Block-upscaling of transport in heterogeneous aquifers

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Abstract One of the most crucial decisions to properly model transport is the choice of upscaled transport parameters (dispersivities and porosity) to be used in a numerical model for a given grid size and problem scale. Here we study block-upscaling of transport parameters of the classical advection-dispersion equation (ADE) to describe the spreading of a nonreactive solute migrating within a single realization of a heterogeneous transmissivity field. We start by assuming that solute transport can be modelled by a local scale ADE, which we employ to solve a concentration field on a finely discretized grid. The latter is taken as the ground truth against which we compare results from an upscaling procedure. The effect of increasing size of (constant, upscaled) transmissivity blocks is assessed upon employing an inverse transport model, the outputs of which are the (constant, upscaled) dispersivities providing a best fit against sampled concentrations at given observation times. Our results provide a set of rules-of-thumb to be used in order to obtain meaningful upscaled parameters.

Keywords heterogeneous media; inverse modelling; numerical modelling; transport; upscaling

INTRODUCTION

Reliable groundwater flow and transport modelling results are needed to properly assess the status of groundwater contamination and the appropriateness of possible remediation scenarios. Most existing modelling codes are based on the assumption that the advection–dispersion equation (ADE) is applicable at some observation scale and describe aquifer properties as distributed over a discrete number of homogeneous regions. Unfortunately, inaccurate modelling of natural variability leads to simulated plumes which poorly represent reality (e.g. Carrera, 1993). Key features which are not modelled by the ADE include: (a) the apparent increase of dispersivity with scale, (b) the strong tailing of breakthrough curves, often showing power law behaviour, and (c) the directional dependence of apparent porosity.

One way to overcome these effects involves solving the ADE at the pore scale. This is a formidable task in itself, since it involves collecting high-resolution threedimensional data sets. Furthermore, one would need to numerically solve flow and transport at a fine scale which would exceed by far today's computers' capacities. A different approach to the problem relies on defining some upscaled parameters to be used in conjunction with appropriate equations, which are capable of reproducing the relevant details of the flow and transport processes at the required scale. The upscaled parameters are typically a result of averaging in the physical space and should incorporate the effect of uncertainty of the smaller scales without the need to actually resolve them.

The objectives of this paper are precisely: (a) to study upscaling to properly model the actual spreading of a nonreactive solute plume, and (b) to provide some insights on the physical meaning of block-upscaled transport parameters, which are employed to provide best estimates of the smaller-scale transport processes.

TRANSPORT UPSCALING

A key question one should answer is the definition of a set of criteria to obtain "reasonable" upscaled results. A first approach to upscaling is based on the macrodispersion concept (Gelhar & Axness, 1983). The resulting transport equation has the same form as the local ADE with a macrodispersion tensor replacing the dispersion tensor. Rubin and co-workers (Rubin *et al.*, 1999) generalized this approach for blockupscaling and model the low frequency fluctuations of the velocity on the numerical grid and the large frequency fluctuations within the macrodispersion tensor. All these approaches are based on ensemble averages. As such, they are applicable only for large spatial (and time) scales, and thus are of limited use for many real problems, where one is typically interested in relatively short distances and travel times. To overcome this problem Kitanidis (1988) introduced the concept of "effective" dispersivity, derived as the average dispersion around the centre of gravity of the solute plume from all (ensemble) realizations rather than the dispersion of the ensemble average of concentration distributions.

Typically, all these approaches are driven by the underlying idea that it is possible to obtain upscaled transport parameters which allow reproduction of the actual plume spreading by matching some predicted spatial or temporal moments of the plume against measurements taken in the field. This might be sufficient for conservative transport, which is the focus of this work, but can be inappropriate in the presence of chemical reactions or biodegradation, when mixing becomes the relevant process. Following this reasoning, we focus on an upscaling procedure which is based on the calibration of upscaled transport parameters upon embedding transport within an inverse modelling algorithm. The latter provides (upscaled) dispersivities and retardation which render the best fit against measured space–time concentration data for a given observation time and block size. The need for including a retardation factor is because we look at a single realization of a heterogeneous field and not at an ensemble, which might change the mean velocity. In this paper we concentrate entirely on the effects on longitudinal dispersivity.

METHODOLOGY

Our approach is based on the assumption that the ADE is valid on a small scale (e.g. pore scale). We then simulate steady-state seepage flow and transport of a nonreactive contaminant within a single realization of the rectangular heterogeneous aquifer depicted in Fig. 1. The field is discretized by 1024×512 square cells of unit side.



no flow, permeable boundary

Fig. 1 Configuration of the simulation. In the upper right corner are the varying block sizes (grey) for the estimation of the upscaled transport parameters indicated.

The boundary conditions are depicted in Fig. 1. Solute is injected uniformly (unit concentration) within a rectangular area of sides 16×8 (Fig. 1), while the initial concentration in the domain is zero. Boundary conditions for the transport problem are reported in Fig. 1. The Gaussian sequential simulator GCOSIM3D (Gómez-Hernández & Journel, 1993) was used to generate one unconditional realization of the ensemble natural logarithm of transmissivity characterized by a unit variance, geometric mean, $T_G = 10^{-3}$ (in consistent units), and spherical correlation with correlation length, $\lambda = 384$. Note that the length of the domain along the dominant flow direction is less than 3λ . Porosity is taken as 0.3, while the longitudinal and transverse dispersivities are respectively taken as $\alpha_L = 10$ and $\alpha_T = 1$ unit length. Flow and transport are solved by finite elements and transport is modelled for a total elapsed time of 6×10^6 time units.

Concentration is then sampled at 561 observation points, uniformly distributed in the domain, to provide an adequate spatial characterization of the plume. These measurements constitute the reference data set against which we analyse the results of the upscaling procedure. Upscaling of transport parameters is performed according to the following steps: (a) a size, *L*, for the (square) upscaled blocks is fixed; (b) the original, fine-scale, transmissivity is upscaled as the geometric mean of the local transmissivities included in a given, large-scale block; (c) inverse modelling of transport (Medina & Carrera, 1996) is then performed for the upscaled transmissivity field. These steps are repeated using the same original field for different upscaled blocks of transmissivity, i.e. $L^* = L/\lambda = 1/24$, 1/12, 1/6, 1/3, 2/3 and ∞ (effective transmissivity; Fig. 2), and for all observation times. A fixed numerical grid, with rectangular 8×4 cells, was used in the inverse procedure, regardless of the value of *L*, to avoid the contribution of grid variability.

For a given observation time, the block-upscaled dispersivity is thus evaluated as the constant parameters rendering a best fit between the concentrations measured on the fine-grid reference field and those simulated on the upscaling domain. This procedure provides the functional dependence of upscaled dispersivities and retardation coefficient on relative block size, L^* , and observation time. It is emphasized that the inverse procedure renders constant transport parameters for each observation time.



Fig. 2 Transmissivity field plotted as $\ln T$ for different block sizes: (a) original field, (b) $L^* = 1/12$, and (c) $L^* = 1/3$.

NUMERICAL RESULTS

Figure 3 depicts the observed plume for the fine-grid reference field at two sampling intervals. The apparent time-dependence of longitudinal dispersivity is then reported in Fig. 4, following two different methodologies: first, as the actual time-derivative of the observation time. While the first definition represents the actual dispersivity if the model would adopt it each time step, the second definition represents the constant dispersivity needed to reproduce the shape of the plume at one certain time step. Both the plume shape and the apparent variation in field dispersivity are typical of anomalous transport.

The influence of the block size on the flow field is evident in Fig. 5, where one can see that while the reference flow lines are still well reproduced when $L^* \approx 1/12$, a choice of $L^* \approx 1/3$ renders a smoothed flow field (in the limit of upscaling to a single block, one would have parallel flow lines).

Figure 6 depicts the dependence of block-scale longitudinal dispersivity estimated by our inverse procedure on the relative block size, L^* , for two different observation times. The values of the longitudinal local-scale and calculated averaged field



Fig. 3 Simulated plume as logarithmic concentrations for two observation times: (a) 7.5×10^5 , and (b) 1.5×10^6 .



Fig. 4 Field dispersivities (actual and averaged) derived from the moments of the simulated plume: calculated as the actual derivative between two time steps and as an average over time. Local dispersivity is given for comparison.



Fig. 5 Comparison of original stream lines (solid lines) and those resulting from the upscaling procedure with block sizes of $L^* = 1/12$ and $L^* = 1/3$ (dashed lines).



Fig. 6 Longitudinal dispersivity against block size for two observation times: (a) 7.5×10^5 , and (b) 1.5×10^6 .

dispersivity (Fig. 4) are also reported for comparison. The salient points to be noted are: (a) increasing L^* generally causes the block-dispersivity to increase; and (b) when $L^* > 1/3$ the inverse procedure renders meaningless block-dispersivity values, as reflected by the apparent decrease of the dispersivity values needed to fit the sampled concentrations for a given observation time.

The ability to obtain a meaningful reproduction of the fine-scale reference concentration field is clearly seen from Fig. 7, which depicts three snapshots of the plume resulting from the inverse procedure for $L^* \approx 1/12$, 1/3 and for the effective T.



Fig. 7 Upscaled plumes as logarithmic concentration for time 1.5×10^6 for three grid discretizations: (a) $L^* = 1/12$, (b) $L^* = 1/3$, and (c) with effective $T(L^* = \infty)$.

Upon comparing these with Fig. 3(b) and on the basis of Fig. 5 one can see that the main features of the plume are well reproduced when $L^* \leq 1/3$, while large (relative to the correlation scale of the underlying local transmissivity field) upscaled blocks are not capable of capturing the salient features of the concentration distribution, thus rendering meaningless the results obtained by the inverse procedure. This is most obvious for the extreme case of using one effective T (Fig. 7(c)) where the upscaled plume moves along the mean flow direction and cannot match the observed original plume.

DISCUSSION

The objective of this paper is to study the meaning of block-upscaling of transport parameters (in particular of longitudinal dispersivity) to reproduce space-time distributions of local-scale concentrations within a single realization of a randomly heterogeneous transmissivity field. Upscaled quantities are here derived as the parameters rendering the best reproduction of the actual concentration field by means of an inverse transport procedure. As such, they are generally a function of the size of the upscaled blocks, *L*, relative to the correlation scale, λ , of the local-scale transmissivity field, and sampling time.

Our results suggest that when the size of the upscaled blocks is small, i.e. $L^* \leq 1/10$, the reference concentration field is well reproduced, without the need to upscale dispersivities or retardation coefficient. For intermediate block sizes $(1/10 < L^* \leq 1/3)$, reproduction of the salient features of the spatial concentration distribution at a given sampling time is possible with constant dispersivity and retardation values. These are increasing functions of L^* and rapidly attain the calculated field dispersivity for small observation times. We conclude that adoption of $L^* > 1/3$ does not allow determination of upscaled transport parameters which are capable of satisfactorily reproducing the

spreading of a contaminant plume within a single local-scale realization of a random transmissivity field due to the lateral shift of the plume's centre of gravity.

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