

A kinetic Monte Carlo Approach to Study Fluid Transport in Porous Networks

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The mechanism of fluid migration in porous networks continues to attract great interest, especially at conditions where the Darcy's law is expected to fail. Fluid transport can be studied by using several computational techniques, such as Molecular Dynamics or Lattice-Boltzmann, each with its own limitations. Molecular Dynamics simulations are used to describe the trajectories of individual atoms and allow us to follow the dynamics of molecular processes in great detail. However, they are incapable of probing large systems for long times, due to computational limitations. Lattice-Boltzmann simulations can provide larger time scale analysis, while accounting the slip boundary condition, at the expense of molecular-level phenomena that might become important in nanopores.

To overcome the current limitations, we implement a stochastic approach to describe fluid transport through porous networks. The pore network is represented as a set of connected finite volumes, and transport is simulated as a random walk of molecules, which hop from voxel to voxel. We validated the method against the diffusion equation along a 1D pore, and against molecular dynamics simulations for transport across a single nanopore. The promising results justified the extension of the model to 1D and 2D pore networks. These models allow us to quantify effects due to pore connectivity, pore features, and presence of other fluids in the resulting permeability.