EXAMPLES OF SUBSURFACE SOLUTE SPREADING DRIVEN BY INHOMOGENEOUS VELOCITY FIELDS

GIOVANNA DARVINI[1],PAOLO SALANDIN[2]

[1]Institute of Hydraulics and Road Infrastructures, Universita' Politecnica delle Marche, Via Brecce Bianche, Ancona, I-60131, Italy
[2]Department of Hydraulic, Maritime, Environmental, and Geotechnical Engineering, University of Padova, Via Loredan 20, Padova, I-35131, Italy

Abstract

The paper deals with the inert solute transport in bounded heterogeneous porous media under nonstationary flow conditions. The nonstationarity of velocity field may originate from the boundary influence in finite domains, flow and solute sources, nonstationarity of medium properties or conditioning of the log-conductivity field to measurements of head or conductivity. In this paper we investigate the combined effect of a nonstationary conductivity field due to the presence of a linear trend in the mean log-conductivity and the impact of boundaries on solute transport. The influence of the initial size of the plume on the evolution of the plume's spatial moments is also considered. Spatial moments of a solute volume of finite initial size are obtained by a Lagrangian analysis starting from the knowledge of the velocity field nonstationary covariance matrices. The latter are evaluated by expanding the hydraulic conductivity and head potential in Taylor series limited to the first-order and by recursive application of the finite element method. The numerical results in terms of particle displacement moments are compared with the known solution available in the literature for unbounded domains and with Monte Carlo simulations expressly developed. The results indicate that ignoring the combined effect of the influence of boundaries, the presence of a mean log-conductivity trend leads to erroneous conclusions on the solute plume dispersion.

1. INTRODUCTION

By dealing with subsurface transport in real-world applications several examples of nonstationarity in natural formations properties have been analyzed in the literature. The medium nonstationarity may be due to distinct geological layers and zones [e.g. Guadagnini et al., 2004] or to the presence of trends in heterogeneity [e.g. Indelman and Rubin, 1995, 1996; Zhang, 1998; Cirpka and Nowak, 2004]. Moreover the medium nonstationarity may be induced by the conditioning procedure of the conductivity field to measurements [e.g. Morales-Casique et al., 2006a,b]. Indelman and Rubin [1995, 1996] analyze the effects of a linear trend in the mean log-conductivity in an unbounded domain. In the first of these papers the flow field statistic was analyzed, while in the latter the motion of a single particle is discussed and general equations for the first two moments of the particle trajectory are derived. From the analytical solution of the transport problem the authors found that a trend parallel to the mean gradient head reduces the particle displacement covariance. The combined effect of a trend of the log-conductivity and the presence of boundaries has been dealt with by Zhang [1998]. In his work the linear, quadratic and periodic trend was considered, but the analysis is limited on the potential head statistics. In this case also as in Indelman and Rubin [1995, 1996], the equations governing the statistical moments were derived by first-order perturbation expansions, but, due to their complexity, they are numerically solved by finite differences technique. Zhang founds that to properly define the potential head spatial variability in a limited domain affected by a trend of hydraulic properties, the influence of boundary conditions cannot be neglected.

The present study explores further the problem, by considering the solute transport in bounded domains in the case of media with a linear trend in the mean log-conductivity parallel to the mean flow direction. By using the Lagrangian approach on transport, we derive the spatial moments of a plume of passive solute from the knowledge of the velocity statistics. The velocity covariances in a nonstationary flow field were obtained by expanding the steady state flow equation in Taylor series limited to first-order and by the recursive application of finite element method. This methodology known as the stochastic finite element method (SFEM) was largely applied in the field of structural engineering [e.g. Kleiber and Hien, 1992]. Few applications in the stochastic subsurface flow and transport field are known to as: to obtain the spatial behavior of the potential head statistical moments [Osnes and Langtangen, 1998]; to discuss the velocity and solute transport statistics in bounded domains with stationary medium [Darvini and Salandin, 2004, 2006] and to develop the chemical species transport [Chaudhuri and Sekhar, 2005]. The results obtained following this approach in the case of a statistically inhomogeneous porous medium are compared with the unbounded solution by Indelman and Rubin [1996] and with evidences resulting from Monte Carlo simulations. Moreover the results given in terms of particle displacement statistics provide a measure of the effect related to the presence of a trend in a bounded domain on the finite size plume evolution.

2. SOLUTE TRANSPORT IN NONSTATIONARY VELOCITY FIELD

We consider the transport of inert solutes in a steady state velocity field $\mathbf{v}(\mathbf{x})$. The latter is determined from the Laplace equation defined on the domain Ω with prescribed conditions on the boundary

$$\nabla K \nabla \Phi = 0 \tag{1}$$

where Φ is the potential head and $K(\mathbf{x})$ is the hydraulic conductivity that is regarded as a random spatial function with lognormal distribution ($Y = \ln K$). The K field is characterized by the expectation $< Y(\mathbf{x}) >$ and by the two-point covariance function $C_Y(\mathbf{x}_1, \mathbf{x}_2)$. In turn, the velocity $\mathbf{v}(\mathbf{x})$ becomes a random space function, whose fluctuating term is $\mathbf{v}'(\mathbf{x}) = \mathbf{v}(\mathbf{x}) - < \mathbf{v}(\mathbf{x}) >$. So that the covariance tensor of the velocity can be written as

$$C_{\mathbf{v}}(\mathbf{x}_1, \mathbf{x}_2) = < \mathbf{v}'(\mathbf{x}_1)\mathbf{v}'(\mathbf{x}_2) >, \tag{2}$$

and for a nonstationary flow field both the statistical moments $< \mathbf{v}(\mathbf{x}) >$ and $C_{\mathbf{v}}(\mathbf{x}_1, \mathbf{x}_2)$ are generally dependent on the position $\mathbf{x}$.

To evaluate the transport of solutes in an inhomogeneous velocity field we apply a classical Lagrangian approach [Dagan, 1989]. Neglecting the pore scale dispersion, the displacement of the particle originating in $\mathbf{x} = \mathbf{a}$ at time $t = t_o$ is defined as

$$X_i(t; \mathbf{a}, t_o) = X_{oi}(t; \mathbf{a}, t_o) + X_i'(t; \mathbf{a}, t_o), \quad i = 1, 2, 3 \tag{3}$$

where X_{oi} is the deterministic zeroth-order component. Following the first-order analysis the fluctuating term X_i'

$$X_i'(t; \mathbf{a}, t_o) = \int_{t_o}^{t} v_i'[X_{oi}(t; \mathbf{a}, t_o)]dt' \tag{4}$$

is computed according to Phythian [1975], while the zeroth-order trajectory X_{oi} can be numerically derived by the usual pathline analysis of the deterministic velocity field. The displacement variances is given by

$$\begin{aligned} X_{ij}(t; \mathbf{a}, \mathbf{b}, t_o) &= < X_i'(t; \mathbf{a}, t_o) X_j'(t; \mathbf{b}, t_o) >= \\ &= < \int_{t_o}^{t} v_i'[\mathbf{X}_o(t'; \mathbf{a}, t_o)]dt' \int_{t_o}^{t} v_j'[\mathbf{X}_o(t''; \mathbf{b}, t_o)]dt'' >= \\ &= \int_{t_o}^{t} dt' \int_{t_o}^{t} dt'' C_{v_{ij}}(t', t''; \mathbf{a}, \mathbf{b}, t_o), \quad i, j = 1, 2, 3. \end{aligned} \tag{5}$$

where according to the first-order analysis $C_{v_{ij}}(t', t''; \mathbf{a}, \mathbf{b}, t_o)$ is the Eulerian velocity covariance evaluated at coordinates $\mathbf{x}_1 = \mathbf{X}_o(t'; \mathbf{a}, t_o)$ and $\mathbf{x}_2 = \mathbf{X}_o(t''; \mathbf{b}, t_o)$.

Although the solute concentration on the injection volume $V_o(\mathbf{x})$ is assumed as spatially constant, in statistically inhomogeneous velocity fields spatial moments of particle trajectory depend on the size of initial solute body volume V_o as well as on its shape and location $\mathbf{x}$. Our interest is in $< R_i >$, the expected value of the trajectory of the center of mass, and in $< S_{ij} >$, the expected value of the second-order spatial moment tensor proportional to the moments of inertia of the solute body. They are respectively defined as:

$$< R_i(t; V_o(\mathbf{x}); t_o) >= \frac{1}{V_o} \int_{V_o} < X_i(t; \mathbf{a}, t_o) > d\mathbf{a}, \tag{6}$$

$$\begin{aligned} < S_{ij}(t; V_o(\mathbf{x}); t_o) > &= \frac{1}{V_o} \int_{V_o} < X_i' X_j' > d\mathbf{a} - < R_i' R_j' > + \\ &+ \frac{1}{V_o} \int_{V_o} < X_i >< X_j > d\mathbf{a} - < R_i >< R_j >, \quad i, j = 1, 2, 3 \end{aligned} \tag{7}$$

where, written as usual $R_i' = R_i - < R_i >$, the uncertainty on the centroid position $R_{ij} =< R_i' R_j' >$ is given by

$$R_{ij}(t; V_o(\mathbf{x}), t_o) = \frac{1}{V_o} \int_{V_o} d\mathbf{a} \frac{1}{V_o} \int_{V_o} d\mathbf{b} < \mathbf{X}_i'(t; \mathbf{a}, t_o) \mathbf{X}_j'(t; \mathbf{b}, t_o) >, \quad i, j = 1, 2, 3. \tag{8}$$

In eq. (7) the difference between last two terms is the moment of inertia of trajectory expectations inside $V_o(\mathbf{x})$ that becomes $S_{ij}(0, V_o)$ in a velocity field where the expected value $< \mathbf{v} >$ is spatially constant.

Equations from (5) to (8) indicate that the spatial moments of a solute plume can be derived from the knowledge of the flow field covariance matrices. Statistics of the velocity that were developed in previous studies [Darvini and Salandin, 2004, 2006] are here applied to analyze the nonergodic transport. We remind only that the solution of flow problem was obtained by expanding the steady state flow equation in Taylor series limited to first-order and deducing the unknowns by the recursive application of finite element method. From the knowledge of the piezometric head mean values and its derivatives in respect to the fluctuating porous media hydraulic conductivity, the statistics of the inhomogeneous velocity field were deduced.

3. NUMERICAL EXPERIMENTS AND DISCUSSION OF RESULTS

Although the general theory described in Section 2 was developed in the more general 3-D case, for sake of simplicity the numerical examples are here developed in a square two-dimensional (x_1, x_2) plane of finite size $L/\lambda = 20$ with the coordinate origin centered at the lower left corner. The hydraulic conductivity $K(\mathbf{x})$ is assumed lognormal $(Y = lnK)$ with expectation $< Y >$, variance σ_Y^2 and exponential isotropic correlation function $\rho_Y(|\mathbf{d}|) = \exp[-|\mathbf{d}|/\lambda]$, where $\mathbf{d} = \mathbf{a} - \mathbf{b}$ is the separation vector and λ the integral scale. The statistical inhomogeneity of porous media manifests itself in a linear trend of expected value $< Y >= ax_1$, while σ_Y^2 and $\rho_Y(|\mathbf{d}|)$ are spatially constant. As boundary conditions we set constant potential head at $x_1 = 0$ and $x_1 = L$ and no-flow conditions along $x_2 = 0$ and $x_2 = L$. The mean flow is direct along the x_1 axis and is constant for a given α. Since the log-conductivity expectation increases like αx_1, the zeroth-order head gradient and the potential head decrease according with

$$\begin{aligned} J_o(x_1) &= J_o(0) exp(-\alpha x_1) \\ \Phi_o(x_1) &= \Phi_o(0) - \frac{J_o(0)}{\alpha}[1 - exp(-\alpha x_1)] \end{aligned} \tag{9}$$

where $J_o(0)$ is the zeroth-order head gradient value at $x_1 = 0$. In the following examples the mean flow and thus $J_o(0)$ are set constant and the potential head $\Phi_o(x_1)$ diminishes as α increases. For the Finite Element discretization we assumed square bilinear elements of constant size $\lambda/4$. A previous study founds that this grid discretization leads reliable solutions on transport problems [Darvini and Salandin, 2006]. On the basis of some preliminary results [Darvini and Salandin, 2005], in the following simulations two different cases are considered, by setting $\alpha = 0$ and 0.2. As a term of comparison we developed a fully non-linear Monte Carlo (MC) analysis. The numerical approach is the same adopted in Salandin and Fiorotto [1998]. The constant edge size of square bilinear elements adopted is $\lambda/8$ and the solute cloud is simulated by use of one particle for each element. The same discretization was adopted to generate the lognormal hydraulic conductivity field with exponential isotropic correlation function.To ensure the velocity covariance and particle statistics convergence the number of Monte Carlo runs was set at $NMC = 20,000$.

By numerical integration of (5) we are able to compute the displacement variance tensor of inert solute. Figure 1 illustrates the dimensionless longitudinal and transverse displacement variances $X_{11}/(\sigma_Y^2\lambda^2)$ and $X_{22}/(\sigma_Y^2\lambda^2)$ evaluated at $\mathbf{x}_0/\lambda = (0.125, 10.125)$ as a function of the dimensionless travel time $t < v_1 > /\lambda$ for $\alpha = 0$ and $\alpha = 0.2$. Figure shows that the introduction of a trend parallel to the mean flow direction leads an increase of the longitudinal dispersion and a reduction of the transverse one compared to

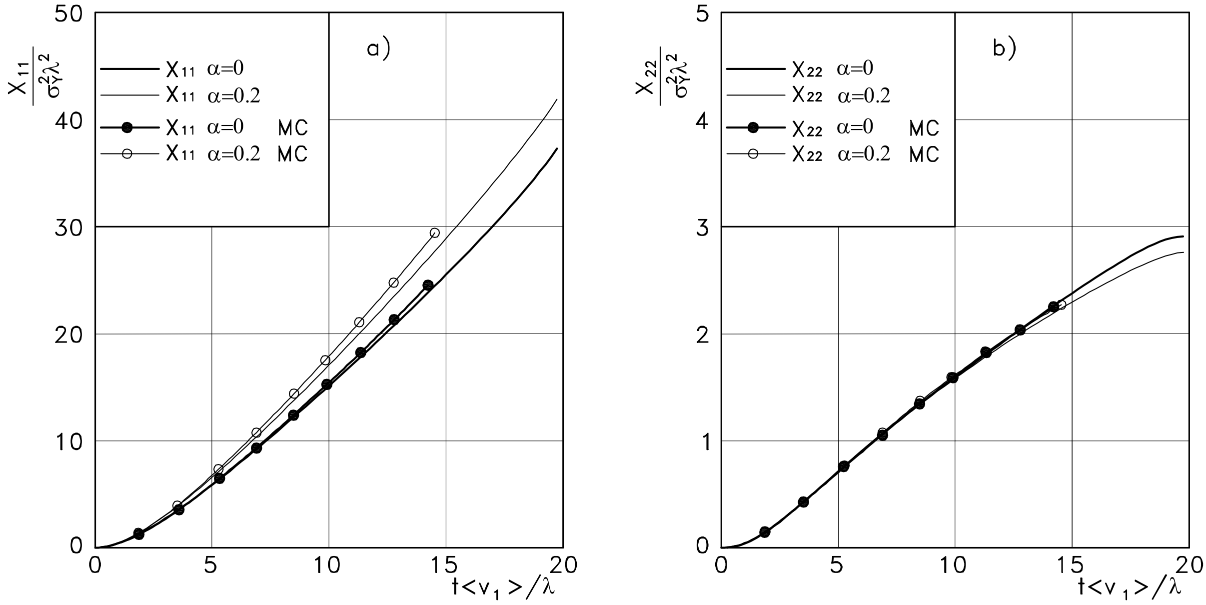

FIGURE 1. Longitudinal (a) and transverse (b) displacement variances as a function of the dimensionless travel time computed at $\mathbf{x}_0/\lambda = (0.125, 10.125)$ for $\alpha = 0$ and $\alpha = 0.2$. Results from Monte Carlo are also shown.

the corresponding values obtained in a stationary log-conductivity field. Note that, due to the finite dimensions of the domain, a Fickian regime is not attained for the dispersion process in absence of any trend also. The comparison with corresponding results of MC simulations shows in all cases a good agreement, but in the MC solution the mean travel time was limited to $\sim 15t < v_1 > /\lambda$ to avoid a loss of particles in the domain of size $L/\lambda = 20$. While the reduction of the transverse displacement variance is in agreement with the results obtained by Indelman and Rubin [1996] for an unbounded domain, the behavior of the X_{11} is opposite. The cited Authors find that a trend parallel to the mean flow direction reduces the longitudinal dispersion, but their solution is unaffected by boundary conditions. Otherwise our result is consistent with the velocity statistics discussed in Darvini and Salandin [2005]. In the bounded domain here considered the presence of a trend leads a reduction of the transverse velocity variability and an increase of the longitudinal one in terms both of the variance and the correlation length in a large portion of the domain.

In Figure 2 the dimensionless values of solute spatial moments $< S_{11} > -S_{11}(0)$ and $< S_{22} > -S_{22}(0)$ are illustrated as a function of the dimensionless travel time $t < v_1 > /\lambda$ for $\alpha = 0$ and $\alpha = 0.2$. The results are obtained by considering a line source normal to the mean flow direction and centered at $\mathbf{x}_o/\lambda = (0.125, 10.125)$. Four different initial sizes of source ($\ell_2/\lambda = 1, 3, 5$ and 10) are considered and compared with the one particle's statistics, that is with the X_{11} and X_{22} time evolution previously described. In absence of any trend the general behavior is well known [Dagan, 1991]. For $\ell_2/\lambda = 1$ the length of the source is equal to the heterogeneity scale: the uncertainty R_{ii} is large and its value

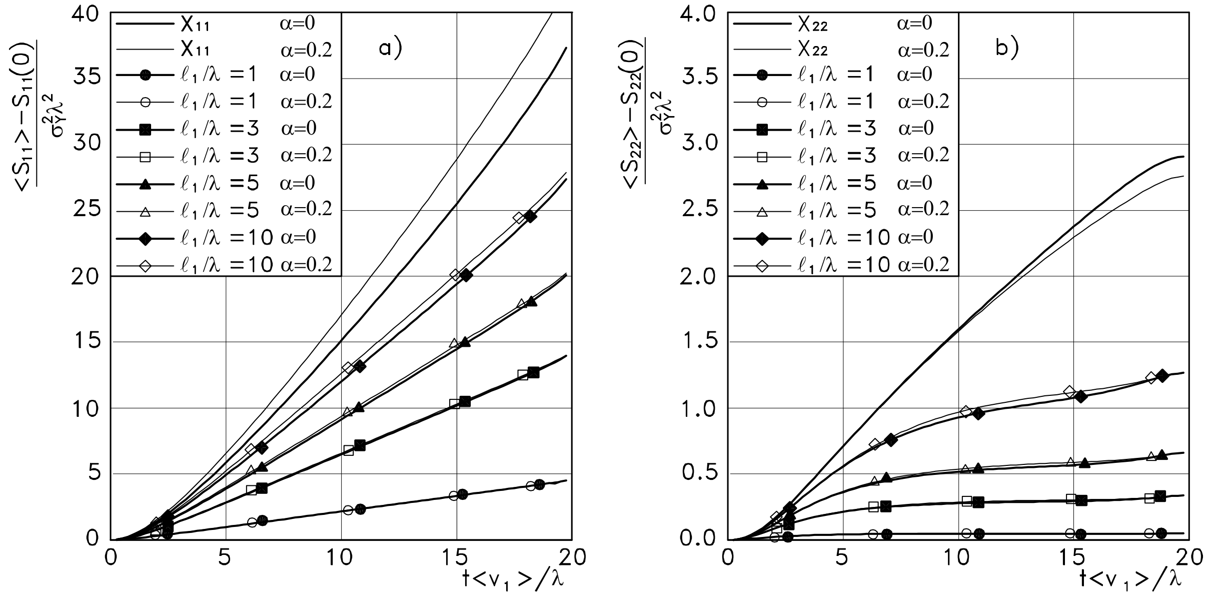

FIGURE 2. Longitudinal (a) and transverse (b) expected values of second spatial moments as a function of travel time for different initial solute source dimensions for $\alpha = 0$ and $\alpha = 0.2$. Line source normal to the mean flow direction centered at $\mathbf{x}_0/\lambda = (0.125, 10.125)$.

approaches the term $(1/V_o)\int_{V_o} X_{ii} d\mathbf{a}$. Thus the expected value of second spatial moment of the centroid of the cloud assumes a limited value as stated from equation (7). This fact means that the centroid of a plume originating from a small source disperses as the single particle. As the ratio ℓ_2/λ increases, more independent trajectories are collected: the uncertainty R_{ii} decreases and $< S_{ii} > -S_{ii}(0)$ increases. In presence of a trend parallel to the mean flow direction, for ℓ_2 comparable with λ and a source located far from the upper and lower boundaries, the spatial mean of the one particle displacement statistics can be considered not affected by the position of the release point along the line normal to the mean flow direction. Thus from $\alpha = 0$ to $\alpha = 0.2$ the increase of the terms $(1/V_o)\int_{V_o} X_{11} d\mathbf{a}$ and R_{11} of the equation (7) is similar and the solute spatial moments $< S_{11} > -S_{11}(0)$ remain substantially unchanged. This fact is true in transverse direction also where both terms reduce. Nevertheless as the length of source line increases, the longitudinal expected value of second spatial moment for $\alpha = 0.2$ becomes larger than that one of the no-trend case. In Figure 2 this behavior is manifest for a solute line whose transverse dimension is large compared to λ. In this case the solute body collects a large number of uncorrelated velocities. The uncertainty about the centroid trajectory R_{11} increases less than the term $(1/V_o)\int_{V_o} X_{11} d\mathbf{a}$ and this fact leads to values of $< S_{11} > -S_{11}(0)$ grater for $\alpha = 0.2$ than in the case $\alpha = 0$. For finite values $\ell_2/\lambda >> 1$ the transverse expectation of second spatial moment $< S_{22} > -S_{22}(0)$ is larger for $\alpha = 0.2$ than in the corresponding no-trend case, while as $\ell_2/\lambda \to \infty$, $S_{22} \to X_{22}$, and an opposite effect is manifest. This complex behavior can be attributed to the combined effect of the trend parallel to the mean flow direction and the role played by the uncertainty R_{22} reduction, the increase of averaging area and the X_{22} small lowering near the right boundary for $\alpha > 0$.

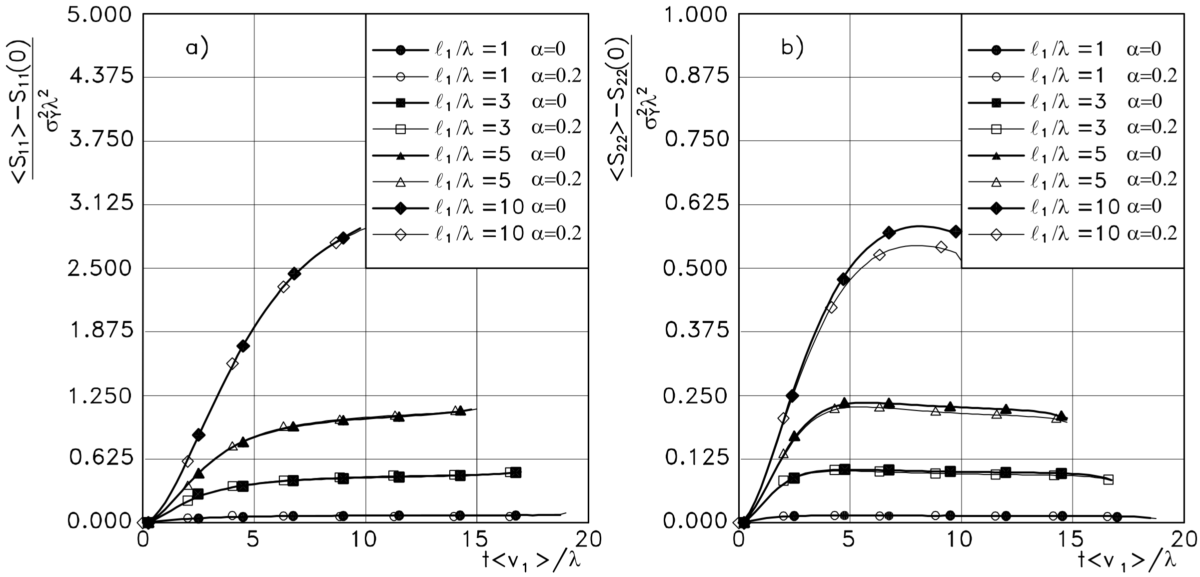

FIGURE 3. Longitudinal (a) and transverse (b) expected values of second spatial moments as a function of travel time for different initial solute source dimensions for $\alpha = 0$ and $\alpha = 0.2$. Line source parallel to the mean flow direction starting from $\mathbf{x}_0/\lambda = (0.125, 10.125)$.

Clearly different is the behavior of $< S_{11} > -S_{11}(0)$ and $< S_{22} > -S_{22}(0)$ for a line source parallel to the mean flow direction. In Figure 3 results for the different initial sizes $\ell_1/\lambda = 1, 3, 5$ and 10 are reported for a line starting from $\mathbf{x}_0/\lambda = (0.125, 10.125)$. Note that, due to the finite size of domain, the computational travel time reduces as the initial plume size increases. While in a stationary flow field for a body of finite length ℓ_1 the particle trajectories become correlated for a time $t > \ell_1/ < v_1 >$, by varying in a limited domain the flow statistics, they remain uncorrelated after $t = \ell_1/ < v_1 >$ also [Darvini and Salandin, 2006]. The presence of a trend equally affects $(1/V_o) \int_{V_o} X_{11} d\mathbf{a}$ and R_{11} and this fact leads a behavior of $< S_{11} > -S_{11}(0)$ as a function of the source initial length similar in two cases. With regard to the transverse second spatial moments, for $\alpha = 0$ moving from $\ell_1/\lambda = 1$ to 10, $(1/V_o) \int_{V_o} X_{22} d\mathbf{a}$ increases and R_{22} reduces. For $\alpha = 0.2$ the increase of the term $(1/V_o) \int_{V_o} X_{22} d\mathbf{a}$ is smaller and the reduction of R_{22} is greater than the case $\alpha = 0$, so that for larger line initial size the presence of a trend leads to values of $< S_{22} > -S_{22}(0)$ smaller than the corresponding no-trend case.

4. CONCLUSIONS

We investigated the combined effects of the spatial nonstationarity of the random log-conductivity field and of boundary conditions on the solute transport in finite domains. We did so through the stochastic finite element method (SFEM) to evaluate according to the first-order approximation the dispersion in spatially inhomogeneous flow fields. In two-dimensional examples proposed the domain is square with constant head and no-flow boundary conditions that ensure a mean constant flux. Numerical simulations and theoretical considerations reported in this note lead to the following major conclusions.

1. A linear trend in the mean log-conductivity parallel to the mean flow direction leads, unlike the result obtained in an unbounded domain, an increase of the one particle residual displacement longitudinal variance while the transversal one reduces slightly.

2. The presence of a trend together with the influence of boundary conditions affects the dispersion of plumes of finite size originating near the imposed piezometric head locations. For a release line normal to the mean flow direction as the initial size increases, the spreading in the presence of a trend is larger than the corresponding no-trend case. Instead for a source line parallel to the mean flow direction the longitudinal spreading is not affected by the trend, while the transverse dispersion is smaller than in the corresponding no-trend case.

3. The comparison of obtained evidences with results of Monte Carlo simulations shows a good agreement and ensures the reliability of the findings here reported.

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