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Effective dispersion in conditioned transmissivity fields

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ABSTRACT

We analyze the impact of conditioning to measurements of hydraulic transmissivity on the transport of a conservative solute. The effects of conditioning on solute transport are widely discussed in the literature, but most of the published works focuses on the reduction of the uncertainty in the prediction of the plume dispersion. In this study both ensemble and effective plume moments are considered for an instantaneous release of a solute through a linear source normal to the mean flow direction, by taking into account different sizes of the source. The analysis, involving a steady and spatially inhomogeneous velocity field, is developed by using the stochastic finite element method. Results show that conditioning reduces the ensemble moment in comparison with the unconditioned case, whereas the effective dispersion may increase because of the contribution of the spatial moments related to the lack of stationarity in the flow field. As the number of conditioning points increases, this effect increases and it is significant in both the longitudinal and transverse directions. Furthermore, we conclude that the moment derived from data collected in the field can be assessed by the conditioned second-order spatial moment only with a dense grid of measured data, and it is manifest for larger initial lengths of the plume. Nevertheless, it seems very likely that the actual dispersion of the plume may be underestimated in practical applications.

1. Introduction

In the stochastic analysis of the groundwater flow and solute transport, measurements of the hydraulic transmissivity are used to infer the spatial statistics of the entire field by the geostatistical approach (e.g. [14]). When the ergodic conditions are met, the stochastic theory provides the behavior of the plume spatial moments as function of the travel time from the knowledge of the expected value and variogram of the transmissivity (e.g. [6]). Otherwise, to ensure site-specific estimates for the solute moments and to reduce uncertainties, the development of a conditioning procedure to measurements is required (e.g. [5,32]).

Conditioning to measured data makes the conditioned transmissivity field inhomogeneous even if the original one is not. Simple theoretical considerations about multigaussian conditioning [6, Section 1.3] show that, starting from a stationary field, the conditioned random function is no more statistically homogeneous and the conditioned mean and covariance become dependent on the spatial position. Obviously, velocity fields derived from the latter are inhomogeneous too, as underlined in several works (e.g. [5,16,22,28]).

The impact of conditioning to available measurements on the transport of a conservative solute is widely discussed in the literature. Most of the published works deals with the reduction of the uncertainty around the solute prediction (e.g. [15,23,31]).

Among others, Zhang and Neuman [33–35] analyzed the conditional spatial moments of a plume, by considering instantaneous sources in two-dimensional mildly-varying log-transmissivity field under uniform prior mean flow. Among the major conclusions, the authors found that, when the number of conditioning points increases, the trajectories of the mean plume centers of mass deviate noticeably from those of the unconditioned plume centers. Furthermore, the second spatial moment of the mean plume about its center of mass is reduced by conditioning techniques. Besides, the density of measurements, the sort of measured data (conductivity or/and head) and the position and the specific value measured of parameters are all important factors for prediction of the solute transport (e.g. [4]).

The reduction of the uncertainty in the transport prediction is also evident from the results of Morales-Casique et al. [20,21] that investigate the effect of the spatial nonstationarity of the flow due to conditioning on log-conductivity data in a finite domain. Their

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results confirm that, for a nonreactive solute plume, the growth of the longitudinal and transverse dispersion, as well as its temporal rates of change, is reduced significantly by conditioning.

Butera and Tanda [3] analyzed the transmissivity conditioning in heterogeneous aquifers subject to uniform recharge. They investigated some cases of few conditioning points with the same transmissivity values and their results show that the mean conditioned trajectory is strongly dependent on the value of the recharge intensity. Moreover, in some of the cases studied, the longitudinal conditioned displacement variance is higher than the unconditioned one, vanishing the advantages of the conditioning process.

All the previous papers focus on the covariance of conditioned trajectories or its temporal derivative, referred to as the ensemble moment of the solute plume as defined by Dagan [7]. In such a paper, the impact of conditioning to transmissivity measurements on the effective moment of the plume is analyzed and some specific results are shown for the first time.

The same topic was tackled by Bellin and Fiori [1] in the case of evolving-scale formations with a large-scale cutoff of the hydraulic transmissivity. They considered the case of a single point of measurement and assumed that the actual particle trajectory deviates slightly from the mean one, which at the zero-order approximation gives a straight line. Their results show that a single measurement of hydraulic transmissivity reduces the difference between ensemble and effective solute moments and the effectiveness in reducing the uncertainty depends on the position of the measurement with respect to the mean trajectory of the plume centroid.

Unlike that work, we analyze the impact of the statistical inhomogeneity of the flow field, stemming from conditioning on transmissivity data, on the mean trajectory of the centroid, and, hence, on the effective dispersion of the plume. The influence of the initial size of the source on the solute spreading has also been investigated. The relevance of this subject is recognized also by several authors (e.g. [17,30]) that discussed the advantage to consider transport information in the inverse models based on transmissivity and piezometric data conditioning.

The velocity field conditioned to available measurements of hydraulic transmissivity is derived by the Stochastic Finite Element Method (SFEM) (e.g. [10,11]). Then, the transport moments of a conservative solute plume are computed from the velocity statistics by a Lagrangian approach limited to the first-order. This approach was recently used to analyze the case of the medium nonstationarity induced by a trend in the mean log-conductivity in bounded domains [9].

Theoretically, the first-order approximation invoked in deriving the flow and transport moments requires the variance of hydraulic log-transmissivity to be much smaller than unit. However, this hypothesis should generally be satisfied with conditioning on measurements [31,36].

An alternative solution developed by classical Monte Carlo (MC) simulations confirms the results obtained by the semi-analytical approach for the effective dispersion in conditioned transmissivity fields.

2. Solute transport in nonstationary velocity field

We briefly recall the derivation of statistical moments of a inert solute plume by the SFEM approach [11].

We consider the transport of an inert solute 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 boundary conditions

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

where Φ is the potential head and $K(\mathbf{x})$ is the transmissivity, taken as a random spatial function with lognormal distribution ($Y = \ln K$). The K field is characterized by the expected value $\langle Y(\mathbf{x})\rangle$ and by the two-point covariance function $C_Y(\mathbf{x}_1, \mathbf{x}_2)$.

By the SFEM approach, the spatial variation of the transmissivity is described by subdividing the whole domain in E elements, and by assuming on each element a different value $K_e, e = 1, \ldots, E$. The first-order expansion in Taylor series limited to the first-order dependence on Y of both K_e and Φ yields the following expressions:

$$K_e = K_{o,e} + \sum_{j=1}^{E} \frac{\partial K_e}{\partial Y_j}\bigg|_o Y'_j, \quad \Phi = \Phi_o + \sum_{j=1}^{E} \frac{\partial \Phi}{\partial Y_j}\bigg|_o Y'_j \tag{2}$$

where $K_{o,e} = \exp(\langle Y_e\rangle)$ is the transmissivity geometric mean, $Y'_j = Y_j - \langle Y_j\rangle$ is the fluctuation of Y, Φ_o is the zeroth-order potential head and $\sum_{j=1}^{E} \frac{\partial \Phi}{\partial Y_j}\big|_o Y'_j$ is the fluctuation of the potential head Φ'.

By considering an arbitrary weight function ξ that satisfies homogenous boundary conditions and by applying the Green's theorem, substitution of (2) in (1) gives the zeroth-order and the first-order equations

$$\sum_{e=1}^{E} \int_{\Omega_e} K_{o,e} \nabla \Phi_o \nabla \xi d\omega = 0 \tag{3}$$

$$\sum_{e=1}^{E} \left(\int_{\Omega_e} K_{o,e} \nabla \frac{\partial \Phi}{\partial Y_j}\bigg|_o \nabla \xi d\omega + \int_{\Omega_e} \frac{\partial K_e}{\partial Y_j}\bigg|_o \nabla \Phi_o \nabla \xi d\omega \right) = 0, \; j = 1, \ldots, E. \tag{4}$$

Numerical solution of Eqs. (3) and (4) with proper boundary conditions provides the unknown zeroth-order potential head Φ_o and derivatives $\partial\Phi/\partial Y_j|_o, j = 1, \ldots, E$ necessary to compute the velocity moments.

Having defined as $\mathbf{v}'(\mathbf{x}) = \mathbf{v}(\mathbf{x}) - \langle \mathbf{v}(\mathbf{x})\rangle$ the fluctuation of the velocity, the expected value is

$$\mathbf{v}_o(\mathbf{x}) = -\frac{1}{n} K_{o,e} \nabla \Phi_o(\mathbf{x}) \tag{5}$$

and the covariance $C_{\mathbf{v}} = \langle \mathbf{v}'(\mathbf{x}_1)\mathbf{v}'(\mathbf{x}_2)\rangle$ is given by:

$$C_{\mathbf{v}}(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{n^2} \sum_{j=1}^{E} \sum_{\ell=1}^{E} \left(-K_{o,e_1} \nabla \frac{\partial \Phi(\mathbf{x}_1)}{\partial Y_j}\bigg|_o - \frac{\partial K_{e_1}}{\partial Y_j}\bigg|_o \nabla \Phi_o(\mathbf{x}_1) \right) \cdot \left(-K_{o,e_2} \nabla \frac{\partial \Phi(\mathbf{x}_2)}{\partial Y_\ell}\bigg|_o - \frac{\partial K_{e_2}}{\partial Y_\ell}\bigg|_o \nabla \Phi_o(\mathbf{x}_2) \right) \langle Y'_j Y'_\ell \rangle, \tag{6}$$

where $\mathbf{x}_1$ and $\mathbf{x}_2$ are the generic position within the elements e_1 and e_2 respectively, and $\langle Y'_j Y'_\ell\rangle$ is the covariance of the log-transmissivity.

By following a classical Lagrangian approach and by neglecting the pore scale dispersion, the trajectory of a single particle starting from $\mathbf{X} = \mathbf{a}$ at time $t = t_o$ is defined as

$$\mathbf{X}(t; \mathbf{a}, t_o) = \mathbf{a} + \int_{t_o}^{t} \mathbf{v}[\mathbf{X}(t'; \mathbf{a}, t_o)] dt' \tag{7}$$

where $\mathbf{v}[\mathbf{X}(t'; \mathbf{a}, t_o)]$ is the Lagrangian velocity.

Sometimes, we name 'macrodispersion' the plume fragmentation that takes place in natural formations due to the heterogeneity of the hydraulic transmissivity, while small scale (e.g. pore scale) effects are usually defined as 'dispersion'. Since the pore scale effects were discarded, for the sake of simplicity and without confusion, in the paper we use just the term 'dispersion'.

According to the linear analysis, the zero-th and the first-order terms of the particle trajectory, $\mathbf{X}_o(t; \mathbf{a}, t_o)$ and $\mathbf{X}'(t; \mathbf{a}, t_o)$ can be obtained as follows

$$\frac{d\mathbf{X}_o}{dt} = \mathbf{v}_o(\mathbf{X}_o)$$

$$\frac{d\mathbf{X}'}{dt} = \mathbf{v}'(\mathbf{X}_o) + (\mathbf{X}' \cdot \nabla)\mathbf{v}_o(\mathbf{X}_o). \tag{8}$$