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Lattice Boltzmann Simulation of Liquid Flow in Nanoporous Media

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A multi-relaxation-time lattice Boltzmann (LB) model for nanoscale liquid flow is developed to investigate the liquid flow characteristics in nanoporous media. The slip length and effective viscosity obtained from molecular dynamics (MD) simulations are adopted to account for the nanoscale effect. First, the LB model for water flow in nanopores is built and water flow characteristics in nanoporous media are investigated. The results show that: (1) the nanoscale effect can either increase or decrease the water flux in nanoporous media, depending on the fluid-solid interaction force; (2) the nanoscale effect impacts the velocity distribution in porous media, making it more uniform in hydrophobic porous media while more heterogeneous in hydrophilic porous media; (3) the end effect caused by the bending of streamlines plays a significant role in water flow in nanoporous media, and neglecting the end effect can greatly overestimate liquid flow ability; and (4) the pore structure also has significant influence on water flow in nanoporous media. With the increase of specific interfacial length, the nanoscale effect increases. In addition, the LB model for oil (octane) flow in quartz nanopores is also established by incorporating the MD simulation results [1]. Oil flow simulation in quartz nanoporous media shows that the conclusions obtained for water flow are also applicable for oil flow.

References

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