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The impact of local diffusion on longitudinal macrodispersivity and its major effect upon anomalous transport in highly heterogeneous aquifers

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ABSTRACT

Flow and transport are solved for a heterogeneous medium modeled as an ensemble of spherical inclusions of uniform radius R and of conductivities K, drawn from a pdf $f(K)$ (Fig. 1). This can be regarded as a particular discretization scheme, allowing for accurate numerical and semi-analytical solutions, for any given univariate $f(Y)$ $(Y = \ln K)$ and integral scale I_Y. The transport is quantified by the longitudinal equivalent macrodispersivity α_{Leq}, for uniform mean flow of velocity U and for a large (ergodic) plume of a conservative solute injected in a vertical plane $(x = 0)$ and moving past a control plane at $x \gg I_Y$. In the past we have solved transport for advection solely for highly heterogeneous media of $\sigma_Y^2 \leqslant 8$. We have found that α_{Leq} increases in a strong nonlinear fashion with σ_Y^2 and transport becomes anomalous for the subordinate model. This effect is explained by the large residence time of solute particles in inclusions of low K.

In the present work we examine the impact of local diffusion as quantified by the Peclet number $Pe = UI_Y/D_0$, where D_0 is the coefficient of molecular diffusion. Transport with diffusion is solved by accurate numerical simulations for flow past spheres of low K and for high $Pe = O(10^2 - 10^4)$. It was found that finite Pe reduces significantly α_{Leq} as compared to advection, for $\sigma_Y^2 \gtrsim 3$ $(Pe = 1000)$ and for $\sigma_Y^2 \gtrsim 1.4$ $(Pe = 100)$, justifying neglection of the effect of diffusion for weak to moderately heterogeneous aquifers (e.g. $\sigma_Y^2 \leqslant 1$). In contrast, diffusion impacts considerably α_{Leq} for large σ_Y^2 due to the removal of solute from low K inclusions. Furthermore, anomalous behavior is eliminated, though α_{Leq} may be still large for $Pe \gg 1$.

1. Introduction

Transport of solutes through aquifers of spatially varying hydraulic conductivity is a topic of recent intensive research. Due to uncertainty it is common to regard the conductivity $K(\mathbf{x})$ as a random field and the equations of water flow and solute transport as stochastic.

We consider modeling of transport of a conservative solute in aquifer steady flow of uniform mean velocity $\mathbf{U}(U, 0, 0)$, in a formation of stationary and isotropic $Y = \ln K$ with variance σ_Y^2.

We assume an unbounded domain and an initial plume of a conservative solute of mass M_0 injected in the formation at time $t = 0$. We are interested in plumes which are large compared to the conductivity integral scale, such that ergodic conditions prevail. The resulting concentration field $C(\mathbf{x}, t)$ can be characterized in terms of different measures. We are concerned here with longitudinal spread and with quantifying the plume by the relative total mass that has moved beyond an arbitrary control plane at x up to time t, i.e. the BTC $M_p(t,x) = (1/M_0)\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_x^{\infty} C(x,y,z,t)\,dx\,dy\,dz$ (e.g. [22,1,11]). The temporal variation is captured by the relative mass flux $\mu(t,x) = \partial M_p/\partial t = (1/M_0)\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_x^{\infty} \partial C/\partial t\,dx\,dy\,dz$ at the control plane and by the associated temporal moments $\mu_p(x) = \int_0^{\infty} t^p \mu(t,x) dt$. We concentrate here on characterizing spreading by the second centered temporal moment $\sigma_t^2(x) = \mu_2 - \mu_1^2$ and by the associated equivalent macrodispersivity $\alpha_{Leq} = U^2\sigma_t^2/2x$ (see e.g. [11]). This is the basic parameter characterizing the spreading mechanism, and it is exhaustive for a Gaussian plume. For plumes which display a non-Gaussian behavior, like those considered in [11], the transport description through σ_t^2 is not exhaustive; still, it represents a first step toward a more complete characterization of transport.

Most previous studies dealing with the above problem is limited to the analysis of weakly heterogeneous media, say $\sigma_Y^2 \leqslant 1$(see, e.g., [12,20,19,7] for a comprehensive view of the literature on the subject, see also the recent books by Zhang [24] and by Rubin [23]). It was found that for realistic values of the Peclet number $Pe = UI_Y/D_0$ (where I_Y is the heterogeneity scale of Y and D_0 the local diffusion or

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dispersion) encountered in applications, local diffusion or dispersion have a small diminishing effect on the longitudinal dispersivity for stationary media, of finite integral scale. However, the impact of transverse diffusion or dispersion becomes very large for stratified media, as shown in the pioneering study of Matheron and de Marsily [18]. Furthermore, the most important component is the transverse one [7], which is more effective in mixing solute among streamtubes. For this reason, the transverse local dispersivity generally leads to an α_{Leq} reduction, a well-known result which traces back to the paper by Matheron and deMarsily [18].

The numerical modeling of transport in a specific alluvial aquifer [17] characterized by large contrast of permeability of different facies, indicates that molecular diffusion may have a significant role upon release of solute from low conductivity zones.

A more systematic investigation of transport in strongly heterogeneous aquifers ($\sigma_Y^2 > 1$) and the effect of local diffusion upon α_{Leq} has been presented recently by the extensive numerical simulations of [5], who have solved flow and transport in 2D media of multi-Gaussian Y, with high accuracy and large size of the flow domain and plume. Thus, they have found that for $Pe = 1000$ the impact of diffusion on α_{Leq} is negligible for $\sigma_Y^2 \leqslant 4$ and significant for $\sigma_Y^2 = 9$. For $Pe = 100$ the effect is more significant with a reduction of α_{Leq} by 10%, 25% and 43% for $\sigma_Y^2 = 4$, 6.25 and 9, respectively. Although the authors offer a qualitative explanation of this effect, it is based on inference rather than a direct examination of the velocity field and concentration distribution. As we shall show in the sequel, determining the effect of diffusion numerically is not a simple matter for large σ_Y^2 and in any case 2D transport is of rather theoretical interest.

In contrast, our aims here are: (i) to investigate transport in formations of 3D structure; (ii) to identify the mechanism by which finite Pe influences longitudinal spreading; (iii) to extend the analysis to formations of non-Gaussian logconductivity for which the advective ($Pe = \infty$) transport is anomalous i.e. α_{Leq} is unbounded, and (iv) to examine the impact of finite Pe on anomalous transport in general.

To achieve these goals we employ a model of structure we have coined as multi-indicator, which we explored extensively in the past (see, e.g., [2,16]), in order to investigate advective transport. The structure is modeled as an ensemble of inclusions of different and independent K (Fig. 1), which can be regarded as a particular scheme of discretization of the K spatial distribution. It can reproduce any univariate pdf $f(K)$ of given integral scale I_Y, by a proper selection of inclusions K values and size R, respectively. However, higher order moments are different for instance from that of multi-Gaussian structures.

The advantages of this model are: (i) it is amenable to very accurate 3D numerical simulations even for large σ_Y^2 and large size of flow domain and solute plume, which are needed in order to eliminate influence of boundaries; the latter is important in order to ensure the stationary and ergodic conditions which are considered in the present study. To our best knowledge numerical studies in the past could not achieve such conditions; (ii) although demanding in terms of computer time and memory, computations could be carried out for a large number of simulations, to cover a wide range of parameters values (σ_Y^2, plume size, travel distance); (iii) we were able to develop an approximate simplified model that was found to lead to accurate results as compared with numerical simulations. It reduced the computation of travel time distributions and particularly of α_{Leq} to a few quadratures. We have compared it recently in the restricted case of 2D transport with the values obtained by [5] and found good agreement for $\sigma_Y^2 \leqslant 6$ [9] and (iv) the approximate, semi-analytical model, permitted us to examine in depth the transport mechanism and to reveal its main features. Gaining this qualitative understanding may be viewed as one the main achievements of our studies.

In the present article we expand our investigations to account for the presence of diffusion, as quantified by a finite Pe, and its influence on transport. We employ the same structural model and the ensuing velocity field, but supplement the solute particles motion by a diffusive component.

This study should be regarded as of a fundamental nature, the aim being to advance the understanding of the role of the basic mechanisms of advection and molecular diffusion and their interplay upon transport in highly heterogeneous aquifers. The assumed conditions of mean uniform flow, stationary structure, ergodic plume and its characterization by the longitudinal macrodispersivity, constitute limitations which do not make yet possible direct use in specific applications. Still, we believe that this is a necessary step, which already may serve a guidance to numerical modelers, for example on how to incorporate molecular diffusion in zones of low permeability and to estimate beforehand its impact.

The plan of the paper is as follows: first we recapitulate briefly our previous work and findings relevant to the present study, we present and analyze next the results of numerical simulations of advective–diffusive transport for isolated inclusions, subsequently we use the results in order to determine α_{Leq} for heterogeneous media made up from an ensemble of inclusions and then anomalous transport is examined in a general manner.

2. Brief recapitulation of previous work on advective solute transport by the multi-indicator model

2.1. The structural model and numerical simulations of advective transport

The 3D heterogeneous medium is modeled by an ensemble of N elements of different $K_i (i = 1, \ldots, N)$ and the setup is illustrated in Fig. 1 (reproduced from [11]). Thus, Fig. 1a depicts the common fine scale discretization of the medium, in which pixels are of correlated K values. Fig. 1b shows a type of multi-indicator model, namely cubical elements of finite size and independent K values that tessellate the space; the size of the elements is proportional to the integral scale of the original field of Fig. 1a. A further simplification is achieved by using a densely packed ensemble of spherical elements (Fig. 1c) of equal radius R. In this case the conductivity of the matrix filling the space between inclusions (30% of the space) is selected to be equal to K_{eff}, the effective one of the medium; we emphasize that in the present setup K_{eff} depends only on the logconductivity pdf. The matrix can be regarded as a swarm of very small spheres which fill the space, of same K distribution as the inclusions of radius R, but of negligible impact upon spreading due to their small dimension.

The inclusions lie in a large ellipsoid which is surrounded by the matrix of effective conductivity, with a uniform velocity field $\mathbf{U}(U, 0, 0)$, applied at infinity. The velocity potential was determined numerically by expanding the interior and exterior one for each inclusion in a series of harmonic functions. The unknown coefficients were determined by matching the normal flux and the head at each inclusion boundary; conservation of mass was satisfied exactly whereas continuity of head was ensured in an approximate manner, but very accurately due to the large number of terms [15]. The velocity field was obtained analytically by differentiation of the potential. Transport was modeled by injecting a large number M of particles along an area A in the injection plane at $x = 0, t = 0$ and by moving them by the fluid velocity until control planes at x is reached. The travel time $\tau_j(x, b_y, b_z)$ $(j = 1, \ldots, M)$ is then recorded, with $y = b_y, z = b_z$ standing for the initial coordinate in A. The plume is of large A at the heterogeneity scale I_Y and can be regarded as ergodic. Then, for a given realization and for uniform mass distribution in A [16] the relationship