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Transport of molecular fluids through three-dimensional porous media

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The main purpose of this study is to extend the analysis which has been made for the double layer theory (summarized by [1]) to situations where the distance between the solid walls is of the order of several molecular diameters. This is of a large interest from a scientific viewpoint and for various engineering applications.

The intermolecular forces and their influence on fluid structure and dynamics can be taken into account by using the mesoscopic scale models based on the Boltzmann equation [2]. The numerical methods derived from these models are less demanding in computational resources than conventional molecular dynamics methods and therefore long time evolution of large samples can be considered.

Three types of fluid particles are considered, namely the anions, the cations and the solvent. They possess a finite diameter which should be at least a few lattice units. The collision frequency between particles is increased by the pair correlation function for hard spheres. The lattice Boltzmann model is built in three dimensions with 19 velocities; it involves two relaxation times. The particle distribution functions are discretized over a basis of Hermite polynomial tensors. Electric forces are included and a Poisson equation is simultaneously solved by a successive over-relaxation method.

The numerical algorithm is detailed; it is devised in order to be able to address any three-dimensional porous media. It involves the determination of the densities of each particle species, of the overall density and of the equilibrium distribution function. Then, the electric forces are determined. Collision operators are applied as well as the boundary conditions. Finally, the propagation step is performed and the algorithm starts a new loop.

The influence of parameters can be illustrated by systematic calculations in a plane Poiseuille configuration. The drastic influence of the ratio between the channel width and the particle sizes on the local densities and the velocities is systematically shown. The differences with the classical double layer theory are illustrated.
Finally, the results of systematic calculations on three-dimensional porous media are presented and discussed.

REFERENCES
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