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An efficient scheme for a phase field model for the moving contact line problem with variable density and viscosity

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ABSTRACT

In this paper, we develop an efficient numerical method for the two phase moving contact line problem with variable density, viscosity, and slip length. The physical model is based on a phase field approach, which consists of a coupled system of the Cahn–Hilliard and Navier–Stokes equations with the generalized Navier boundary condition [1,2,5]. To overcome the difficulties due to large density and viscosity ratio, the Navier–Stokes equations are solved by a splitting method based on a pressure Poisson equation [11], while the Cahn–Hilliard equation is solved by a convex splitting method. We show that the method is stable under certain conditions. The linearized schemes are easy to implement and introduce only mild CFL time constraint. Numerical tests are carried out to verify the accuracy, stability and efficiency of the schemes. The method allows us to simulate the interface problems with extremely small interface thickness. Three dimensional simulations are included to validate the efficiency of the method.

1. Introduction

Moving contact line problem, where the fluid–fluid interface intersects the solid wall, is a classical problem that occurs in many physical phenomena. It is well known that classical hydrodynamical models with no-slip boundary condition lead to nonphysical singularity in the vicinity of the contact line [3]. A phase field model with generalized Navier boundary condition (GNBC) is proposed in [1,3] to resolve the issue. It is shown that the numerical results based on the GNBC can reproduce quantitatively the results from the MD simulation. This indicates that the new model can accurately describe the behavior near the contact line. The model involves a coupled system of the Cahn–Hilliard and Navier–Stokes equations.

$$\frac{\partial \phi}{\partial t} + \mathbf{v}\cdot\nabla\phi = M\nabla^2\mu, \tag{1.1}$$

$$\rho\left[\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{v}\right] = -\nabla p + \nabla\cdot\left[\eta D(\mathbf{v})\right] + \mu\nabla\phi + \rho\mathbf{g}_{ext}, \tag{1.2}$$

$$\nabla\cdot\mathbf{v} = 0, \tag{1.3}$$

here p is the pressure, $\eta D(\mathbf{v}) = \eta(\nabla\mathbf{v} + \nabla\mathbf{v}^T)$ denotes the viscous part of the stress tensor, ρ, η are the fluid mass density and viscosity; $\rho\mathbf{g}_{ext}$ is the external body force density, and M is the phenomenological mobility coefficient; $\mu = -K\nabla^2\phi - r\phi + u\phi^3$ is the chemical potential, and $\mu\nabla\phi$ is the capillary force; K, r, u are the parameters that are related to the

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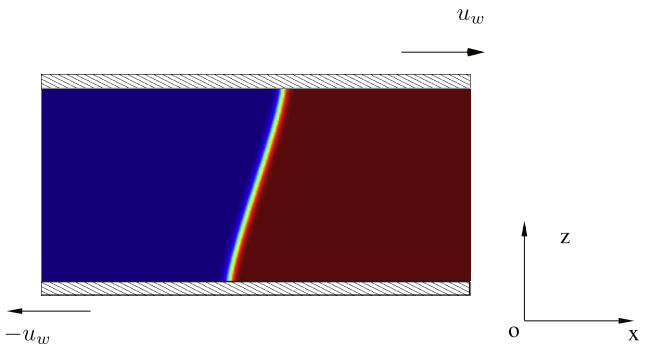

Fig. 1. Two-phase Couette flow with wall speed u_w.

interface profile thickness $\xi = \sqrt{K/r}$, the interfacial tension $\gamma = 2\sqrt{2}r^2\xi/3u$, and the two homogeneous equilibrium phases $\phi_\pm = \pm\sqrt{r/u}$ ($=\pm 1$ in our case).

To describe the motion of the contact line, Eq. (1.2) is supplemented with the generalized Navier boundary condition at top and bottom boundaries (Fig. 1).

$$\beta v_x^{slip} = -\eta\partial_n v_x + L(\phi)\partial_x\phi, \tag{1.4}$$

where $L(\phi) = K\partial_n\phi + \partial\gamma_{wf}(\phi)/\partial\phi$, and $\gamma_{wf}(\phi) = -\frac{1}{2}\gamma\cos\theta_s^{surf}\sin(\frac{\pi}{2}\phi)$, θ_s^{surf} is the static contact angle; β is the slip coefficient; $v_x^{slip} = v_x - u_w$ is the slip velocity, u_w is the wall speed. The velocity field is denoted by $\mathbf{v} = (v_x, v_z)$ (see Fig. 1), where v_x, v_z are velocities along x, z directions, $\mathbf{n}, \boldsymbol{\tau}$ are unit vectors orthogonal and tangential to the boundaries, $v_n := \mathbf{v}\cdot\mathbf{n}$, $v_\tau := \mathbf{v}\cdot\boldsymbol{\tau}$. In addition, a relaxation boundary condition is imposed on the phase field variable ϕ at the top and bottom boundaries:

$$\frac{\partial\phi}{\partial t} + v_x\partial_x\phi = -\Gamma\big[L(\phi)\big], \tag{1.5}$$

where Γ is a (positive) phenomenological parameter, together with the following impermeability conditions:

$$v_z = 0, \qquad \partial_n\mu = 0. \tag{1.6}$$

Here the variable density, viscosity and slip length are taken to be the volume average of those for the two flows, i.e.,

$$\rho = \rho_L\left(\frac{1+\phi}{2}\right) + \rho_G\left(\frac{1-\phi}{2}\right), \qquad \eta = \eta_L\left(\frac{1+\phi}{2}\right) + \eta_G\left(\frac{1-\phi}{2}\right).$$

Although this may be inconsistent with the continuity equation $\rho_t + \nabla\cdot(\rho\mathbf{v}) = 0$ (when ρ is not a constant), it is shown in [8] that the total mass is still conserved if the boundary conditions (1.6) are imposed.

There have been many work on developing efficient numerical methods for two phase flow with general variable density and viscosity [7–11,13–15]. However, most of the work were on models for problems where the interface does not intersect with the boundary. The main difficulty in those problems comes from the high (fourth) order derivatives and strong nonlinearity in the Cahn–Hilliard equation which introduces a strong stability constraint for the time step. Extra complexity is introduced in the moving contact line model due to the generalized Navier boundary condition (1.4). For two phase system with equal density and viscosity, we have developed an efficient gradient stable scheme [5]. The scheme is unconditionally stable and has the property of total energy decaying. Another efficient scheme based on a least square/finite element method is also proposed in [6].

Solving Navier–Stokes equations with large density ratios using projection method can be very time consuming since it requires solving a variable-coefficient stiffness matrix (with very large condition number) at each time step. Guermond and Salgado [11] proposed a splitting method for Navier–Stokes equations with variable density based on penalty techniques, which only requires solving pressure Poisson equation with constant coefficient per time step.

In this paper, we develop a gradient stable scheme for the system (1.1)–(1.6). The scheme is based on a convex splitting of the bulk free energy functional and the surface energy, and a splitting method based on the pressure Poisson equation for Navier–Stokes equations. We show, under certain conditions, the scheme has the total energy decaying property and is stable. Numerical tests are carried out to verify the stability, accuracy and efficiency of the scheme. We also compared the performance of two types of Navier–Stokes solvers. It is verified that, the splitting scheme based on pressure Poisson equation has similar accuracy as the projection method, but the splitting scheme is significantly more efficient in terms of computational cost, making it more favorable in large scale simulations.

The rest of the paper is organized as follows. In Section 2, we derive the energy law for the PDE system. The numerical scheme and discrete energy law are derived in Section 3. Numerical tests are performed and the results are analyzed in Section 4. The paper concludes in Section 5 with a few remarks.