Mesoscopic simulations of multi-phase flows: static and dynamics

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The physical behavior of a class of mesoscopic models, based on a discrete version of the Boltzmann equation (lattice Boltzmann equation) for multiphase flows is analyzed. In particular, an extended pseudo-potential method is developed, which permits to tune the equation of state and surface tension independently of each other [1]. We specialize it to describe the wetting/dewetting transition of fluids in presence of nanoscopic grooves etched on the boundaries [2]. This approach permits to retain the essential supra-molecular details of fluid-solid interactions without surrendering -actually boosting- the computational efficiency of continuum methods. The method is used to analyze the importance of conspiring effects between hydrophobicity and roughness on the global mass flow rate of the microchannel. The mesoscopic method is also compared quantitatively against Molecular Dynamics (MD) results of Cottin-Bizonne *et al.* [3].
Results on the dynamics of contact line for diffusive interfaces is also studied at changing the large-scale geometry. The method predicts the existence of a critical capillary number for the entrapment transition (wetting failure) in agreement with lubrication theory.
The extended scenario developed in this work clarifies the theoretical foundations of the Shan-Chen methodology [4] for the lattice Boltzmann equation and enhances its applicability and flexibility for the simulation of multiphase flows with more realistic density ratios.

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