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Generalized Mixed-Cell Mass Balance Solute Transport Modeling in Pore-Scale Disordered Networks: A New Semi-Analytical Approach

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Introduction

Accurately predicting (non-reactive or reactive) solute transport migration, at multiple scales, in subsurface aquifers is identified among urgent societal and scientific challenges in water resources engineering and environmental pollution [1]. In particular, pore-scale models are essential tools to bridge the gap between the pore and REV scales at which observable macroscopic behavior of solute transport processes become apparent. While challenges do persist in this field, we derive cutting-edge pore scale semi-analytical formulation for solute transport modelling in disordered networks. Continuous concentration profiles along pore throats are calculated analytically, a posteriori, from time-dependent numerically simulated concentrations in neighboring pores. A double Laplace transform method is applied to governing advection-diffusion equations in network elements by enforcing mass flux continuity along their interfaces. We show that these solutions involve a time-dependent convolution product kernels or interpolating functions expressed as convergent exponentially decreasing series of locally embedded pore-throat geometrical and flow properties. Explicit dependence of interpolating kernels on the local Péclet numbers leads to a generalized numerical scheme for accurate simulation of solute transport processes in pore networks. Indeed, widely used numerical schemes in the literature [2-7] are equivalent to the asymptotic (long-time) form of our general scheme for extremely small or high Péclet numbers. Therefore, we demonstrate for the first-time that previously adopted numerical schemes for mass balance in pore networks [2-7] may overlook pore scale dynamics for a full range of intermediate Péclet numbers occurring in subsurface aquifers. These findings are illustrated by analysis of simulated concentration distributions in a benchmark pore network extracted from Berea sandstone three-dimensional pore space image. Our findings [8]

provide additional insights into the understanding of pore-scale solute transport processes to further improve the predictive capability of existing mixed-cell mass balance network models.

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