CFD Simulation of Microscopic Two-phase Fluid Motion on Solid Body with Edges and Heterogeneously-wetted Surface Using Phase-field Model

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ABSTRACT

Wettability of solid surface to multiphase fluid plays an important role in control of motions of bubbles and droplets on the surface. In micro/nano engineering, the surface is often designed to be heterogeneously dry and wetted by fine-textured imprinting and by self-assemble mono-layered film coating. It is important to predict the fluid motions on the surface for optimizing performance of fluidic MEMS (micro-electro mechanical systems) devices and micro-fabrication processes for MEMS-IC integration, and also for controlling heat and mass transfer through porous media (e.g. sandstone). Computational fluid dynamics (CFD) simulation facilitates us to better understand such microscopic fluid flows because it is difficult to experimentally or theoretically analyse them in 3D.

Our objective in this study is to examine the applicability of a CFD method [1, 2] to simulation of motions of microscopic two-phase fluid on solid surfaces with edges for evaluating fluidic devices and for predicting underground fluid flows. The method adopts phase-field model (PFM) [3-5] for interface dynamics and lattice-Boltzmann model (LBM) [2, 6] as numerical solution scheme. Based on the free-energy theory, PFM reproduces an interface as a finite volumetric zone between different phases without imposing topological constraints on interface as phase boundary. The contact angle is obtained from a potential of the surface through a simple boundary condition of the gradient of the order parameter. As a result, the PFM approach does not necessarily require conventional algorithms for advection and reconstruction of interfaces [3]. LBM assumes that a fluid consists of fictitious mesoscopic particles repeating collisions with each other and rectilinear translations with an isotropic discrete velocity set. One of main features of a semi-Lagrangian LBM scheme is the simple particle-kinematic operation in discrete conservation form on an isotropic spatial lattice, which is useful for high-performance computing [6]. The PFM-LBM CFD method therefore has an attractive advantage over the others, efficient simulation of complex motions of multiple fluid particles on partially-wetted and textured surfaces [1, 2]. The major findings in preliminary immiscible liquid-liquid simulations are as follows: (1) the method simulated well departure of droplet from flat solid surface due to buoyancy in agreement with semi-empirical prediction; (2) the droplet had larger static contact angle on a textured hydrophobic surface than on the flat one in a similar way with experimental data.

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