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Lattice Boltzmann Simulation of Solute Transport in Heterogeneous Porous Media with Conduits to Estimate Macroscopic Continuous Time Random Walk Model Parameters *

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We use Lattice Boltzmann models to simulate solute transport in porous media traversed by open fractures or other conduits. Our particular interest is to simulate moderate Reynolds number flow in the conduits to study the effect of eddy mixing and matrix diffusion on solute breakthrough curve. These "double-porosity" systems represent an area of significant interest in environmental fluid mechanics. We fit the resulting solute breakthrough curves (BTCs) with macroscopic Continuous Time Random Walk (CTRW) models. CTRW is a non-perturbative upscaling method effectively used to model a wide range of transport phenomena in heterogeneous media. In this approach, the impact of system fluctuations on effective transport is modeled by a joint probability density function $\psi(s,t)$ which describes each particle transition over a distance and direction, s and time t and characterizes the random walk both in space and time. The associated effective transport PDE is characterized by a time memory term, which is a functional of the transition time distribution. The porous media are simulated using a real numbered solids fraction that damps the inertial components of the flow leading to a Darcy's Law solution. Solute transport in the porous medium is simulated with anisotropic dispersion. In the open conduits, standard fluid flow and diffusive transport are solved. The combination of Lattice Boltzmann methods and CTRW models will help elucidate the relationship between the microscopic parameters of the flow (micro-geometry, Reynolds numbers) and the macroscopic parameters of transport. Our ultimate goal is the application of the CTRW models to large-scale hydro-geological systems.

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