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

Olav Galteland, Bjørn Hafskjold, Dick Bedeaux and Signe Kjelstrup
PorLab, Department of Chemistry, Norwegian University of Science and Technology, Trondheim, Norway
olav.galteland@ntnu.no

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.

Acknowledgement

The calculation power is granted by The Norwegian Metacenter of Computational Science (NOTUR). Thanks to the Research Council of Norway through its Centres of Excellence funding scheme, project number 262644, PoreLab.

References