

## On the concept of block effective macrodispersivity

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**Abstract** A method for computing block-effective macrodispersivities is presented. The block-effective macrodispersivities model the effects of the numerical sub-grid scale variability, which are wiped out progressively in the process of grid coarsening. The goal is to represent the effects of sub-grid scale variability on mixing through coefficients that depend on the grid scales and the plume scales, as well as pore-scale dispersivity and travel time. This allows for more efficient and accurate numerical modelling, since numerical grid blocks can be set at scales larger than just a tiny fraction of the integral scale. This paper shows that the critical scales for constraining the numerical grid block's scales are those of the solute body.

### INTRODUCTION

Stochastic modelling of concentration often calls for Monte Carlo simulation. To capture accurately the effects of spatial variability, a very fine grid is required, with a typical grid block scale being equal to only a fraction of the conductivity's integral scale. The ensuing computational burden may be very large at times, and the tendency is to reduce the effort by increasing the grid block scale. The loss of resolution results in homogenization of relatively large areas, and in eliminating the sub-grid scale variability from consideration. Hence measures should be taken to account for the effects which are eliminated by homogenization.

In principle, one can homogenize the entire flow domain and solve the differential equation for the mean concentration and concentration variance instead. In this case, the velocity field is represented through its expected value, and the effects of heterogeneity through the macrodispersivity tensor. For consistency, the effects of heterogeneity should not be reproduced on the grid, and the measurements collected at the site need to be ignored (at least partly, since they will be used for inference of the geostatistical models), thus ignoring an expensive source of information. Additionally, the concentration's uncertainty is not adequately represented through its mean and variance.

An alternative hybrid approach is proposed which incorporates the benefits of the power of the Monte Carlo approach (e.g. the entire probability distribution function of the concentration can be computed instead of mean and variance), is conditional to measurements, and at the same time allows homogenization over portions of the domain through the use of block-effective macrodispersivities.

### TECHNICAL APPROACH

The common approach to numerical modelling can be characterized through the following length scales:  $I_T$ , the integral scale of the hydrogeological variable, for

example  $Y$  can be the commonly-used log conductivity; and  $L_G$ , the characteristic length scale of the grid block.  $L_G \ll I_Y$  is commonly taken, and the common recommendation is to take  $L_G \sim 0.25I_Y$ . This allows accurate capture of the effects of spatial variability. If measurements are available, they can be used for conditioning. Another length scale is  $L_H$ , the length scale characterizing the variability of the pressure head. It is usually much larger than  $I_Y$  due to physical constraints, and is not considered as a constraining factor in grid design. Finally, the length scales of the solute body  $\ell_i$ ,  $i = 1, \dots, m$ , with  $m$  being the space dimensionality, are recognized only indirectly. It is accepted that if  $L_G \ll I_Y$ , the flow domain can be used for modelling solute bodies of any size.

Solving the advection–dispersion equation for the mean and variance of the concentration allows working with  $L_G > I_Y$ , as long as  $\ell_i$  are exceedingly large, much larger than  $I_Y$ , which is a major drawback. In this situation, the solute body is insensitive to local parameter configuration, and there is no need to condition the numerical grid on measurements.

We are interested in situations where  $\ell_i$  are not large. In this case, it is necessary to condition the grid on the measurements, but is it also necessary to generate a grid such that  $L_G \ll I_Y$ ? We introduce new length scales  $\lambda_i$ ,  $i = 1, \dots, m$ , which may be proportional to the average spacing between measurements. We consider the spectral density function  $S_Y(k_i)$  where  $k_i$ ,  $i = 1, \dots, m$ , is the wave number vector. According to Nyquist sampling theorem, the  $\lambda_i$  define upper cut-off values on the wave numbers which are reproduced on the grid. Sampling the  $Y$  field with spacing  $\lambda_i$  reproduces, in essence, the low wave number portion of  $S_Y$ , and wipes out the spectrum corresponding to the large wave numbers. The wiped-out sub-grid variability needs to be accounted for in support of the choice of grid blocks of dimension  $\lambda_i$ . “In essence” here means that the grid scale is not necessarily a sharp low-pass filter, and some of the high wave number spectra are folded into the low wave number ones.

Our proposal (Rubin *et al.*, 1999) is to take  $L_{G,i} \sim \lambda_i$ . The  $Y$  values at the grid nodes can be generated conditional to measurements. This will capture the low wave-number portion of the spectral density function. In parallel, block-effective macrodispersivities will be used to account for the sub-grid variability, conditional to the simulated low-wave numbers.

Note that the plume’s scale is also a filter. For demonstration, consider the case of a plume smaller than the grid block. Mixing is not affected by the entire sub-grid scale variability. Consequently, block-effective macrodispersivities that account for the entire sub-grid scale variability will overestimate dispersion.

## RESULTS AND CONCLUSIONS

Representing the numerical grid as a low-pass filter, the portion of the spectral density function which is reproduced by generating  $Y$  values over nodes with spacing  $\lambda_i$  is:

$$S_N(k_i) = \begin{cases} S_Y(k_i) & \text{for } k_i \leq \frac{\pi}{\lambda_i} \quad i = 1, \dots, m \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

Other filter types can be used as well. The effects of the invisible portion of  $S_Y$  are obtained by “freezing” the large wave numbers and conditioning the low wave numbers on the large ones. The conditional spectra are then employed either in a Lagrangian or Eulerian framework to develop the block-effective macrodispersivities.

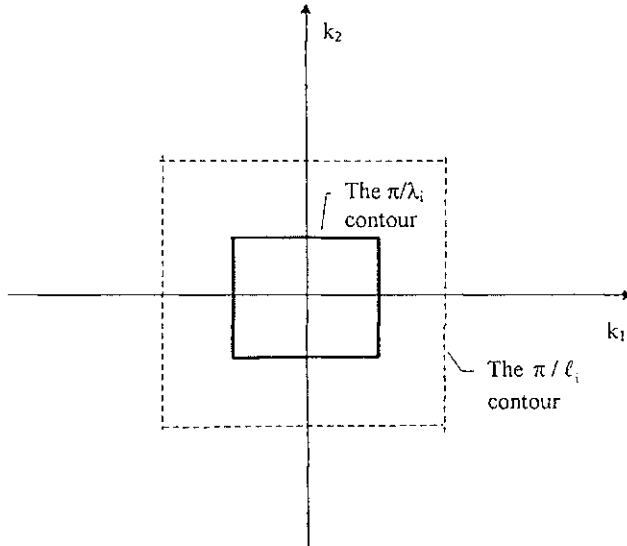
In the case of small variability in the log conductivity, with steady state flow and uniform in the average flow, the block-effective macrodispersion tensor for a plume smaller than the grid block is:

$$\tilde{D}_{ij}(t) = D_{ij}^*(t) - \frac{1}{(2\pi)^{m/2}} \int_0^t \int_{\Omega_i} \int_{\Omega_m} e^{-ik \cdot U t'} U_q U_p \left\{ \delta_{jq} - \frac{k_j k_q}{k^2} \right\} \left\{ \delta_{ip} - \frac{k_i k_p}{k^2} \right\} C_Y(k) dk_1 dk_m \Bigg] dt' \tag{2}$$

with:

$$\Omega_i = \begin{cases} \ell_i(t) & \text{as long as } \ell_i(t) < \lambda_i \\ \lambda_i & \text{otherwise} \end{cases}$$

based on the separation of wave numbers shown in Fig. 1. Here  $t$  denotes travel time,  $U_q = K_G J_q / \phi$ , where  $K_G$  is the geometric mean log conductivity,  $J_q$  is the mean head gradient in the  $q$ th direction, and  $\phi$  is porosity.  $D_{ij}^*$  is the macrodispersion coefficient applicable for large plumes, and it is obtained by integrating the second term on the right-hand side from negative infinity to infinity (cf. Dagan, 1984). Additional modifications are possibly to account for the effects of pore-scale dispersion (Rubin *et al.*, 1999).

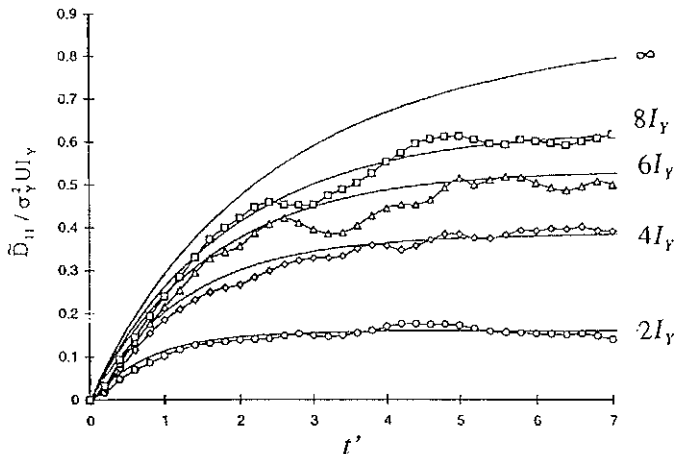


**Fig. 1** The effects of the sub-grid variability on dispersion in the case of a small plume (i.e. smaller than the grid block’s scales). The plume is affected by the wave numbers outside the dashed line. The block effective dispersion coefficients need to account only for these wave numbers. The effects of the wave numbers in the strip between the solid line and dashed line should be eliminated. That strip will keep decreasing in size as the plume increases in dimension.

For  $\ell_i > \lambda_i$  the block-effective dispersivity does not depend on  $\ell_i$  (although total mixing does, of course). The  $\ell_i$  will filter out the effects of the low wave numbers which are modelled directly on the grid. For  $\ell_i < \lambda_i$  the block effective dispersivity does depend on  $\ell_i$ . This transforms equation (2) into a nonlinear relationship since  $\ell_i$  are not known *a priori* at any  $t > 0$ .

Macrodispersivities model the dispersion of the mean concentration plumes. To predict an experiment, the solute body needs to be very large compared to the integral scale of the complete spectra. In the case of block effective dispersivity, the sub-grid scale variability is characterized by a much smaller integral scale, and consequently, modelling of an experiment is also possible for small plumes.

Figure 2 compares the theoretical longitudinal block effective dispersion coefficient in two-dimensional flow in a domain where the spatial variability is characterized by an exponential spatial covariance, with numerical simulations. Results are shown for several block dimensions, given in integral scales of the log conductivity, and good agreement is found. These results corresponds to the  $\ell_i > \lambda_i$  case.



**Fig. 2** Time dependence of the block-effective longitudinal macrodispersion coefficients for various  $\lambda_i$ . The horizontal scale is non-dimensional time. Here  $t'$  is non-dimensional travel time, defined as  $tUL_y$ , where  $U$  is the mean velocity.

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