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Numerical Simulation for Moving Contact Line with Continuous Finite Element Schemes

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Abstract. In this paper, we compute a phase field (diffuse interface) model of Cahn-Hilliard type for moving contact line problems governing the motion of isothermal multiphase incompressible fluids. The generalized Navier boundary condition proposed by Qian et al. [1] is adopted here. We discretize model equations using a continuous finite element method in space and a modified midpoint scheme in time. We apply a penalty formulation to the continuity equation which may increase the stability in the pressure variable. Two kinds of immiscible fluids in a pipe and droplet displacement with a moving contact line under the effect of pressure driven shear flow are studied using a relatively coarse grid. We also derive the discrete energy law for the droplet displacement case, which is slightly different due to the boundary conditions. The accuracy and stability of the scheme are validated by examples, results and estimate order.

AMS subject classifications: 65M60, 76T10

Key words: Two-phase flow, generalized Navier boundary condition, continuous finite elements, moving contact line.

1 Introduction

Multiphase flows are common in our lives, for example, gas bubbles trapped and droplet of oil moved in water, biological fluids, and cells in blood, etc.. They play an important

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role in engineering, biological and applications. For example, the inclusion removal of melted materials is carried out with the help of bubble flotation [2]. When a bubble rises to the edge of a container the interface changes its geometric property. This forms moving contact line problem. Moving contact line, where the fluid-fluid interface intersects the solid wall has been extensively studied by researchers both theoretically and experimentally. Norman and Miksis [3] investigated the dynamics of a gas bubble with a moving contact line rising in an inclined channel. Luo et al. [4] carried out a numerical simulation on the Poiseuille flow of two immiscible fluids between two parallel plates with undulating solid surface and showed the effect of the surface roughness on the motion of two phase flow. The formation of bubbles on an orifice plate was studied by Chen et al. [5]. In their works, two models are considered where one is a stick-slip model and the other one assumes that the apparent contact angle is linearly related to the velocity. Fuentes and Cerro [6] presented a model for two immiscible fluids, considering force balance and inertia effect. Nikolayev et al. [7] proposed a model that took into account of heterogeneities of the solid surface and the inertia effect. Zahedi et al. [8] applied the idea of driving contact line movement by enforcing the equilibrium contact angle at the boundary to that in the traditional model and solved the new model by a conservative level set method. Gerbeau and Lelivre [9] numerically simulated two immiscible fluids between two parallel walls and performed a stability analysis in the energy norm with the consideration of the gravity and surface tension effects. Xu and Wang [10] analyzed the effect of the roughness of the rough surface on moving contact line. Jacqmin [11] investigated moving contact line dynamics of CHW (Cahn-Hilliard-van der Waals) diffuse mean-field interface. The convection or the diffusion driven by chemical potential gradients would cause the change of the interface. This phase field model was compared with the classical sharp interface model.

The change of the contact line as the fluid flows is of great interest where the boundary condition of a moving contact line is crucial. A no-slip condition holds on the boundary may lead to a force singularity in the vicinity of the contact line. This is why moving contact line problems are more complicated than normal multiphase flow problems. Several works have been carried out to eliminate the singularity. The most popular viewpoint is to relax the no-slip condition by introducing a new parameter called slip length [12]. With this viewpoint, Qian et al. [1] proposed the generalized Navier boundary condition (GNBC) based on the molecular dynamics theory. With the help of GNBC that can be derived variationally from the principle of minimum energy dissipation [21], they successfully simulated the moving contact line in two chemically patterned channels. Several numerical methods have been developed for moving contact line problem, for example, immersed interface method [13], finite element method [14,25], the volume of fluid method [15], a hybrid atomistic-continuum method [16] and moving mesh spectral method [17], etc. have been applied to moving contact line problems over the years. In addition, to construct a stable scheme, the energy of the system was made decreasing with time under certain conditions [19].