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Modeling impacts of subscale heterogeneities on dispersive solute transport in subsurface systems

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ABSTRACT

Previous works in the literature demonstrated that dispersion increases with heterogeneities and travel distance in heterogeneous reservoirs. However, it remains challenging to quantify the effects of subscale heterogeneities on dispersion. Scale-up of input dispersivity and other reservoir attributes to the transport modeling scale should account for subscale heterogeneity and its variability.

A method is proposed to quantify the uncertainties in reservoir attributes and dispersivity introduced by scale-up. A random walk particle tracking (RWPT) method, which is not prone to numerical dispersion, is used for transport modeling. First, to scale-up rock properties including porosity and permeability, volume variance at the transport modeling scale is computed corresponding to a given spatial correlation model; numerous sets of "conditioning data" are sampled from probability distributions whose mean is the block average of the actual measure values and the variance is the variance of block mean. Stochastic simulations are subsequently performed to generate multiple realizations at the transport modeling scale. Next, multiple sub-grid geostatistical realizations depicting detailed fine-scale heterogeneities and of the same physical sizes as the transport modeling grid block are subjected to RWPT simulation. Effective longitudinal and transverse (horizontal) dispersivities in two-dimensional models are determined simultaneously by matching the corresponding breakthrough concentration history for each realization with an equivalent medium consisting of averaged homogeneous rock properties. Aggregating results derived with all realizations, we generate probability distributions of scaled-up dispersivities conditional to particular averaged rock properties, from which values representative of the transport modeling scale are randomly drawn.

The method is applied to model a tracer injection process. Results obtained from coarse-scale models, where reservoir properties and dispersivities are populated with the proposed approach, are compared to those obtained from fine-scale models. Our results verify that dispersivity increases with scale and demonstrate that (1) uncertainty distributions in recovery obtained by accounting for variability owing to scale-up capture the actual fine-scale behavior; and (2) ignoring sub-scale uncertainties would underestimate the ensuing uncertainty in recovery performance. An important contribution of this work is that it presents a quantitative and systematic procedure to scale-up both rock and flow-related properties. It reinforces the notion that deterministic conditioning data does not exist in reservoir modeling.

1. Introduction

Dispersion in porous media results from the interplay between convective spreading and diffusion (Perkins and Johnston, 1963). Convective spreading occurs because of

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variations in path lengths and solute particles following different streamlines (Jha et al., 2011). Diffusion, on the other hand, is the process whereby random motion of solute particles is involved in a net movement corresponding to the concentration gradient and is described by Fick's law. It is enhanced by additional mixing caused by concentration gradients as a result of uneven fluid velocities (Aronofsky and Heller, 1957). Presence of local velocity gradients due to multi-scale heterogeneous rock properties can enhance mixing (Lake, 1989).

It has been extensively reported in the literature that dispersivity increases with distance (Gelhar et al., 1992; Fleurant and Van Der Lee, 2001) and time (Binning and Celia, 2002). This scale-dependent behavior is usually described as non-Fickian, anomalous, or non-Gaussian (Berkowitz et al., 2000; John, 2008), characterized by early breakthrough and long- or heavy-tailed effluent histories at the late times. Heavy-tailed nature of breakthrough concentration (BTC) profiles has been also observed under convergent radial flow around injectors and producers (Pedretti et al., 2014). Under converging flow, heavy-tailed behavior of transport heavily depends on the vertical architecture and connectivity patterns between the injecting and producing locations. Jha et al. (2011) observed that diffusion is an important element in Fickian transport because it helps to ensure that movement of solute particles is independent and random (particles are moving from regions of low-velocity to high-velocity and vice versa). In case of realistic parabolic velocity profile in pore throat (similar to flow between two parallel plates), the velocities of particles near the porous material surface are not independent (due to no-slip boundary conditions at the solid surfaces) and in the absence of diffusion, solute particles near the low velocity region cannot move into main flow stream. In other words, without diffusion, each solute particle would follow the same streamline without interacting with particles from other stream lines. The randomness introduced by diffusion has allowed particles near the solid porous material with low velocity to switch between different streamlines and acquire independent velocity.

At the reservoir or field scale, non-Fickian behavior can be explained by both large-scale heterogeneity and unresolved sub-scale heterogeneities. Gylling et al. (1999), Becker and Shapiro (2003), and Gouze et al. (2008) attributed non-Fickian dispersion to long-range spatial correlation of geological features (e.g., increase in correlation in the permeability field), resulting in velocities to be correlated over large distances. A common example would be fractured formations with dual porous systems (Bijeljic et al., 2013). Non-Fickian dispersion may also be explained by the temporal correlations of the solute motion due to mass transfers in small-scale geological structures (Dentz et al., 2004; Le Borgne and Gouze, 2008). As noted by Le Borgne and Gouze (2008), it is most probable that both spatial correlations controlled by large-scale structures and temporal correlations controlled by small-scale structures lead to non-Fickian transport in some heterogeneous reservoirs. Since heterogeneity varies as a function of scales, description of dispersion must account for impacts of heterogeneity and scale (Arya et al., 1988; Gelhar et al., 1992; Mahadevan et al., 2003; Berkowitz et al., 2006; Jha et al., 2009, 2011; John et al., 2010).

Several studies (Aronofsky and Heller, 1957; Scheidegger, 1988; Berkowitz et al., 2006; Jha et al., 2011) discussed the specific issues about applicability of classical advection–dispersion equation (ADE) for modeling transport behavior of both Fickian and non-Fickian characteristics. The existence of preferential flow paths was clearly shown in laboratory-scale systems (Hoffman et al., 1996; Oswald et al., 1997). Some experimental studies also revealed systematic deviation between experimental BTCs and ADE predictions. Levy and Berkowitz (2003) also measured the BTCs in homogeneous meter-length flow cells and observed non-Fickian dispersion behavior in terms of early-time and late-time arrivals (tails). The classical ADE formulation is not suitable for modeling non-Fickian transport because dispersion is modeled as a sum of diffusion and convective spreading, which act independently from each other, ignoring the mixing introduced by the interaction of these two mechanisms.

Other issue in the solute transport modeling is the numerical dispersion (artificial dispersion). Numerical dispersion is the result of truncation error and generally overwhelms physical dispersion (Lantz, 1971; Fanchi, 1983; Haajizadeh et al., 1999; Binning and Celia, 2002). Many numerical schemes generate significant numerical dispersion and, therefore, lead to an overestimation of transverse mixing. Although numerical dispersion could be partially decreased by choosing proper discretization scheme (e.g., mesh size and time steps) and incorporating higher-order approximation, it still poses a significant challenge when used to analyze effects of physical dispersion. Advection dominated problems often suffer from numerical dispersion and numerical oscillations (instabilities) (Zheng and Bennett, 2002; Salamon et al., 2006a; Hoteit et al., 2002; Fleurant and Van Der Lee, 2001). These problems could be solved by selecting higher grid resolution and small time steps. These numerical problems can also be alleviated by choosing appropriate numerical scheme and better flux approximations, resulting in long executions times even with the CPUs available these days (Liu et al., 2004; Salamon et al., 2006a). Alternative method of solving partial differential equation (ADE) is particle tracking (Lagrangian method) based approach. Particle tracking is a grid-free approach capable of eliminating numerical dispersion (Salamon et al., 2006a; Jha et al., 2009; John et al., 2010). Its computational requirement is also less as compared to FD/FV/FE-based simulator, since particles move independently and parallel computing formulation is favorable.

Particle tracking formulations can be classified into a number of categories: (1) random walk particle tracking (RWPT) or classical random walk (CRW); and (2) continuous time random walk (CTRW). In RWPT, each transit time step $\tau = \Delta t$ is considered as discrete, constant, and deterministic whereas transition length vector ξ is independent and identically distributed (i.i.d.) random variables with zero mean and unit variance (Salamon et al., 2006a). In CTRW, each τ and ξ are random variables following a probability density function $\psi(\tau, \xi) = \psi_s(\xi)\, \psi_t(\tau)$, where both τ and ξ are independent, stationary stochastic processes (Srinivasan et al., 2010).

Different approaches were described in the literature for representing sub-scale effects in coarse-scale continuum flow simulations. Barker and Fayers (1994) introduced pseudo(effective) coefficients, referred to as α-factors, in the flux terms of the transport equation to relate compositions of fluids leaving a grid block to the average compositions within the grid block. Efendiev et al. (2000) derived expressions for