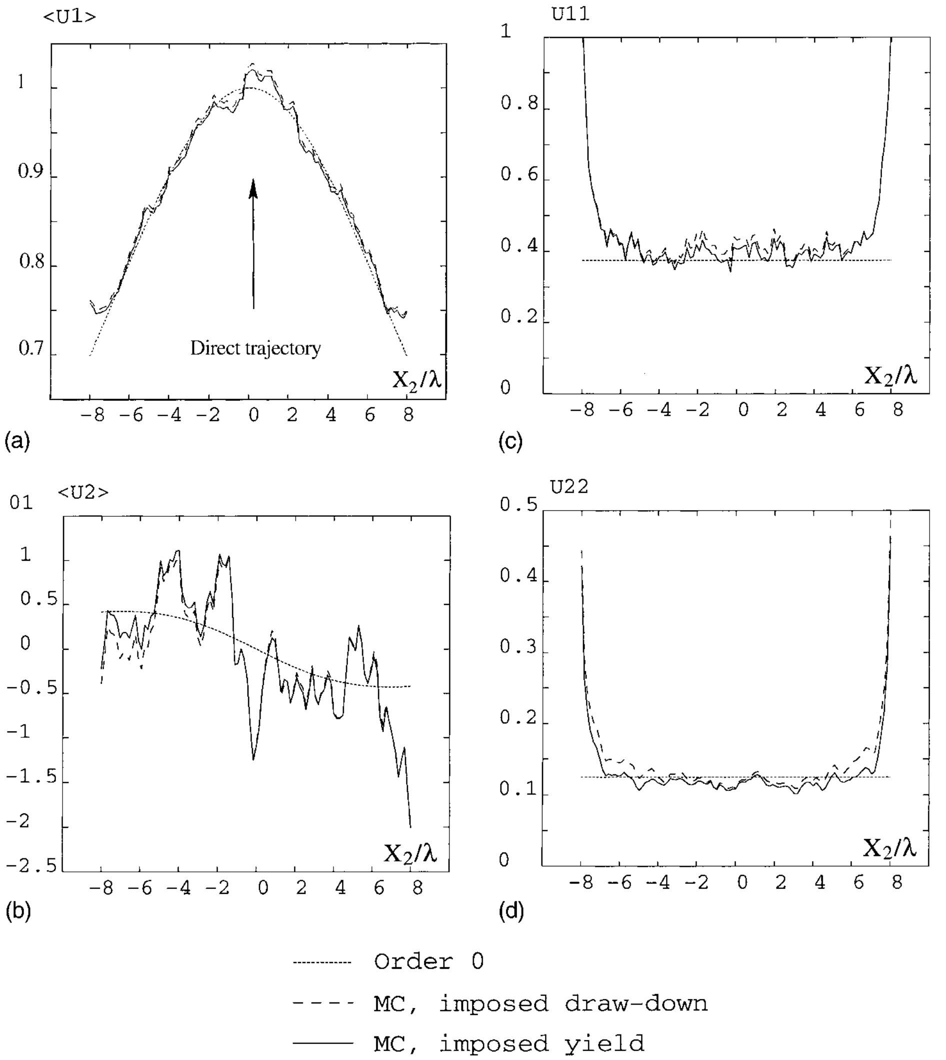

Figure 6. Dipolar flow: First and second normalized moments of Darcy's velocity along axis two ($x_1 = 0$). Notation : $U = \| \langle \vec{U} \rangle \|$, $\langle U_i \rangle \equiv \langle U_i \rangle / U$ and $u_{ii} \equiv u_{ii}/U^2\sigma_y^2$. The direct trajectory is along the axis 1 (see Figure (a)). (a) Mean longitudinal velocity; (b) mean transverse velocity; (c) longitudinal velocity variance; (d) transverse velocity variance.

longitudinal displacement, but fails to predict correctly the transverse spreading. It is interesting to notice how transverse dispersion depends on the injection boundary type (both wells are of same boundary type, but it has been seen above that the nature of the pumping well had little impact on dispersion), by a factor of 2; imposed-head condition at the injection well producing a wider dispersion than imposed-flux condition.

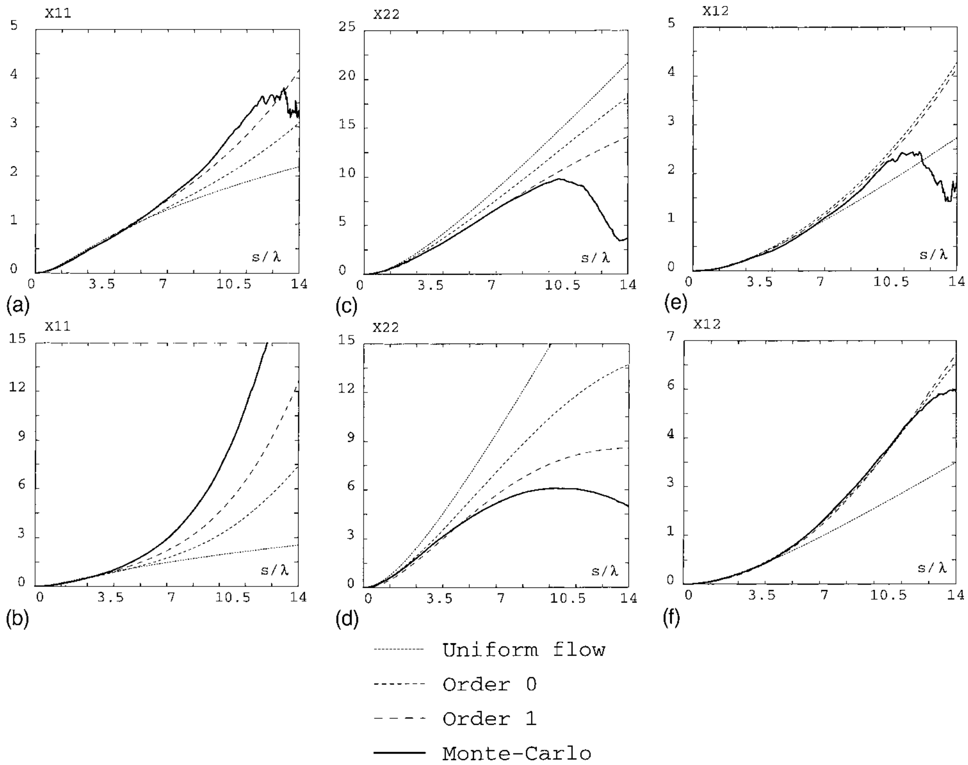

Figure 7. Normalized displacement variances, $X_{ii} \equiv X_{ii}/\sigma_Y^2\lambda^2$, as functions of the dimensionless curvilinear abcissa, for the turning flows. $\sigma_Y = 0.5$. (a) X_{11}, turning flow ($\varepsilon = 1/34$); (d) X_{11}, turning flow ($\varepsilon = 1/20$); (b) X_{22}, turning flow ($\varepsilon = 1/34$); (e) X_{22}, turning flow ($\varepsilon = 1/20$); (c) X_{12}, turning flow ($\varepsilon = 1/34$); (f) X_{12}, turning flow ($\varepsilon = 1/20$).

3.3. BREAKTHROUGH CURVES

We present here, for the two cases involving wells, the probability density functions (pdf) of arrival time τ, equivalent, from the stochastic point of view, to the breakthrough curves (Figures 9(a) and 9(b)). They are calculated by derivation of the repartition function F_τ of arrival time, which is itself obtained by analytical integration of position probability density function f_X over the half-plane 'behind' the pumping well. The main, and unfortunately very questionable, assumption made for f_X calculation is its gaussianity. This assumption is dictated by the position moments availability, since only the first two of them are available. The gaussian distribution is convenient because its writing as a function of position mean and variance is straight-forward: $\vec{M}_X$ and $\overline{\overline{C}}_X$ being the time-dependent average vector and covariance tensor of particle position $\vec{X}$ for a given model, the position probability density function at point $\vec{\zeta}$ and at time t has the following form:

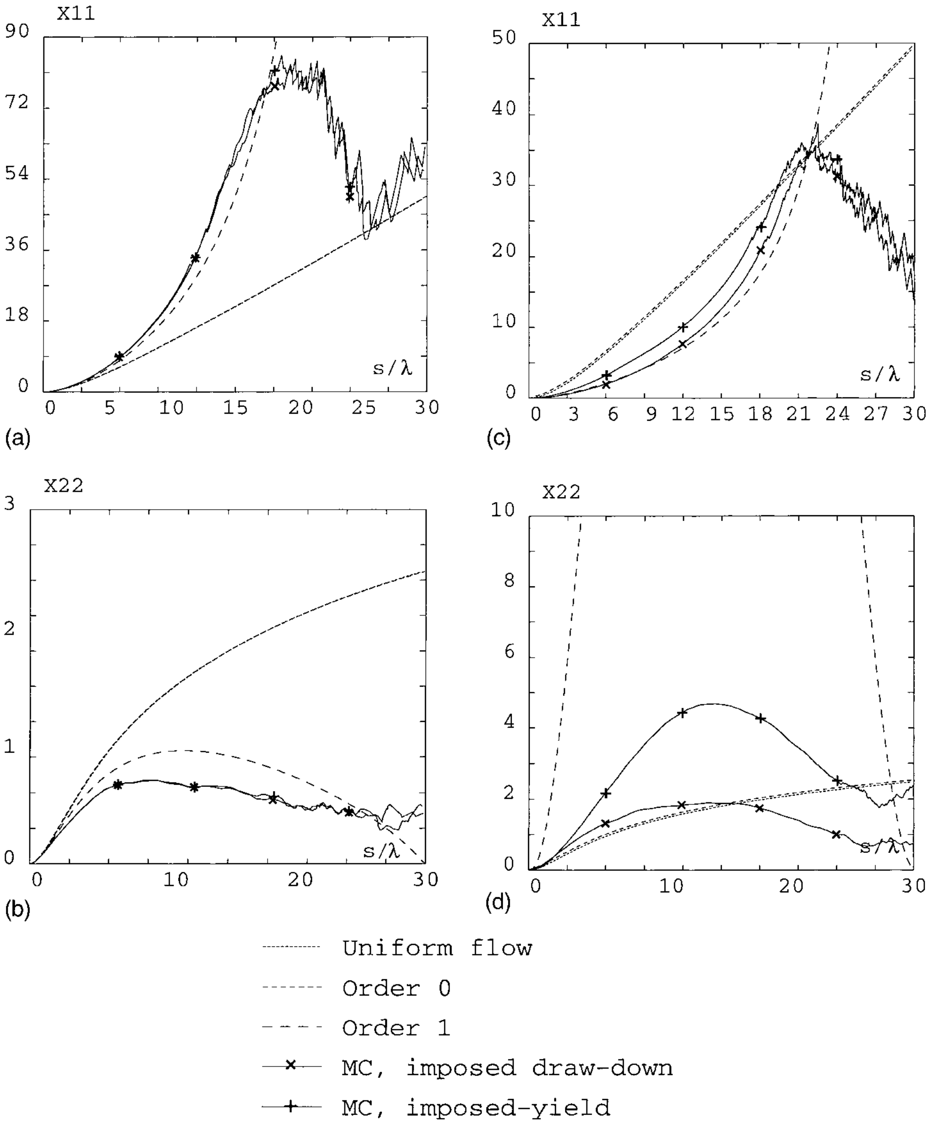

Figure 8. Normalized displacement variances, $X_{ii} \equiv X_{ii}/\sigma_Y^2\lambda^2$, as functions of the dimensionless curvilinear abcissa, (a) and (b): for the single pumping; (c) and (d): for the dual pumping case. $\sigma_Y = 0.5$ (a) X_{11}, radial convergent flow (release distance $= 30\lambda$); (b) X_{22}, radial convergent flow (release distance $= 30\lambda$); (c) X_{11}, dipolar flow; (d) X_{22}, dipolar flow.

$$f_X(\vec{\zeta}, t) = \frac{1}{2\pi\sqrt{|C_X|}} \exp\left(-\frac{1}{2}[{}^t\vec{\mu} C_X^{-1} \vec{\mu}]\right), \tag{18}$$

where $\vec{\mu} = \vec{\zeta} - \vec{M}_X(t)$, and $C_X = \overline{\overline{C}}_X(t)$.

Moreover, and whatever the shape of the position pdf, the theoretical arrival time density probability function is

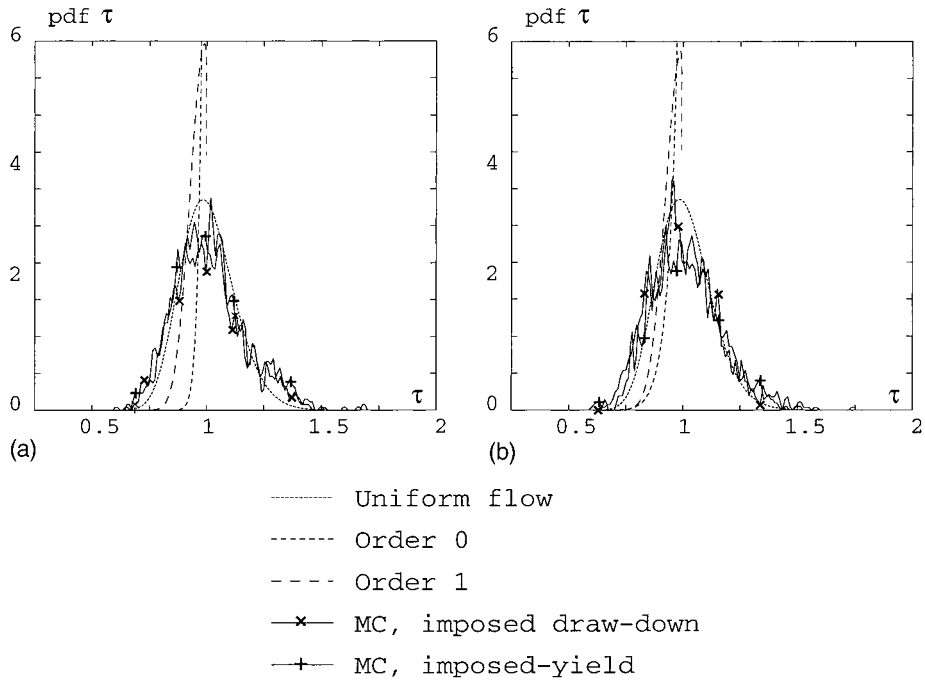

Figure 9. Arrival time probability density function. Arrival time τ has been normalized by its mean. $\sigma_Y = 0.5$. (a) Radial convergent flow (release distance $=30\lambda$); (b) dipolar flow.

$$f_\tau = \frac{\partial F_\tau}{\partial \tau}, \tag{19}$$

with the following estimation of F, based on its expression for the crossing of a fictive plane in uniform flow (Dagan, 1989):

$$F_\tau(\tau) = \int_{\zeta_2} \int_{\zeta_1 > X_{\text{pumping}}} f_X(\vec{\zeta}, \tau) d\vec{\zeta}, \tag{20}$$

Using Equations (18) and (20) leads to the classical result:

$$F_\tau(\tau) = \frac{1}{2}\text{erfc}\frac{s(\tau)}{\sqrt{2X_{11}(s(\tau))}}. \tag{21}$$

Zeroth and first-order predictions do not give a good fit for both types of pumping: they are based on the mean trajectory which ends, by definition, at the pumping well. They are thus not defined after that time. Moreover, they strongly underestimate the spreading of the arrival time (the first order model is slightly better). Then this underestimation cannot be explained by the misfit of longitudinal position variance. It obviously comes from the non-gaussianity of position pdf in the vicinity of the pumping well, whereas it is the basic hypothesis of the aforedescribed model. This effect is plain and easily understood when one thinks that the available positions are limited to the abscissa of the well, whereas a gaussian distribution would induce the presence of the tracer behind and around the pumping well.

On the other hand, arrival time pdf given by the uniform flow model leads to a very good fit. The velocity of the equivalent uniform flow was chosen such as to honor the mean arrival time. This result confirms what Lenda and Zuber put forward previously without demonstration (Lenda and Zuber, 1970; Zuber, 1974). A similar result has been proved later by (Indelman and Dagan, 1999) in radially divergent flows. Although the problem was not totally the same, the similarity is strong enough to suggest that the result we found is not coincidental, but should be cautiously limited to single well or dipolar wells situations. Though this model heavily misestimates position moments versus travel distance, its predictions are closer to Monte-Carlo results than any other model if position moments are plotted versus travel time instead (not represented). Therefore, with exclusive interest on breakthrough curves, the uniform flow equivalence model has proved itself very efficient.

In order to simulate more closely the migration of a plume, a second particle has been released at the top-right corner of the square-shaped injection well (see Figure 1(c)). Arrival time statistics have been derived and combined to the first particle's arrival time pdf (Figure 10). As expected, arrival times of the second point are shifted to longer time, more dispersed, and with a lower maximum. The resulting probability law is nearly twice larger, with a shifted mean, and, of course, a lower maximum. From this, it is possible to induce that arrival time pdf of a whole plume, defined at $t = 0$ by an infinite number of particles equally positioned around the injection well, would be substantially more scattered with a later mean. The uniform flow model, unchanged, would be definitely far from reality. This needs to be verified, though difficult to do, computationally speaking, because it theoretically

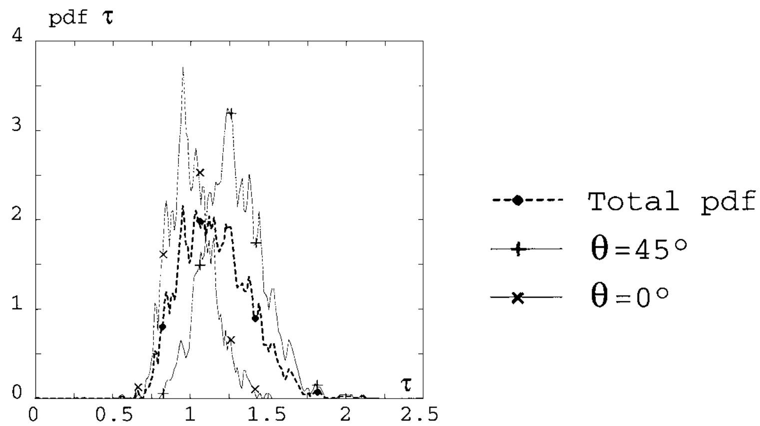

Figure 10. Arrival time distribution law for a plume (*dashed line*) simulated by two release points (*continuous lines*) situated initially around the injection well at two different angles θ. Arrival time τ has been normalized by the mean arrival time of the shorter trajectory.

requires an infinite domain of study. Limiting the study to a smaller distribution of launched particles, say 10 particles between 0 and 120° still represents a very heavy computation that has not been performed.

4. Conclusion

This study of flow and transport in three different types of nonuniform flows in stationary transmissivity fields by Monte-Carlo simulations has shown that transport processes are strongly affected by the type of flow: position variances cannot be approximated by the uniform flow assumption unless the nonuniformity is very weak. The hypothesis of locally uniform flow (zeroth order of scale separation) increases moderately the quality of the prediction in the case of the turning flow, but is of no use in the single well case nor in the two-well dipolar case. Taking into account explicitly the velocity gradient in the evaluation of position variances (first order of scale separation) improves significantly the predictions. Highly nonuniform turning flows (scale separation gauge ε higher than 0.03) are still not handled theoretically, as well as dipolar fields with respect to transverse dispersion. These configurations require higher order terms in the ε Taylor's expansion of the mean velocity. Besides this, due to its nonuniformity, the flow is stochastically nonstationary. It can nevertheless be considered locally uniform and stationary if one is only interested in head and Darcy's velocity variances.

Boundary conditions, as well as wells nature (imposed flux or imposed head) also affect kinematics and transport variables. Their effect are qualitatively very similar to those observed in uniform flow (CEA internal report), with the exception of transverse velocity variance which is not affected by the wells. The nature of the well(s) has a long range effect on transport, though it is not clearly seen with just one pumping well. In the dipolar case, the longitudinal and transverse dispersions are weaker when the water flux is imposed at the injection well than when the draw-down is imposed. This is particularly true for transverse dispersion.

Finally, the uniform flow assumption can be used for practical purpose in the interpretation of arrival time statistics obtained by single-well pumping tests: transport in the neighborhood of a pumping well acts surprisingly closely like in a uniform flow honoring the mean arrival time. This means that measurement of longitudinal dispersivity from tracer test with a single pumping well can be used in uniform flow problems. Previous results of Lenda and Zuber (1970) are therefore confirmed. This is of great importance as most of the field hydrogeologists use the Lenda et Zuber assumption in order to determine transport parameters.

This conclusion can be extended to the dipole test for the particle following the straight trajectory from the injection well to the pumping well. It is unfortunately not applicable to an entire plume released all around the injection well. Further study is required to link the dispersivity obtained by fitting breakthrough curve obtained by a dipole test, using the uniform flow assumption, to the dispersivity corresponding to an actual uniform flow in the same medium. The present study has shown that these two dispersivities were very different. Use of an upscaled model – that is constant asymptotic dispersivity in an homogeneous medium with a deterministic Darcy's velocity – in the fitting of dispersivity to breakthrough curves, as it is done today, can bring significant enhancement, but the validity of this method still needs to be checked. This should be kept in mind by field experimentalists when they deduce dispersivities from tracer experiments, and by modelers when they use constant dispersivities. The dispersion model presented here works well for all the investigated flow fields, except for the transverse dispersion in a radial divergent flow field. No improvement can be presented at the present time. These results show implicitly that the assumption made on the normalized velocity covariance, covariance equal to that of the uniform flow, seems to be valid. Finally let us emphasize that the uniform flow assumption, used by many hydrogeologists, gives a very good approximation of the arrival time probability density function, and consequently a good measure of the longitudinal dispersivity in an uniform flow field.

Appendix A. Derivation of Velocity Mean and Fluctuations in 2D Flows

We detail here the expression of velocity mean and fluctuations up to second-order in σ_Y in 2D flows by the perturbation method. This derivation is inspired from, and essentially limited to (Dagan, 1989; Gelhar, 1993; Grenier, 1996). The meaningness of this development is questionable since some high-order terms may become infinite, or, as a matter of fact, greater that lower-order terms. It is nevertheless assumed here that neglecting terms of order higher that 2 or 3 is a pertinent process. In any case, σ_Y should be lower than unity.

Let Y, H and $\vec{U}$ be log-transmissivity, hydraulic head and darcy's velocity respectively. $\langle\rangle$ brackets denote ensemble mean, and low-case variables y, h and $\vec{u}$ fluctuations. The numbers in exponent parenthesis specify order in σ_Y of the current variable. Therefore, the asymptotic expansion being limited to the second order, the hydraulic variables read:

$$\begin{aligned} Y &= \langle Y\rangle + y &&= Y^{(0)} + Y^{(1)}, \\ H &= \langle H\rangle + h &&= H^{(0)} + H^{(1)} + H^{(2)}, \\ \vec{U} &= \langle \vec{U}\rangle + \vec{u} &&= \vec{U}^{(0)} + \vec{U}^{(1)} + \vec{U}^{(2)}. \end{aligned} \tag{22}$$

Darcy's law can be expressed as

$$\vec{U} = -\mathrm{e}^{Y}\vec{\nabla} H, \tag{23}$$

so that the water mass conservation (without recharge since uniform flow is assumed):

$$\mathrm{div}\vec{U} = 0 \quad \text{with boundary conditions} \tag{24}$$

associated to the approximation

$$\mathrm{e}^{Y} \simeq T_G\left(1 + y + \frac{y^2}{2}\right), \tag{25}$$

where $T_G = \mathrm{e}^{\langle Y \rangle}$, may be rewritten as:

$$\operatorname{div}\left[\left(1 + y + \frac{y^2}{2}\right)(\vec{\nabla} H^{(0)} + \vec{\nabla} H^{(1)} + \vec{\nabla} H^{(2)})\right] = 0 \qquad (26)$$

In the case where boundary conditions are deterministic, they can be fully applied to the zeroth-order reduction of Equation (26), leaving null value imposed to higher order head. The identification of order zero, one and two in Equation (26) leads to the three following equations:

$$\Delta H^{(0)} = 0, \quad \text{with deterministic boundary conditions} \qquad (27)$$

$$\operatorname{div}(y\vec{\nabla} H^{(0)} + \vec{\nabla} H^{(1)}) = 0 \quad \text{with } H^{(1)} = 0 \quad \text{at the boundaries} \qquad (28)$$

$$\operatorname{div}\left(\frac{y^2}{2}\vec{\nabla} H^{(0)} + y\vec{\nabla} H^{(1)} + \vec{\nabla} H^{(2)}\right) = 0 \quad \text{with } H^{(2)} = 0 \quad \text{at the boundaries} \qquad (29)$$

Equations (27) and (28) give

$$\Delta H^{(1)} + \vec{\nabla} y \cdot \vec{\nabla} H^{(0)} = 0, \quad \text{with } H^{(1)} = 0 \quad \text{at the boundaries} \qquad (30)$$

which, in turn, changes Equation (29) to:

$$\Delta H^{(2)} + \vec{\nabla} y \cdot \vec{\nabla} H^{(1)} = 0, \quad \text{with } H^{(2)} = 0 \quad \text{at the boundaries.} \qquad (31)$$

It is now possible to identify the means and fluctuations of the different orders of H. Equation (27) shows that $H^{(0)}$ has no fluctuation: $\langle H^{(0)} \rangle = H^{(0)}$ and $h^{(0)} = 0$, so that (from Equation (30), $H^{(1)}$ is pure fluctuation: $\langle H^{(1)} \rangle = 0$ and $h^{(1)} = H^{(1)}$. Summarizing Equations (27), (28) and (31), taking respectively the mean and the fluctuation of the results, and discarding any third-order term, the equations governing total mean head and fluctuations become:

$$\Delta \langle H \rangle = -\langle \vec{\nabla} y \cdot \vec{\nabla} h^{(1)} \rangle \quad \text{with deterministic boundary conditions} \qquad (32)$$

$$\Delta h = -\vec{\nabla} y \cdot \vec{\nabla} H^{(0)} - (\vec{\nabla} y \cdot \vec{\nabla} h^{(1)} - \langle \vec{\nabla} y \cdot \vec{\nabla} h^{(1)} \rangle) \quad \text{with } h = 0 \quad \text{at the boundaries.} \qquad (33)$$

The right-hand term in Equation (32) is the second-order mean head laplacian $\langle \Delta H^{(2)} \rangle$, that makes head differ from its sole zeroth-order approximation. It is null in uniform flows. Although it is certainly non-null in nonuniform flows, since it must depend on location because of the space-dependency of $\langle \vec{\nabla} H^{(0)} \rangle$ in Equation (30), it is not sure how strong it is. Similarly, the right-hand term in parenthesis in Equation (33) is the second-order head fluctuation laplacian $\Delta h^{(2)}$, usually neglected, but a priori non-null. For the same reason as for its mean, head fluctuations yield a space-dependency due to flow nonuniformity. There is thus an influence, though its strength might be low, of flow nonuniformity on velocity fluctuations.

Writing Equation (23) with the approximation (25) and the expansion (22), we obtain, by identification, the following expansion terms of $\vec{U}$:

$$\vec{U}^{(0)} = -T_G \vec{\nabla} H^{(0)}, \tag{34}$$

$$\vec{U}^{(1)} = -T_G (y \vec{\nabla} H^{(0)} + \vec{\nabla} H^{(1)}), \tag{35}$$

$$\vec{U}^{(2)} = -T_G \left(\frac{y^2}{2} \vec{\nabla} H^{(1)} + y \vec{\nabla} H^{(1)} + \vec{\nabla} H^{(2)} \right). \tag{36}$$

Splitting the sum of Equations (34), (35) and (36) between mean and fluctuations, and knowing that $H^{(0)}$ has no fluctuation, and $H^{(1)}$ has zero mean, yields:

$$\langle \vec{U} \rangle = -T_G \left[\left(1 + \frac{\sigma_y^2}{2} \right) \langle \vec{\nabla} H^{(0)} \rangle + \langle y \vec{\nabla} h^{(1)} \rangle + \langle \vec{\nabla} H^{(2)} \rangle \right], \tag{37}$$

$$\begin{aligned} \vec{u} \;=\; -T_G \Bigg[& \left(y + \frac{y^2 - \sigma_y^2}{2} \right) \langle \vec{\nabla} H^{(0)} \rangle + \vec{\nabla} h^{(1)} + \\ & + \langle \vec{\nabla} H^{(2)} \rangle + (y \vec{\nabla} h^{(1)} - \langle y \vec{\nabla} h^{(1)} \rangle) + \vec{\nabla} h^{(2)} \Bigg]. \end{aligned} \tag{38}$$

In uniform flows, (Dagan, 1989; Gelhar, 1993) proved that $\langle y \vec{\nabla} h^{(1)} \rangle = -(\sigma_y^2/2) \langle \vec{\nabla} H^{(0)} \rangle = cste$, and thus, by Equation (31), that $\langle H^{(2)} = 0 \rangle$. In a nonuniform flow, $\langle \vec{\nabla} H^{(0)} \rangle$ being spatially variable, these relations are not true anymore, but the contribution of the incriminated terms is of order two only. At the first order, we have the simple following expressions for head and velocity:

$$\begin{aligned} &\langle H \rangle = \langle H^{(0)} \rangle \quad \text{and} \quad \Delta \langle H \rangle = 0 \qquad \text{with deterministic boundary conditions} \\ &h = h^{(1)} \quad \text{and} \quad \Delta h = -\vec{\nabla} y \cdot \vec{\nabla} \langle H \rangle \qquad \text{with } h = 0 \text{ at the boundaries} \\ &\langle \vec{U} \rangle = -T_G \vec{\nabla} \langle H \rangle, \\ &\vec{u} = -T_G (y \vec{\nabla} \langle H \rangle + \vec{\nabla} h), \end{aligned} \tag{39}$$

where we recognize the expression of velocity mean chosen in paragraph (2.2), Equation (8).

Appendix B. Derivation of Position Variances in a Turning Flow Without Recharge

We present here, as an example, how expressions (9), (11) and (12) were obtained for the turning flow case. The interested reader can process alike to verify the two other expressions of $g(s)$ in (12) for the other cases.

Starting from the mean velocity field (2), the gradient matrix of $\langle\vec{U}\rangle$ is very simple:

$$\vec{\nabla} \otimes \langle\vec{U}(\vec{X})\rangle = \frac{U_0}{Y_m}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{40}$$

Equation (7) can be explicitly rewritten:

$$\begin{cases} \dfrac{\mathrm{d}x_1}{\mathrm{d}t} = u_1(\langle\vec{X}(t)\rangle) + Ax_1, \\ \dfrac{\mathrm{d}x_2}{\mathrm{d}t} = u_2(\langle\vec{X}(t)\rangle) - Ax_2, \end{cases} \tag{41}$$

where $A = U_0/Y_m$. Solving (41) yields displacement expressions (null at $t = 0$):

$$\begin{aligned} x_1(t) &= \int_{t'=0}^{t} u_1(\langle\vec{X}(t')\rangle)\frac{\mathrm{e}^{At}}{\mathrm{e}^{At'}}\,\mathrm{d}t', \\ x_2(t) &= \int_{t'=0}^{t} u_2(\langle\vec{X}(t')\rangle)\frac{\mathrm{e}^{At'}}{\mathrm{e}^{At}}\,\mathrm{d}t', \end{aligned} \tag{42}$$

Then, replacing temporal variables by curvilinear abscissa along the mean trajectory, and with the convention $f[\langle\vec{X}(t)\rangle] = f[s(t)]$, we can write the position variances:

$$\begin{aligned} \langle x_1^2(s)\rangle &= \iint_{s',s''=0}^{s} \frac{\langle u_1(s')u_1(s'')\rangle}{\|\langle\vec{U}(s')\rangle\|\|\langle\vec{U}(s'')\rangle\|}\frac{\mathrm{e}^{At(s)}}{\mathrm{e}^{At(s')}}\frac{\mathrm{e}^{At(s)}}{\mathrm{e}^{At(s'')}}\,\mathrm{d}s'\,\mathrm{d}s'' \\ \langle x_1x_2(s)\rangle &= \iint_{s',s''=0}^{s} \frac{\langle u_1(s')u_2(s'')\rangle}{\|\langle\vec{U}(s')\rangle\|\|\langle\vec{U}(s'')\rangle\|}\frac{\mathrm{e}^{At(s')}}{\mathrm{e}^{At(s'')}}\,\mathrm{d}s'\,\mathrm{d}s'', \\ \langle x_2^2(s)\rangle &= \iint_{s',s''=0}^{s} \frac{\langle u_2(s')u_2(s'')\rangle}{\|\langle\vec{U}(s')\rangle\|\|\langle\vec{U}(s'')\rangle\|}\frac{\mathrm{e}^{At(s')}}{\mathrm{e}^{At(s)}}\frac{\mathrm{e}^{At(s'')}}{\mathrm{e}^{At(s)}}\,\mathrm{d}s'\,\mathrm{d}s''. \end{aligned} \tag{43}$$

Writing $g(s) = \exp(U_0t(s)/L)$, these expressions can be rewritten in the more concise form:

$$\begin{aligned} \langle x_1^2(s)\rangle &= \iint_{s',s''=0}^{s} u_{11}^*\frac{g(s)}{g(s')}\frac{g(s)}{g(s'')}\,\mathrm{d}s'\mathrm{d}s'', \\ \langle x_1x_2(s)\rangle &= \iint_{s',s''=0}^{s} u_{12}^*\frac{g(s')}{g(s'')}\,\mathrm{d}s'\mathrm{d}s'', \\ \langle x_2^2(s)\rangle &= \iint_{s',s''=0}^{s} u_{22}^*\frac{g(s')}{g(s)}\frac{g(s'')}{g(s)}\,\mathrm{d}s'\mathrm{d}s''. \end{aligned} \tag{44}$$

in which we recognize expression (9), with the dimensionless velocity fluctuation covariance u_{ij}^* defined by Equation (10).

These position covariances have a finite range of a few λ (Rubin, 1991). According to the scale separation approximation, stating that the range of variation of the mean velocity is very large compared to λ, the mean velocity can be considered locally uniform in the estimation of u^*_{ij}. Consequently, save for a base change from the tangent base to the reference base, it is equal to the normalised velocity covariance $u^*_{ij}|_{\text{unif}}$ in a uniform flow. Using the tensorial notation, we now have the following expression for the velocity covariance matrix:

$$[u^*_{ij}(s', s'')] = \overline{\overline{P}}(s')[u^*_{ij}(\vec{r})]|_{\text{unif}}\overline{\overline{P}}(s''), \tag{45}$$

where $\overline{\overline{P}}(s)$ is the transfer matrix from an orthonormal reference basis to the orthonormal local mean tangent base.

$$\overline{\overline{P}}(s) = \frac{1}{U}\begin{bmatrix} U_1 & -U_2 \\ U_2 & U_1 \end{bmatrix}, \tag{46}$$

where U_1, U_2 and U are components and norm of velocity mean at point $\langle \vec{X}(s(t))\rangle$. $\overline{\overline{P}}$ depends only on $\langle \vec{U}\rangle$ direction at the point of the mean trajectory reached after a travel distance s. ${}^t\overline{\overline{P}}$ is the transposition of $\overline{\overline{P}}$.

The equivalent separation distance $\vec{r}$ is not the real separation $\vec{X}(s'') - \vec{X}(s')$, but is located on the tangent with a length which can be alternatively expressed as a function of time: $\vec{r} = \overline{X''} - \vec{X}(s') = (\| \langle \vec{U}(s')\rangle \| (t'' - t'); 0)$ in the local base, or, preferentially, relatively to travel distance: $\vec{r} = (s'' - s'; 0)$ (see Figure 11). Although this latter choice does not come directly under zeroth-order scale separation, it is a slight enhancement to the model because transport quantities such as velocity covariances, dispersivity and position variances depend on travel distances

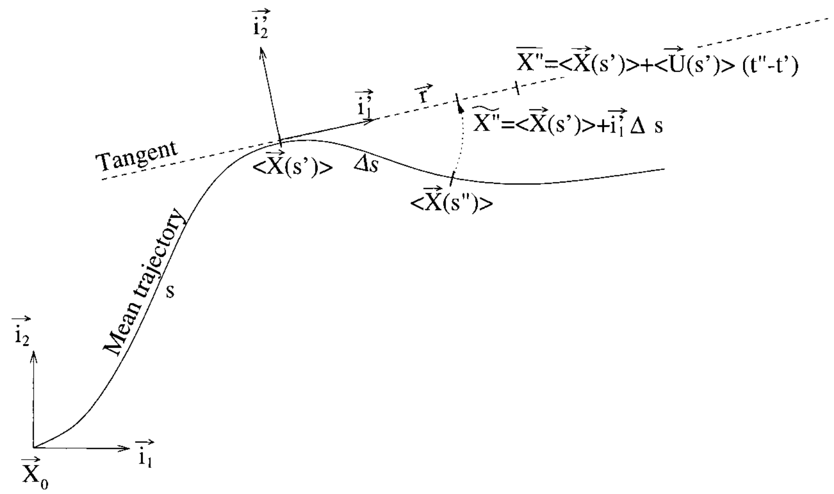

Figure 11. Scheme of zeroth-order separation scale for velocity covariance separation vector. The trajectory is locally approximated by its tangent, with a constant velocity $\langle \vec{U}(s')\rangle$ taken at the first integration point. $\overline{X''}$ is the approached position of the second integration point $\vec{X}(s'')$ if time-separation is chosen. In our case, the travel distance as been prefered, and $\vec{X}(s'')$ has been approximated by $\widetilde{X''}$ instead.

rather than time ; the latter introducing an apparent dependence on the norm of the mean velocity.

Expressions (43) can then be numerically calculated by double integration, using the velocity covariances given in (Rubin, 1991).

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