Non-Isothermal Transport in Porous Media Studied by Non-Equilibrium Molecular Dynamics Simulations

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Darcy's law is an empirical law that describes isothermal mass transport through a porous medium in a pressure gradient. It has been known for a long time that there are cases where Darcy's law does not apply, also for single phase flow with small pore sizes and low pressure gradients [1–4]. Non-equilibrium molecular dynamics simulation is an excellent tool to study flow in porous media. We have used a modified Lennard-Jones/Spline potential which makes it possible to model a wide range of systems with varying pore sizes, interface tensions, and fluid viscosity. The Reflective Particle Method has been used to create a pressure gradient [5] and the Nosé-Hoover thermostat has been used to create a temperature gradient across the porous medium. We present results for single and two-phase flow varying the contact of wetting fluid, porosity, average pore diameter, and interface tensions. The results are interpreted using non-equilibrium thermodynamics for porous media, a new theory.

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