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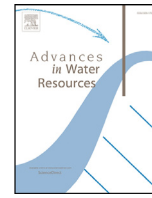

Upscaling of solute transport in disordered porous media by wavelet transformations

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ABSTRACT

Modeling flow and solute transport in large-scale (e.g. on the order of 10^3 m heterogeneous porous media involves substantial computational burden. A common approach to alleviate the problem is to utilize an upscaling method that generates models that require less intensive computations. The method must also preserve the important properties of the spatial distribution of the hydraulic conductivity (K) field. We use an upscaling method based on the wavelet transformations (WTs) that coarsens the computational grid based on the spatial distribution of K. The technique is applied to a porous formation with broadly distributed and correlated K values, and the governing equation for solute transport in the formation is solved numerically. The WT upscaling preserves the resolution of the initial highly-resolved computational grid in the high K zones, as well as that of the zones with sharp contrasts between the neighboring K, whereas the low-K zones are averaged out. To demonstrate the accuracy of the method, we simulate fluid flow and nonreactive solute transport in both the high-resolution and upscaled grids, and compare the concentration profiles and the breakthrough times. The results indicate that the WT upscaling of a K field generates non-uniform upscaled grids with a number of grid blocks that on average is about two percent of the number of the blocks in the original high-resolution computational grids, while the concentration profiles, the breakthrough times and the second moment of the concentration distribution, computed for both models, are virtually identical. A systematic parametric study is also carried out in order to investigate the sensitivity of the method to the broadness of the K field, the nature of the correlations in the field (positive versus negative), and the size of the computational grid. As the broadness of the K field and the size of the computational domain increase, better agreement between the results for the high-resolution and upscaled models is obtained.

1. Introduction

It is of fundamental and practical importance to incorporate the spatial heterogeneity of porous geological formations in the models of flow and transport in such media (Dagan et al., 1989; Rubin, 2003; Sahimi, 2011). At the field scale (e.g. orders of $10^2 - 10^3$ m), subsurface properties, such as the permeability, vary many orders of magnitude across multiple length scales (e.g. from 1 m to 10^3 m or larger) (Dagan et al., 1989; Rubin, 2003; Sahimi, 2011). It is well recognized that the spatial fluctuations of the permeability field, i.e. many orders of magnitude difference between permeability values, have a significant role in the spreading rates of solute plumes, as well as estimates of their early or late arrival times. Thus, neglecting the effect of subsurface heterogeneity, and in particular the spatial distribution of the permeability, in numerical simulation leads to erroneous prediction of solute transport, which will have severe consequences for health risk assessment (de Barros and Rubin, 2008; Maxwell et al., 1999), the likelihood of extreme events (de Barros and Fiori, 2014; Dentz and Tartakovsky, 2010; Henri et al., 2015), and for reactive mixing (Dentz et al., 2011; Luo et al., 2008).

In general, to obtain accurate predictions for solute mixing at the field scale and calculate the properties that characterize the process, such as the distribution of travel times and the dispersion coefficients, numerical simulation of flow and transport in large-scale porous media requires a computational grid with high enough resolution to represent the variability of the hydrogeological properties (Ababou et al., 1989; de Dreuzy et al., 2007). Simulation with such high-resolution computational grids entails solving

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several million discretized equations over thousands of time steps, leading to a very high computational burden. The resolution of the grid depends, of course, on the available data that are used to construct the grid blocks. But, for the same of argument we consider blocks whose linear size is 1 m. Thus, numerical simulation of solute transport at the field scale might become prohibitively expensive, particularly when such highly-resolved models are subject to uncertainty and must be cast within a Monte Carlo sampling (Rubin, 2003; Sahimi, 2011). As a result, a key aspect of the simulation is how to distribute the limited computational resources in an efficient manner in order to reduce the simulation cost (Leube et al., 2013; 2012; Moslehi et al., 2015). To alleviate the computational burden, upscaling methods are used.

Upscaling flow and transport in heterogeneous porous formations has been studied intensively for several decades. One may divide the existing methods into those that are based on volume (Wang and Kitanidis, 1999; Whitaker, 1999; Wood et al., 2003; Wood and Valdés-Parada, 2013), ensemble (Koch and Brady, 1985; Rubinstein and Torquato, 1989), or stochastic averaging (Attinger, 2003; Dagan, 1984; Gelhar and Axness, 1983; Neuman et al., 1987; Rubin et al., 1999). In the context of stochastic averaging, many analytical methods have been developed to evaluate the effective transport properties in a coarse-scale heterogeneous model, including analytical perturbation (de Barros and Dentz, 2016; de Barros and Rubin, 2011; Gelhar and Axness, 1983; Gutjahr et al., 1978) and self-consistent (Dagan et al., 1989; Fiori et al., 2011; Rubin and Gómez-Hernández, 1990) methods. Alternatively, numerical simulations (Ababou, 1988; Desbarats, 1987; Warren et al., 1961) and the renormalization group transformations (King, 1989; King et al., 1993; Mukhopadhyay and Sahimi, 2000) have been employed to compute the effective conductivity of field-scale porous media. Such works were reviewed by Renard and De Marsily (1997), Wen and Gómez-Hernández (1996), and Sahimi (2011).

In general, most of the coarsening process is carried out by homogenizing the aquifer's model through, for example, its hydraulic conductivity or the permeability attributed to the blocks of a highly-resolved computational grid such that the upscaled permeability or conductivity field has identical symmetries as those of the fine-scale field, as defined earlier (Desbarats, 1992; Durlofsky, 1991; Kitanidis, 1990). The size of the upscaled grid blocks is determined by considering the available computational resources. A drawback associated with the homogenization techniques is that they coarsen the subsurface domain uniformly, which often leads to large errors in the predictions for the flow and transport properties, especially in the presence of fractured regions or sink and source. This is because many homogeneization methods average out the effects of extreme events, such as fast flow paths or large flow barriers. To address this issue, Durlofsky et al. (1997) proposed to first scale up the permeability field by a homogenization technique and then identify the high-velocity regions by solving for single-phase flow in the homogenized grid. Such regions are then discretized to the fine scale in order to capture the small-scale variability that the field contains. Although the issue of uniform blocks is addressed, the single-phase flow should still be computed prior to the upscaling process.

An alternative method for upscaling is based on the wavelet transforms (WTs) (Ebrahimi and Sahimi, 2002; 2004; 2006; Heidarinasab et al., 2004; Mehrabi and Sahimi, 1997; Rasaei and Sahimi, 2008; 2009; Sahimi, 2003), which have been used to upscale heterogeneous porous media by coarsening the permeability or hydraulic conductivity field. The method upscales the high-resolution geological model of a porous formation non-uniformly, which leads to preserving the important information on the spatial distribution of the permeability field at all the relevant length scales, but coarsens those parts of the computational grid that contribute little to the flow field. Thus, the number of grid blocks in the computational grid and, hence, the number of flow and transport equations to be solved are reduced drastically without sacrificing any crucial information about the conductivity or permeability field. Use of the WTs in various applications has been the subject of intensive research over the past 25 years (Chui, 1992; Heidarinasab et al., 2004; Holschneider, 1995; Meyer, 1992; Nievergelt and Nievergelt, 1999; Sahimi, 2003), including the simulation of flow and transport in large-scale porous media, such as oil reservoir (Kikani et al., 1998; Lu et al., 2000; Moridis et al., 1996; Rasaei and Sahimi, 2008, 2009; Sahimi, 2003; Sahimi and Hashemi, 2001).

The focus of this study is to extend the upscaling method by the WTs, introduced originally by Mehrabi and Sahimi (1997) and Ebrahimi and Sahimi (2002), to upscaling of solute transport in disordered porous media. Their work focused on upscaling a permeability or conductivity field. In contrast, our primary goal is to investigate the effect of multiple features, i.e. structural and geometrical parameters, in the conductivity field on the overall transport behavior, such as the arrival time, peak concentration and spatial moments, and to demonstrate how geostatistical parameters characterizing the heterogeneous fields influence the performance of the upscaling using wavelet transformation. Furthermore, we used the upscaled field to reconstruct the second central spatial moment of the plume that represents global features of the transport process. The spatial moment analysis has not be been analyzed in the previous works related to WTs. We show that upscaling by the WTs efficiently coarsens the computational grid for simulating solute transport in subsurface domains, and reduces substantially the number of grid blocks. To demonstrate the accuracy of the upscaling procedure via the WTs, flow and transport are simulated in both the fine-resolution and the upscaled computational grids, and the results are compared.

The rest of this paper is structured as follows. In Section 2 we formulate the class of problem under investigation. Section 3 describes the details pertaining to the WTs and the methodology used for upscaling of the hydraulic conductivity or permeability field. We then present the details of the numerical simulations in Section 4. The results are presented and discussed in Section 5, where we test systematically the performance of the WT upscaling for a variety of disordered porous formations. The last section summarizes the paper.

2. Problem statement

We consider a fully-saturated steady-state flow of an incompressible and Newtonian fluid through a heterogeneous geological formation. The hydraulic conductivity $K(\mathbf{x})$ is spatially distributed, where $\mathbf{x}$ represents the Cartesian coordinate system. We assume that the flow is slow enough that the fluid velocity $\mathbf{v}(\mathbf{x})$ follows the Darcy's law

$$\mathbf{v}(\mathbf{x}) = \frac{K(\mathbf{x})}{\mathcal{P}} \nabla \varphi(\mathbf{x}) \,, \tag{1}$$

where $\varphi(\mathbf{x})$ is the hydraulic head, and $\mathcal{P}$ is the porosity of the medium, assumed to be uniform. As usual, the hydraulic head is computed by solving the flow equation

$$\nabla \cdot [K(\mathbf{x}) \nabla \varphi(\mathbf{x})] = 0 \,. \tag{2}$$

A constant hydraulic gradient in the mean sense is imposed on the system such that, on average, the flow is uniform along the longitudinal direction. An inert solute is released and advected and dispersed by the fluctuating velocity field and diffusion. The spatiotemporal evolution of the concentration field is governed by the advection-dispersion equation,

$$\frac{\partial C(\mathbf{x}, t)}{\partial t} + \mathbf{v}(\mathbf{x}) \cdot \nabla C(\mathbf{x}, t) = \nabla \cdot [\mathbf{D}_o(\mathbf{x}) \nabla C(\mathbf{x}, t)] \,, \tag{3}$$