Modeling and simulation of three-component flows on solid surface

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Abstract

Moving contact line problem, which occurs when the fluid-fluid interface intersects with solid substrate, has been a classical problem that has received extensive attention over the last several decades. It has been shown that classical hydrodynamic equations with no-slip boundary conditions can lead to nonphysical singularity in the vicinity of the contact line. Recently, the generalized Navier boundary condition(GNBC) is introduced to the problem of two component flows on solid substrates. A continuum phase field model which couples the Cahn-Hilliard and Navier-Stokes equations with GNBC is proposed. It is shown that the numerical results based on the continuum hydrodynamic model with GNBC can quantitatively reproduce the results form the molecular dynamic(MD) simulations, which imply that GNBC is quite accurate in describing the behavior of fluids near the contact line. In this work, we extend the moving contact line problem to three component flows. The model is also based on the Cahn-Hilliard and Navier-Stokes system, and the idea of GNBC is extended to problems with three phases. We show that, to model the three component system, the bulk free energy and the boundary energy have to be carefully chosen so that the model is well-posed and consistent with the two component system. In the aspect of numerics, we design an efficient adaptive finite element method for the system. Several numerical results are presented: including the spreading of liquid lens between two phases, the buoyancy driven drop through a fluid-fluid interface, spreading of a compound droplet on a stationary substrate, and the dynamics of a compound droplet on a substrate under shear flows.

Keywords: Phase field, Three phase flow, Contact line, Adaptive finite element