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Three-dimensional analysis of spreading and mixing of miscible compound in heterogeneous variable-aperture fracture

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Abstract

As mass transport mechanisms, the spreading and mixing (dilution) processes of miscible contaminated compounds are fundamental to understanding reactive transport behaviors and transverse dispersion. In this study, the spreading and dilution processes of a miscible contaminated compound in a three-dimensional self-affine rough fracture were simulated with the coupled lattice Boltzmann method (LBM). Moment analysis and the Shannon entropy (dilution index) were employed to analyze the spreading and mixing processes, respectively. The corresponding results showed that the spreading process was anisotropic due to the heterogeneous aperture distribution. A compound was transported faster in a large aperture region than in a small aperture region due to the occurrence of preferential flow. Both the spreading and mixing processes were highly dependent on the fluid flow velocity and molecular diffusion. The calculated results of the dilution index showed that increasing the fluid flow velocity and molecular diffusion coefficient led to a higher increasing rate of the dilution index.

Keywords: Mixing; Spreading; Solute transport; Three-dimensional fracture; Self-affinity; Hurst exponent

1. Introduction

The investigation of spreading and mixing processes in the subsurface is important in many scientific disciplines, technical applications, and engineering practices, including contaminant hydrology, nuclear waste storage, groundwater remediation, and reservoir engineering (Qian et al., 2011; Yang et al., 2012; Mondal and Sleep, 2013; Cai et al., 2010). In groundwater environments, the mass transport of a miscible contaminated compound is complex due to the geological formations in the subsurface. Characterization of the spreading and mixing processes of miscible compounds is significant to quantification and description of the chemical and biological reactions in both porous media and fractures. According to Rolle et al. (2009) and Kitanidis (1994), spreading caused by the variability of advection velocity refers to the change of compound cloud shape, while dilution refers to the change of water volume occupied by the solute, which is the only process allowing mass exchange between different streamlines and resulting in the decrease of the peak concentration in breakthrough curves. Insufficient or incomplete mixing of a compound often has a certain influence on the overall and local rates of chemical reaction. In particular, since only the mixing process transverse to the flow directions is dispersive, the mixing process plays an important role in transverse dispersion of the compound cloud. Therefore, it is important to understand and quantify the spreading and mixing processes of compounds in the subsurface.

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A large number of numerical and experimental studies have shown that the heterogeneous nature of geological formations has a significant influence on the spreading and mixing processes of compounds. Rolle and Kitanidis (2014) used a pore-scale numerical model to study the effects of compound-specific dilution on transient transport and solute breakthrough. Because characterizing a dilution process from integrated measurements of solute breakthrough is challenging, they modified the dilution index, introduced by Kitanidis (1994), and proposed a transient flux-related dilution index to measure the dilution breakthrough curve. Hochstetler et al. (2013) studied the effects of compound-specific transverse mixing on steady-state reactive plumes by comparing pore-scale simulations with Darcy-scale experiments. Ballarini et al. (2014) evaluated the effect of heterogeneities on transverse mixing in bench-scale tank experiments by analyzing the spatial moment and dilution index of the compound tracer. The results showed that the magnitude of permeability had a significant influence on the spreading and dilution processes; as in heterogeneous porous media, a non-uniform flow velocity field occurred in the natural fracture due to the heterogeneous aperture distribution. Cirpka et al. (2015) described the quantitative assessment of transverse mixing and its enhancement in three-dimensional (3D) heterogeneous anisotropic porous media. They used a quantitative method to analyze transverse mixing based on the spreading and dilution processes. Although many studies have shown that the heterogeneity of porous media has a significant influence on the spreading and dilution processes, and, consequently, transverse dispersion is highly dependent on the heterogeneity of the geological formation, studies of the spreading and dilution processes in rough fractures are still limited. Recently, Dou and Zhou (2014) described the miscible compound transport in a two-dimensional (2D) single rough fracture. The results showed that the slow mass exchange through solute molecular diffusion between mobile and immobile regions, which was caused by the roughness of the fracture, resulted in a long breakthrough tailing. However, they did not analyze the spreading and mixing processes.

The Navier-Stokes equation has typically been used to solve the non-uniform flow velocity field. Recently, lots of numerical methods have shown that, as an alternative to directly solving the Navier-Stokes equation, the lattice Boltzmann method (LBM) can simulate the non-uniform flow velocity by solving the discrete Boltzmann equation (Chen et al., 2013). Much effort has been devoted to designing different boundary conditions for the LBM, such as the periodic boundary condition, pressure boundary condition, and bounce-back boundary condition. For the geometric model used in this study, the LBM has natural advantages over other conventional computational fluid dynamics (CFD) methods, especially in dealing with the boundary of a self-affine rough fracture wall. In addition, Dou and Zhou (2014) have proved that a coupled LBM model is capable of simulating the miscible compound transport.

The main objective of this study was to simulate the spreading and mixing processes of a compound in a 3D rough fracture and investigate the influence of non-uniform flow velocity and molecular diffusion on the spreading and mixing processes. The non-uniform flow velocity and compound concentration fields were obtained by solving the Navier-Stokes equation and the advection-diffusion equation through a coupled LBM model, respectively. A 3D rough fracture was generated using the technique of successive random additions. The spreading and mixing processes of the compound were analyzed by calculating the spatial moment and original dilution index for different molecular diffusion coefficients in different average fluid flow velocity fields.

2. Method

2.1. Numerical model

In this study, a coupled LBM model was developed to simulate the miscible compound transport in a 3D rough fracture. The coupled LBM model used two particle distribution functions to represent the pure water and the miscible compound, respectively:

$$f_i(\boldsymbol{X}+\boldsymbol{e}_i\Delta t, t+\Delta t) - f_i(\boldsymbol{X},t) = -\frac{\Delta t}{\tau}\left[f_i(\boldsymbol{X},t) - f_{\mathrm{eq}i}(\boldsymbol{X},t)\right] \quad (1)$$

$$g_i(\boldsymbol{X}+\boldsymbol{e}_i\Delta t, t+\Delta t) - g_i(\boldsymbol{X},t) = -\frac{\Delta t}{\tau_{\mathrm{D}}}\left[g_i(\boldsymbol{X},t) - g_{\mathrm{eq}i}(\boldsymbol{X},t)\right] \quad (2)$$

where $f_i(\boldsymbol{X},t)$ and $g_i(\boldsymbol{X},t)$ are the distribution functions of fluid particles and compound particles, respectively, at spatial position $\boldsymbol{X}$ and time t with velocity vector $\boldsymbol{e}_i$, respectively; the subscript i is the number of particles; τ and τ_{D} are the non-dimensional relaxation times related to the kinematic viscosity, $\upsilon = c_{\mathrm{s}}^2(\tau - 0.5\Delta t)$, and the molecular diffusion coefficient, $D_{\mathrm{f}} = c_{\mathrm{s}}^2(\tau_{\mathrm{D}} - 0.5\Delta t)$, respectively; c_{s} is the lattice sound speed; and $f_{\mathrm{eq}i}(\boldsymbol{X},t)$ and $g_{\mathrm{eq}i}(\boldsymbol{X},t)$ are the equilibrium distribution functions for fluid particles and compound particles, respectively, defined as

$$f_{\mathrm{eq}i}(\boldsymbol{X},t) = \omega_i\rho_{\mathrm{f}}\left[1 + \frac{\boldsymbol{e}_i\cdot\boldsymbol{u}_{\mathrm{eq}}}{c_{\mathrm{s}}^2} + \frac{(\boldsymbol{e}_i\cdot\boldsymbol{u}_{\mathrm{eq}})^2}{2c_{\mathrm{s}}^4} - \frac{\boldsymbol{u}_{\mathrm{eq}}^2}{2c_{\mathrm{s}}^2}\right] \quad (3)$$

$$g_{\mathrm{eq}i}(\boldsymbol{X},t) = \omega_i C\left[1 + \frac{\boldsymbol{e}_i\cdot\boldsymbol{u}_{\mathrm{eq}}}{c_{\mathrm{s}}^2} + \frac{(\boldsymbol{e}_i\cdot\boldsymbol{u}_{\mathrm{eq}})^2}{2c_{\mathrm{s}}^4} - \frac{\boldsymbol{u}_{\mathrm{eq}}^2}{2c_{\mathrm{s}}^2}\right] \quad (4)$$

where $\boldsymbol{u}_{\mathrm{eq}}$ is the local equilibrium velocity, ρ_{f} is the fluid density, and C is the compound concentration. In this study, the D3Q19 model and corresponding weight ω_i were employed to simulate the particle movement for each node. The fluid density, compound concentration, fluid pressure p, and fluid velocity $\boldsymbol{u}$ in the absence of any additional forces are given by the following:

$$\rho_{\mathrm{f}} = \sum_{i=0}^{18} f_i \quad (5)$$