A Stochastic Approach to Estimate Block Dispersivities that Includes the Effect of Mass Transfer Between Grid Blocks

D. Fernàndez-Garcia and J. J. Gómez-Hernández

Abstract Efficiency constraints force the use of a coarse discretization of the numerical transport model compared with the detailed scale required for the most adequate description of the physical properties. Upscaling encompasses the methods that transfer small-scale information to the computational scale. The loss of small-scale information of aquifer properties to construct a numerical model by upscaling largely modifies the true heterogeneous structure of the aquifer compromising the final predictions of solute transport. Within this context, we present extensive Monte Carlo solute transport simulations in heterogeneous porous media to investigate the impact of upscaling on the evolution of solute plumes, and we analyzed the benefits of using enhanced block dispersion tensors in the advection-dispersion equation to compensate for the loss of information. In doing this, we show that when enhancing the block dispersion tensor to compensate for the loss of small-scale information, mass transfer between grid blocks is in turn amplified largely reducing macrodispersion in the upscaled model. We conclude that block dispersivities should consider not only the fluctuation of aquifer properties inside the block but also the simultaneous effect of enhanced mass transfer between all blocks of the numerical model. Then, using a stochastic approach, we present a new concept of block dispersivity that accounts for both effects: block heterogeneity and mass transfer between grid blocks. As a result, we quantified the amount of contribution that mass transfer effects has on block dispersivity.

1 Introduction

In order to efficiently make solute transport predictions in real field settings, complex transport models cannot afford to describe heterogeneity at the necessary detail scale required for an adequate description of the underlying processes. As a result, models are often used with a coarse grid discretization of the media. This implies a

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simplification of the physical problem, since not all the subgrid information on the spatial variability of the parameters is transferred to the numerical grid. In this context, upscaling is used to transfer small-scale information to the computational scale.

We present Monte Carlo solute transport simulations in heterogeneous porous media to investigate the impact of upscaling on the evolution of solute plumes. We show that usual upscaled transport models can largely underestimate the spreading of solute plumes even if block dispersivities are calculated as being representative of within-block heterogeneity. Two major effects were identified that can restrict the growth of the solute plume in the numerical upscaled model: (i) tensorial nature of hydraulic conductivity; and (ii) mass transfer effects between blocks of the numerical model. This paper focuses on the latter effect. In particular, we investigate the concept of block dispersivity and its relation with mass transfer between grid blocks.

2 Computational Investigations

2.1 Design of Solute Transport Monte Carlo Simulations

Transport simulations consider a square bidimensional confined aquifer with uniform mean flow in the x-direction. The domain extends 240 units in the x and y directions. Boundary conditions were no-flux for boundaries parallel to the mean flow and constant-head otherwise (mean hydraulic gradient J equal to 0.01). At the small scale, the hydraulic conductivity tensor is isotropic. The aquifer is heterogeneous and described by a spatially varying hydraulic conductivity such that the $\ln K(\mathbf{x})$ follows a multi-Gaussian random function. The geometric mean of the $\ln K(\mathbf{x})$ field is $K_G = 1$. The random function model is described by an isotropic exponential covariance function with the correlation scale (λ) set to 4 units. A very fine grid is used to generate a reference $\ln K(\mathbf{x})$ field through the GCOSIM3D code (Gómez-Hernández and Journel 1993) representing the real aquifer. The resolution of the fine-scale model is 4 grid-cells per correlation scale. The Monte Carlo transport simulation scheme consists in 50 realizations for each $\sigma^2_{\ln K}$ that ranged from 0.06 to 4. Each realization of the $\ln K(\mathbf{x})$ field is upscaled to a resolution referred to as 30-by-30, which correspond to the upscaling process of transferring the small-scale information (240×240 cells) to a regular computational grid of 30×30 blocks. For simplicity, at the fine-scale the transport model is purely advective. After upscaling, at the coarse-scale, solute transport is governed by the advection-dispersion equation that is used with an equivalent block hydraulic conductivity tensor and an equivalent block dispersivity tensor.

The impact of upscaling was then evaluated by comparing Monte Carlo solute transport simulations of a large plume moving through the reference $\ln K(\mathbf{x})$ fields with their corresponding upscaled model. A seven-point finite difference groundwater flow model, MODFLOW2000 (Harbaugh et al. 2000) was used to solve the flow problem and a transport code based on the Random Walk Particle Method (Fernàndez-Garcia et al. 2005) was used to simulate solute transport. Transport simulations start by injecting a large number of particles (5,000) equidistantly distributed in a line transverse to the mean flow direction. This line is 35λ long and is centered with respect to the transverse dimension (Fig. 1). The first arrival time and the position of particles passing through 20 control planes transverse to the mean flow direction and located at several distances away from the source were tracked until particles exited the lower constant head boundary. This allowed measuring longitudinal macrodispersivity at control planes. We calculate macrodispersivities from Monte Carlo simulations by using the method of temporal moments as applied to particle tracking transport codes in Fernàndez-Garcia et al. (2005).

We note that the objective of this work is not to examine the performance of solute transport under different choices of boundary and initial conditions, but to evaluate transport behavior with a change of support scale under the same conditions. Thus, we consistently estimate block properties (upscaling rule) and solute transport behavior always using a slug injection to ultimately estimate transport behavior/properties through flux-averaged concentrations.

2.2 Upscaling Methodology

The selected method for the calculation of block hydraulic conductivities $\mathbf{K}_b$ is known as the Simple Laplacian method with skin (Wen and Gómez-Hernández 1996). For a given realization of the lnK(**x**) field, the region being upscaled is isolated from the rest

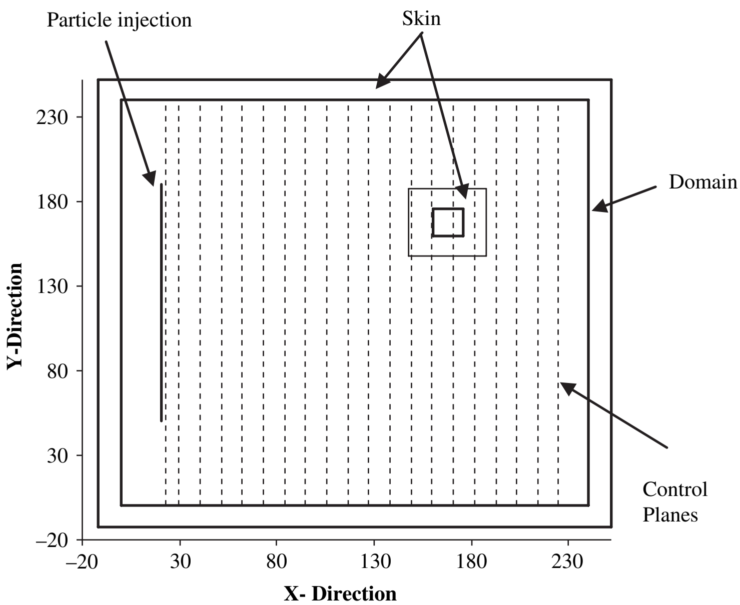

Fig. 1 Sketch of transport simulations showing the initial location of particles, the control planes where mass fluxes are measured

of the system. This region not only comprises the portion of the heterogeneous aquifer delineated by the grid-block, but also includes a small portion of the heterogeneous aquifer adjacent to the grid-block referred to as the skin (Fig. 1). The skin is designed to approximately emulate the original water head boundary conditions on the grid-block without having to solve the flow problem for the entire domain. In this work, the skin spans over 3λ to minimize boundary effects and block hydraulic conductivity $\mathbf{K}_b$ is assumed to be a diagonal second-order tensor with principal directions parallel to the block sides. The principal components were calculated as

$$K_{b,ii}(\mathbf{x}) = \frac{\int_{V(\mathbf{x})} q_i(\mathbf{u})d\mathbf{u}}{\int_{V(\mathbf{x})} -\partial h/\partial x_i(\mathbf{u})d\mathbf{u}} \tag{1}$$

where V(x) denotes the volume of the grid-block the centroids of which is at **x**, **q** is the darcy velocity, and h is the piezometric head. We considered a diagonal $\mathbf{K}_b$ tensor for being the usual assumption underlying most benchmark groundwater flow models. We proposed a numerical method that evaluates block dispersivities by simulating a natural-gradient tracer test inside the isolated block region, so that the solute tracer only samples the block heterogeneity. This choice stems from the fact that field tracer tests are often attempted as a means of estimating input dispersivities for transport models. For each isolated block with skin, steady-state flow is achieved using the needed boundary conditions (i.e. linearly varying pressure head at the block boundaries) to originate a mean flux equal to the block averaged one. Then, a Dirac-input tracer line source is injected in a line transverse to the block averaged flux and situated at the upgradient limit of the block. Block dispersivity values, A_L and A_T, are estimated from the mass flux breakthrough curve by the method of temporal moments as,

$$A_L = \frac{L}{2}\frac{\sigma_t^2}{T_a^2} - \alpha_L \tag{2}$$

$$A_T = \frac{\sigma_y^2}{2L} - \alpha_T \tag{3}$$

where L is the size of the block in the mean flow direction, α_L and α_T are respectively the longitudinal and transverse local dispersivity, $\sigma^2{}_t$ is the variance of travel times of particles exiting the block, $\sigma^2{}_y$ is the variance of transverse displacements of particles exiting the block, and T_a is the mean arrival time.

2.3 Simulation Results

Figure 2 shows the scale-dependence of longitudinal dispersivity as a function of travel distances for different $\sigma^2{}_{\ln K}$ and transport models. We distinguish two important features. At early times, when particles have still not travelled through various

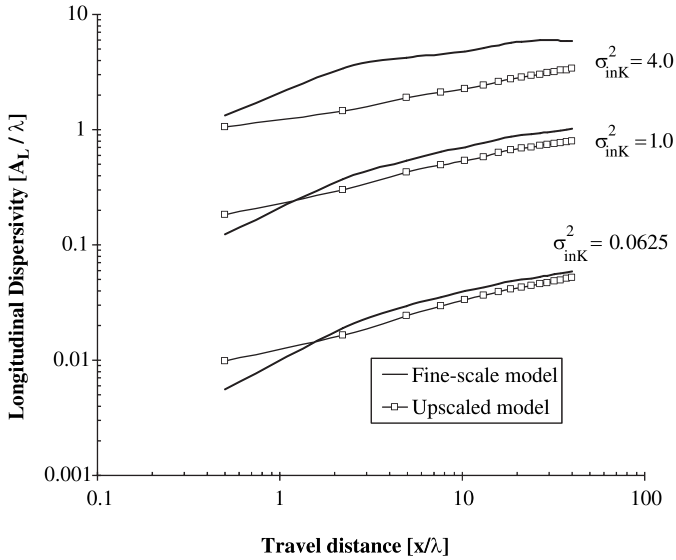

Fig. 2 Comparison of the scale-dependence of longitudinal macrodispersivity obtained from fine-scale simulations with those for the upscaled model

grid-blocks, dispersivities are larger than those corresponding to the fine-scale model mainly because block dispersivity was not considered a time-dependent parameter but represents the time-average behavior within a block. This effect rapidly vanishes when particles passes through few blocks.

At late times, block dispersivity approaches an asymptotic dispersivity value that is significantly smaller than those for the fine-scale model. Asymptotic behavior is seen in all cases yet not clearly appreciated in Fig. 2 because we used logarithmic scales. This can be attributed to several effects (Fernàndez-Garcia and Gómez-Hernández 2006). Among them, we suspect that mass transfer interaction between grid-blocks of the numerical model and the tensorial nature of hydraulic conductivity can largely affect the behavior of solute transport in the upscaled model. For instance, it is suspected that when enhancing the block dispersion tensor to compensate for the loss of velocity variability through upscaling, transverse mass transfer between grid blocks is in turn amplified reducing macrodispersion. This issue is analyzed in the following sections based on the small perturbation stochastic approach.

3 A Stochastic Approach to Estimate Block Dispersivities

3.1 General Formulation

This section presents a novel stochastic approach to the problem of upscaling dispersivity in heterogeneous formations. Considering a nonreactive solute plume moving through a stationary lnK random field under steady-state mean uniform flow parallel to the x_1 coordinate, the effective spatial moments of a solute at large travel distances are written as (e.g., Gelhar and Axness 1983)

$$\lim_{x_1\to\infty}\frac{1}{2}\frac{M_{ij}(x_{m,1})}{x_{m,1}} = \left(\alpha_i + \frac{\tau D_d\phi}{q_m,\,1}\right)\delta_{ij} + \sigma_f^2\lambda_1 B_{ij}(\alpha_i,\lambda_i) \tag{4}$$

where $x_{m,1}$ is the mean travel distance, M_{ij} is the effective spatial moment tensor, α_i are the local dispersivity coefficients, ϕ is the porosity, τ is the tortuosity, $\sigma^2{}_{\ln K}$ is the variance of the natural log of K, λ_i are the correlation scales in the ith-direction, and B_{ij} is a real function expressed as

$$B_{ij} = \frac{1}{\sigma_{\ln K^2\lambda_1}}\int_{-\infty}^{+\infty}\frac{1}{q_{m,1}^2\beta(\mathbf{k})}S_{q_iq_j}(\mathbf{k})d\,\mathbf{k} \tag{5}$$

$$\beta(\mathbf{k}) = ik_1 + \alpha_i k_i^2 \tag{6}$$

where $S_{\mathbf{qq}}$ is the spectrum of the darcy velocity field. Einstein's convention is used. Following Dagan (1994), the basic requirement for upscaling is that the statistics of the spatial moments at the fine-scale should be the same as those obtained in the upscaled model,

$$\frac{1}{2}\frac{M_{ij}(x_{m,1})}{x_{m,1}} = \frac{1}{2}\frac{M_{ij}^m(x_{m,1})}{x_{m,1}} \tag{7}$$

where the superscript m denotes that the quantity is related to the simulated values given by the numerical model. The problem is reduced to resolve M^m. To achieve this, we view the process of upscaling the hydraulic conductivity field as a filtering process. The filter is such that suppresses the high frequency lnK fluctuations that cannot be represented by the numerical model. We used a low-pass filter function denoted as $F_g(\mathbf{k})$. In commercial groundwater systems based on the classical advection-dispersion equation, the increase in block dispersivity to account for a coarse discretization is directly translated in the large time growth of spatial moments as

$$\lim_{x_1\to\infty}\frac{1}{2}\frac{M_{ij}(x_{m,1})}{x_{m,1}} = \left(\alpha_i + \frac{\tau D_d\phi}{q_{m,1}}\right)\delta_{ij} + A_i^b\delta_{ij} + \sigma_f^2\lambda_1 B_{ij}^m(A_i^b,\alpha_i,\lambda_i) \tag{8}$$

$$B_{ij}^m = \frac{1}{\sigma_{\ln K}^2\lambda_1}\int_{-\infty}^{+\infty}\frac{1}{q_{m,1}^2}\beta^m(\mathbf{k})F_g(\mathbf{k})S_{q_iq_j}(\mathbf{k})d\,\mathbf{k} \tag{9}$$

$$\beta^m(\mathbf{k}) = ik_1 + \alpha_i k_i^2 + A_i^b k_i^2 \tag{10}$$

where A^b denotes the increase in block dispersivity due to block heterogeneity. Since the terms (real part) multiplying the velocity spectrum in the integration of B_{ij} and $B^m{}_{ij}$ are all even functions, and knowing that $S_{\mathbf{qq}}$ is odd if $i\neq j$, in this case, the requirement of upscaling (at large travel distances) is fulfilled and reduced to the following nonlinear system of n equations with n unknowns ($A^b{}_i$) , being n the dimension of the problem,

$$\sigma^2_{\ln K}\lambda_1 B_{ii}(\alpha_i, \lambda_i) = A^b_i + \sigma^2_{\ln K}\lambda_1 B^m_{ii}(A^b_i, \alpha_i, \lambda_i, F_g) \quad i = 1, \ldots, n \tag{11}$$

3.2 Evaluating Mass Transfer Effects on Block Dispersivity

In this section we discuss the influence of mass transfer effects on block-effective dispersivities for the case of a two-dimensional aquifer with an isotropic exponential covariance function. We only focus on the underestimation of the longitudinal spatial moment due to mass transfer effects in the upscaled model. Thus, the objective is not to exactly solve the coupled system of equations but to understand and quantified mass transfer effects in modeling solute transport with a numerical code. Assuming an isotropic dispersivity, i.e., $A^b{}_i = A^b$ and $\alpha_i = \alpha$, the problem of upscaling dispersivity is simplified to find the root of the following equation,

$$\sigma^2_{\ln K}\lambda_1 B_{11}(\alpha, \lambda) - A^b - \sigma^2_{\ln K}\lambda_1 B^m_{11}(A^b, \alpha, \lambda, F_g) = 0 \tag{12}$$

To obtain simple analytical expressions of B^m, we employed a low-pass filter function similar to Rubin's Nyquist model (Rubin et al. 1999), defined as a function that takes the value of unity if $|\mathbf{k}| \leq \pi/\Delta$, where Δ is the domain discretization, assumed constant for all directions. It can be shown that this definition, which is mathematically convenient, yields analytical solutions which effectively behave as Rubin's Nyquist model for negligible mass transfer (A^b approaching zero in $B^m{}_{11}$). Defining $\varepsilon = (\alpha + A^b)/\lambda$ and $\xi = \pi/(\Delta/\lambda)$, using the relationship between the velocity spectrum and the lnK spectrum (Gelhar and Axness 1983), and expressing B_{11} in polar coordinates, we obtain after integration,

$$B^m_{11}(\varepsilon, \xi) = \frac{1}{2}\int_0^{\xi} (-3\varepsilon z - 2\varepsilon^3 z^3 + 2(1 + \varepsilon^2 z^2)^{3/2})(1 + z^2)^{-3/2} dz \tag{13}$$

Using (13) in (12), we solve for A^b by means of finding the root of equation (12). Knowing that $\alpha << A^b$ for general aquifer conditions, we consider α negligible in the analysis. We quantified the contribution of mass transfer to block dispersivity using the relative increase in A^b due to mass transfer defined as,

$$\varepsilon_r = \frac{A^b(\varepsilon, \Delta) - A^b(\varepsilon = 0, \Delta)}{A^b(\varepsilon = 0, \Delta)} \times 100 \tag{14}$$

Figure 3 shows the relative increase in A^b due to mass transfer effects as a function of the size of grid-block, Δ/λ, and degree of heterogeneity, $\sigma^2{}_{\ln K}$, for the case of

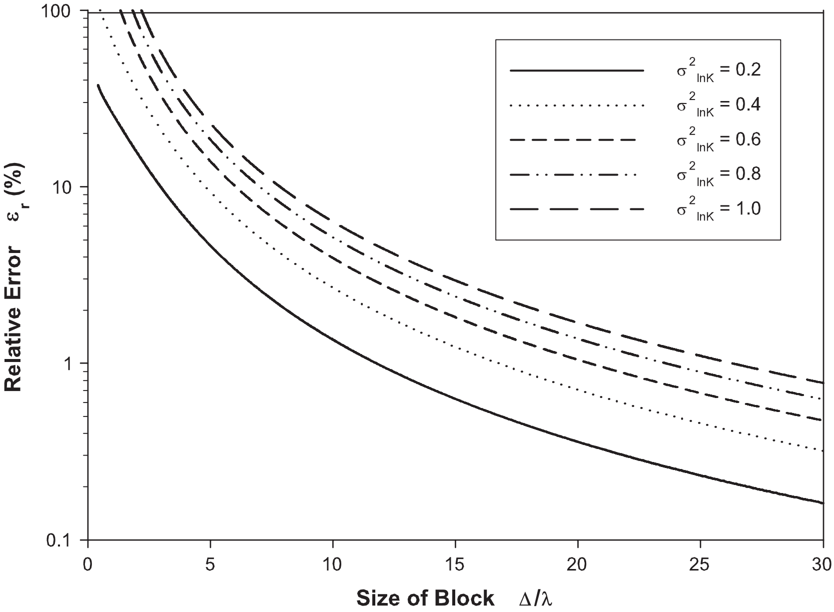

Fig. 3 Relative increase in block dispersivity due to mass transfer as a function of size of grid-block and degree of heterogeneity for the case of a two-dimensional isotropic exponential covariance function

a two-dimensional isotropic exponential covariance function. The relative contribution of mass transfer decays with block size and σ^2_{lnK}. Note that as Δ/λ approaches zero from the right ε_r tends to infinity because block dispersivity with negligible mass transfer $A^b(\varepsilon{=}0,\Delta)$ approaches zero faster than $A^b(\varepsilon,\Delta)$. For the usual case of block sizes of few correlation scales, we see that the contribution of mass transfer is very important, for instance, ε_r is about 57 per cent for the case of $\Delta/\lambda{=}3$ and $\sigma^2_{\mathrm{lnK}}{=}1$.

We note that in realistic modeling applications the form of the dispersivity tensor is usually anisotropic with $A_1^b/A_2^b \approx 10$. In this case, mass transfer effects can be significantly decreased, being less dramatic. Nonetheless, our combined numerical-analytical approach suggests that mass transfer interaction between blocks of the numerical model should be taken into consideration when quantifying block dispersivity values.

4 Conclusions

We used an analytical stochastic approach combined with Monte Carlo simulations to study the meaning of block dispersivity as frequently utilize in modeling contaminant transport. Specifically, we focus on the relationship between mass transfer between blocks of the numerical model and block dispersivities. We found that block dispersivities used as input in transport models should not only reflect the underlying heterogeneous structure filtered out by the model but also consider the effect of mass transfer and the interaction between grid-blocks of the numerical model. These effects are estimated to be significant with decreasing block size and increasing degree of heterogeneity.

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