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Reduced-Order Direct Numerical Simulation of Solute Transport in Porous Media[1] YASHAR MEHMANI, HAMDI TCHELEPI, Stanford University — Pore-scale models are an important tool for analyzing fluid dynamics in porous materials (e.g., rocks, soils, fuel cells). Current direct numerical simulation (DNS) techniques, while very accurate, are computationally prohibitive for sample sizes that are statistically representative of the porous structure. Reduced-order approaches such as pore-network models (PNM) aim to approximate the pore-space geometry and physics to remedy this problem. Predictions from current techniques, however, have not always been successful. This work focuses on single-phase transport of a passive solute under advection-dominated regimes and delineates the minimum set of approximations that consistently produce accurate PNM predictions. Novel network extraction (discretization) and particle simulation techniques are developed and compared to high-fidelity DNS simulations for a wide range of micromodel heterogeneities and a single sphere pack. Moreover, common modeling assumptions in the literature are analyzed and shown that they can lead to first-order errors under advection-dominated regimes. This work has implications for optimizing material design and operations in manufactured (electrodes) and natural (rocks) porous media pertaining to energy systems.

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