On the use of the concept of block-scale macrodispersion for numerical simulation of flow and transport in heterogeneous formations

ALBERTO BELLIN[1], ALISON LAWRENCE[2] and YORAM RUBIN[2]

1. *Dipartimento di Ingegneria Civile ed Ambientale, Università di Trento, via Mesiano 77, 38050 Trento, ITALY*
2. *Department of Civil and Environmental Engineering, University of California at Berkeley, Berkeley, California 94720, USA*

Abstract The use of the block-scale macrodispersivity concept to model the effects of the unresolved sub-grid hydraulic property variations, which are progressively wiped-out with the coarsening of the computational grid, is discussed by means of an example. In stochastic modeling, a computational grid with block sizes of only a fraction of the log-conductivity integral scale should be used to reproduce accurately the hydraulic property variations. To reduce the ensuing computational effort of Monte Carlo simulations, we propose simulating solute spreading using larger grid blocks, while reproducing the effect of the sub-grid spatial variability of the hydraulic conductivity, which is not captured directly on the grid, by Brownian motion with the time-dependent effective block-scale dispersion tensor. The resulting plume moments compare very well with those obtained using fine grid blocks, showing that the block-scale dispersivity concept provides a valid alternative to the traditional upscaling techniques for reducing the computational burden of numerical simulations without compromising accuracy.

Introduction

The spreading of solutes in natural formations is controlled by hydraulic property variations acting on a multiplicity of continuous and discrete scales. Stochastic modeling is often used to account for both the variations of the hydraulic conductivity, K, and uncertainty. The latter accounts for incomplete information on the actual hydraulic property variations. To capture accurately the spatial variability of K, a very fine grid is required, with typical dimensions being only a fraction of the log-conductivity integral scale. The ensuing computational burden is one of the main drawbacks limiting the use of stochastic modeling in applications, and its relevance increases when stochastic modeling calls for Monte Carlo simulations. The tendency is to reduce the computational cost by using larger grid block scales, and reducing the resolution. Using large grid blocks is permitted only if measures are introduced to account for the loss of resolution caused by the homogenization.

The idea of using an upscaled macrodispersion coefficient was explored by Dagan (1994) and pursued further by Rubin et al. (1999), who derived and discussed the block dispersion coefficient for ergodic plumes. In Bellin et al. (2001, submitted), a method is proposed which reproduces the large-scale variability directly on the grid, and models the unresolved small-scale variations through suitable block-scale effective macrodispersion coefficients, which depend on both plume and block scales. In this paper, we summarize those calculations and show an example of the results.

The block-scale dispersion coefficient

We start by considering that the following length scales are important in numerical modeling of transport in heterogeneous formations: I_Y, the integral scale of the hydraulic log-conductivity, $Y=lnK$, which represents the hydraulic property variations of the geological formation; the characteristic size of the source, l; the characteristic size of the grid-blocks, Δ; and the length representing the characteristic scale of the variability reproduced directly on the grid, l, which corresponds to the highest observable frequency $f = 1/(2l)$. In applications, the latter can be roughly defined as the dimension of the zone of uniform hydraulic conductivity. The spreading of the plume is controlled by the interplay between these scales of variability. Following Rubin et al. (1999) we assume that the local fluctuation of Y from its expected value, m_Y, can be split into two components

$$Y' = \overline{Y} + \widetilde{Y}, \tag{1}$$

where $\overline{Y}$ is the zero-mean fluctuation representing the variations captured by simulations, and $\widetilde{Y}$ represents the subgrid variability, such that l is proportional to $I_{\overline{Y}}$, the integral scale of $\overline{Y}$.

Monte Carlo simulations use repeated solutions of flow and transport in which the hydraulic conductivity is homogenized over volumes as large as the grid blocks, neglecting the hydraulic property variations at scales smaller than l. To avoid this problem, blocks with size equal to only a fraction of I_Y are used in numerical simulations, leading to a large computational cost, compared with traditional models.

In a recent paper Rubin et al. (1999) introduced the concept of block-scale macrodispersion to represent the effects on the plume of the wiped-out variability. According to Rubin et al. (1999), the macrodispersion tensor D_{ij} is composed of two terms: the large-scale macrodispersion tensor $\overline{D}_{ij}$ representing hydraulic property variations at scales larger than l, and the block-size macrodispersion tensor $\widetilde{D}_{ij}$ modeling the wiped-out small-scale variability

$$D_{ij}(t) = \overline{D}_{ij}(t) + \widetilde{D}_{ij}(t); \tag{2}$$

For a constant mean velocity vector $\mathbf{U}$ parallel to the $x_1$direction, $\overline{D}_{ij}$ and $\widetilde{D}_{ij}$ assume the following expressions

$$\overline{D}_{ij}(t) = \frac{U^2}{(2p)^{m/2}} \int_0^t \left[\int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} e^{-ik_1 U t'} \left(d_{1i} - \frac{k_1 k_i}{k^2} \right) \left(d_{1j} - \frac{k_1 k_j}{k^2} \right) F(\mathbf{k}) \hat{C}_Y(\mathbf{k}) d\mathbf{k} \right] dt', \tag{3}$$

and

$$\tilde{D}_{ij}(t)=\frac{U^2}{(2p)^{m/2}}\int_0^t\left[\int_{-\infty}^{\infty}....\int_{-\infty}^{\infty}e^{-ik_1Ut'}\left(d_{1i}-\frac{k_1k_i}{k^2}\right)\left(d_{1j}-\frac{k_1k_j}{k^2}\right)(1-F(\mathbf{k}))\hat{C}_Y(\mathbf{k})d\mathbf{k}\right]dt'; \quad (4)$$

where $\hat{C}_Y$ is the Fourier transform of the log-conductivity covariance function, d is the Kronecker delta, k_i, $i=1,..,m$, with m representing the space dimensionality, are the components of the wavelengths $\mathbf{k}$, and $d\mathbf{k}=dk_1...dk_m$. In (3) and (4) F is the following filter

$$F(\mathbf{k})=\begin{cases}1 & \text{for } |k_i|\le \pi/\lambda_i\ ,i=1,...m\\ 0 & \text{otherwise}\end{cases}. \quad (5)$$

In Monte Carlo simulations $\overline{D}_{ij}$ is modeled through the variations of the hydraulic conductivity reproduced directly on the grid, and $\tilde{D}_{ij}$ represents the effects on the plume spreading of the wiped-out variability. In this paper, we propose to model the wiped-out variability through the diffusive term of the advection-dispersion equation with the dispersion coefficient given by (4). In principle, this allows using larger blocks in the numerical simulations, reducing the computational effort without compromising accuracy.

In the next section, we show with an example how this can be accomplished. There are of course limits to the maximum block's size that can be employed in numerical simulations, which are discussed in detail in the work by Bellin et al. (2001, submitted).

An example of application

We consider here, as an example, a two-dimensional isotropic formation with the following model of the hydraulic property variations

$$C_Y(r)=s_Y^2e^{-r'},\quad r'=\sqrt{\frac{r_1^2+r_2^2}{I_Y^2}}\ , \quad (6)$$

where r_i, $i=1,2$, is the i-th component of the two-point separation distance. The hydraulic conductivity is first generated over a regular grid with spacing $D_1=D_2=0.25I_Y$, by using HYDRO_GEN, the generator of random functions developed by Bellin and Rubin (1996), and then it is filtered to remove fluctuations at frequencies larger than $f=1/(2l)$ obtaining $\overline{Y}$. Flow is solved by the Galerkin's method with triangular elements and linear shape functions. Additional information concerning the Galerkin's scheme and its implementation in heterogeneous formation can be found in the paper by Bellin et al. (1992). Furthermore, in numerical simulations the size of the computational grid blocks, Δ, is assumed as large as l.

We consider here the case of an instantaneous release of solute with constant concentration, C_0, within the surface A_0. Transport is solved in a Lagrangian framework in which the total mass of solute is divided into a large number, *NP*, of non-interacting particles, which are displaced according to the following particle tracking algorithm

$$X_{j,i}^{(k)}(t) = X_{j,i}^{(k)}(t-\Delta t) + v_i^{(k)}[\mathbf{X}_j^{(k)}(t-\Delta t)] + \sqrt{2\,\tilde{D}_{ii}(t)\,\Delta t}\; e_{j,i}^{(k)} \qquad (7)$$

where, $X_{j,i}$ is the *i*-th component of the trajectory of particle number *j*, v_i is the Eulerian velocity computed numerically from the solution of the flow equation, Δt is the time step used to solve the transport problem, and $e_{j,i}$ is a normally distributed random number with mean zero and unit variance. Here and in the following, the exponent *(k)* is used to indicate quantities computed in the *k*-th Monte Carlo realization. The second term on the right-hand side of (7) simulates the convective effects resulting from the variability reproduced on the grid, and the third term reproduces the macro-dispersive effects of the wiped-out variability. We neglect pore-scale dispersion, which only effects the plume moments appreciably for large traveling distances (Fiori, 1996).

We describe the plume behavior through the longitudinal effective second order moment, $< S_{11} >$, which in the Lagrangian framework used in this work is computed as follows:

$$\begin{aligned} < S_{11}(t) > &= \frac{1}{MC}\sum_{k=1}^{MC} S_{11}^{(k)}(t) = \frac{1}{MC}\sum_{k=1}^{MC}\frac{1}{NP}\sum_{j=1}^{NP}\left[X_{j,1}^{(k)}(t) - R_1^{(k)}(t)\right]^2 \\ R_1^{(k)}(t) &= \frac{1}{NP}\sum_{j=1}^{NP} X_{j,1}^{(k)}(t) \end{aligned} \quad , \qquad (8)$$

where $R_1^{(k)}$ is the longitudinal component of the trajectory of the plume centroid in the *k*-th Monte Carlo realization, and *MC* is the number of Monte Carlo realizations determined such that convergence of ensemble statistics is ensured. It can be shown that the moments (8) converge to the exact solutions as the number of particles grows large. The numerical moments computed by (8) are compared with analytical first-order solutions.

Figure 1 shows $< S_{11} >$ obtained from numerical simulations conducted with several block sizes and with the wiped-out variability simulated through $\tilde{D}_{ij}$ (4). The source area is rectangular with sides $l_1 = I_Y$ and $l = 10 I_Y$ along the longitudinal and transverse directions, respectively. The first order solution is obtained for vanishing longitudinal source size and $l = 10 I_Y$.

The two cases $\Delta = l = 2 I_Y$ and $\Delta = l = 6 I_Y$ show a relative difference varying between 5.1% and 7.4%, for $tU / I_Y > 5$, such that it can be neglected in applications. Additional numerical simulations showed that this difference reduces further, being comprised between 2.2% and 2.9%, when the case $l = 6 I_Y$ is simulated with $\Delta = 4 I_Y$, such that $\Delta / I_{\bar{Y}} = 1.2$ as for $\Delta = l = 2 I_Y$.

We compare now large- and fine-grid simulations, with the latter obtained by using blocks of size $\Delta_{fg} / I_Y = 0.25$, which is dictated by the need to reproduce the hydraulic conductivity field over the grid with a negligible wiped-out variability (Bellin et al, 1992). Fine grid simulations are then conducted by setting $\tilde{D}_{ii} = 0$ in (7). The relative difference, which for $\Delta = l = 2I_Y$ and $tU / I_Y > 5$ varies between 8.6% and 12.7%, with the smaller value observed at the larger times, is between 15.1% and 19.5% for $\Delta = l = 6I_Y$.

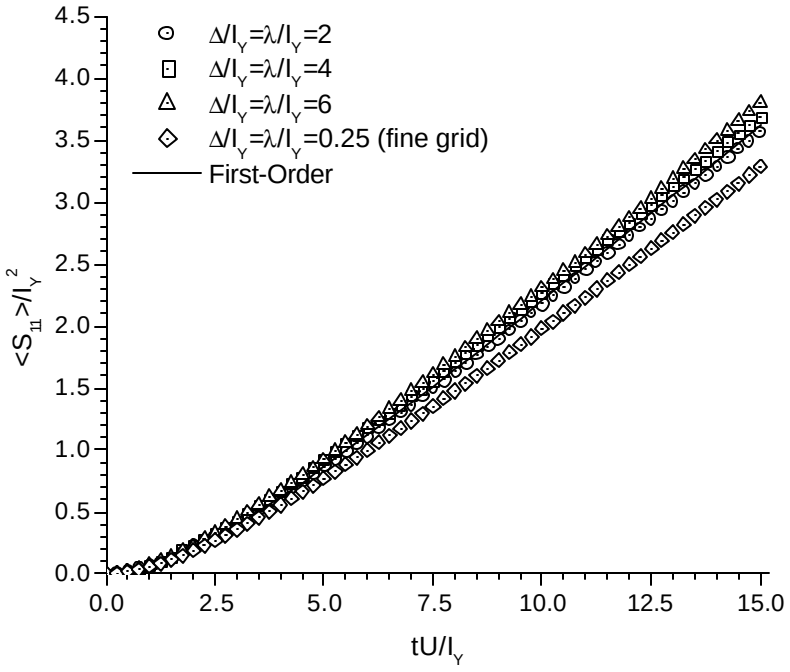

Figure 1: Comparison between the longitudinal second-order plume moments obtained with several block sizes. The first-order solution, obtained in absence of wiped-out variability, and the fine-grid numerical solution are also shown. In all cases, the transverse source size is $l / I_Y = 10$ and $s_Y^2 = 0.2$. Results are obtained with 2000 Monte Carlo realizations.

These differences originate from the neglected terms of order higher than s_Y^2 in (4), which are instead included in the fine grid simulations, leading to numerical simulations which disregard the non-linear effects of the wiped-out variability on the solute spreading, and of the progressive deterioration of accuracy of the numerical simulations as the block's size grows large. The latter is the consequence of the fact that the same level of accuracy in the reproduction of $\overline{Y}$ is obtained only if Δ is set in such a way as to maintain constant the ratio $\Delta / I_{\overline{Y}}$, and $I_{\overline{Y}}$, the integral scale of $\overline{Y}$, increases less than linearly with l (Rubin et al., 1999), such that doubling l results in a smaller relative increment of $I_{\overline{Y}}$. Thus, if Δ is set equal to l, simulations conducted with a large l suffer form a less accurate reproduction of the large-scale variations, $\overline{Y}$. To separate the

two effects, we repeated the simulations imposing the condition $\Delta / I_{\bar{Y}} = 0.25$, which leads to grid's sizes of $\Delta / I_Y = 0.4, 0.6$ and 0.8 for the three values of l considered in this paper. In doing that, the ratio $R_\Delta = \Delta / \Delta_{fg}$ is 1.6 for $l / I_Y = 2$, and it reaches the values of 2.4 and 3.2 for $l / I_Y = 4$ and $l / I_Y = 6$, respectively. The resulting moments are shown in Figure 2. The relative differences between large- and fine-grid simulations reduce with respect to the cases shown in Figure 1, varying between 2.2% and 4.6% for $l = 2I_Y$, and between 6.9% and 9.7% for $l = 6I_Y$. In both cases, the smaller relative difference is observed at the larger times. The case $l = 4I_Y$ lies in between the other two cases. Furthermore, Figure 2 shows that the numerical $< S_{11} >$ is larger than the corresponding fine-grid solution and that as l increases it approaches the first-order solution. This result shows that the effects on the solute spreading of the wiped-out variability can be reproduced through (4) with the above limitation for the grid's size, although the relative importance of the neglected higher-order terms increases with l, as more variability is reproduced through $\tilde{D}_{ij}$.

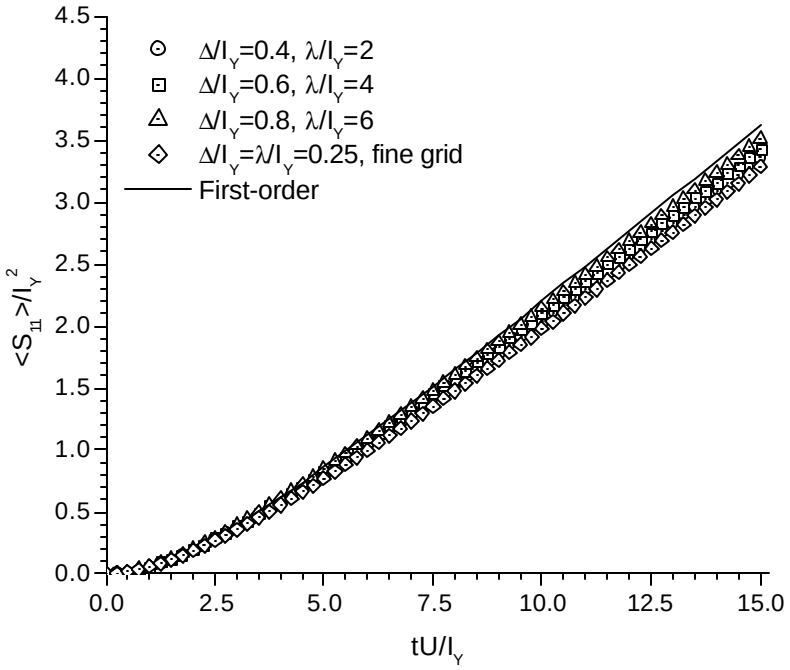

Figure 2: Comparison between the longitudinal second-order plume moments obtained while maintaining constant the ratio $\Delta / I_{\bar{Y}}$. The first-order solution, obtained in absence of wiped-out variability, and the fine-grid numerical solution are also shown. In all cases, the transverse source size is $l / I_Y = 10$ and $s_Y^2 = 0.2$. Results are obtained with 2000 Monte Carlo realizations.

In the remaining part of this paper, we discuss the results of an exercise conducted to verify if the concept of block-scale dispersivity can be used in simulations conditional to log-conductivity measurements. A more detailed discussion is presented in Bellin et al.

(2001, submitted). The actual longitudinal second-order moment, S_{11}, obtained numerically from a realization of K, which is assumed as the true picture of the aquifer, is compared with $< S_{11} >$ obtained from Monte Carlo simulations conditional to the measurements of *K* extracted from the same reference field. Measurements are taken over a regular grid with spacing $d = 2 I_Y$ in both longitudinal and transverse directions, $l = 2 I_Y$, and the block's size is fixed at $\Delta = 0.4 I_Y$. Numerical results discussed in Bellin et al. (2001, submitted) show that $< S_{11} >$, conditional to the measurements, reproduces the main features of the actual moment, S_{11}, much better than the corresponding unconditional moment. However, as l increases, the difference between conditional and unconditional moments vanishes, since $\tilde{D}_{ij}$, (4), is obtained for the unconditional case. Furthermore, the one-standard deviation interval of confidence increases with the travel distance, leading to the conclusion that uncertainty increases with the travel distance. The unconditional moments show a more regular behavior, which for $tU / I_Y > 4$, differs from that of the actual moment. The impact of the spacing between measurements is further discussed in Bellin et al. (2001, submitted).

The main conclusion that can be drawn from this work is that the block-scale macrodispersion coefficients can be used to model the wiped-out variations occurring when blocks larger than a fraction of I_Y are used in numerical simulations. This leads to the reduction of the computational cost of the numerical simulations. The need to obtain an accurate reproduction of $\bar{Y}$ poses a limitation to the grid size, which cannot exceed $0.25 I_{\bar{Y}}$, if the simulations are conducted with the objective of making the results independent from l. However, numerical simulations showed that from a practical point of view, block sizes as large as $1.2 I_{\bar{Y}}$ can be used if a moderate difference of about 2% between cases with different values of l can be accepted. However, it should be noted that higher-order effects are captured only for the variations reproduced on the grid, such that numerical and first-order solutions for $< S_{11} >$ tend to converge to the same result when l grows large.

Acknowledgments: The first author acknowledges the support of the program MURST-COFIN99 N. 9908168131_006: "Metodologie innovative per il monitoraggio, la gestione ed il controllo quali-quantitativo delle acque sotterranee." The second and the third authors acknowledge support from the National Science Foundation through grant EAR 9628306.

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