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Numerical approximations for a phase-field moving contact line model with variable densities and viscosities

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ABSTRACT

We consider the numerical approximations of a two-phase hydrodynamics coupled phase-field model that incorporates the variable densities, viscosities and moving contact line boundary conditions. The model is a nonlinear, coupled system that consists of incompressible Navier–Stokes equations with the generalized Navier boundary condition, and the Cahn–Hilliard equations with moving contact line boundary conditions. By some subtle explicit–implicit treatments to nonlinear terms, we develop two efficient, unconditionally energy stable numerical schemes, in particular, a linear decoupled energy stable scheme for the system with static contact line condition, and a nonlinear energy stable scheme for the system with dynamic contact line condition. An efficient spectral-Galerkin spatial discretization is implemented to verify the accuracy and efficiency of proposed schemes. Various numerical results show that the proposed schemes are efficient and accurate.

1. Introduction

Mixtures of two or more immiscible fluid components with different physical properties are widely used in many science and engineering applications. When the interface of a fluid mixture touches the solid wall, a physical process called “moving contact line” (MCL) occurs. Appearing in many applications (e.g., spray cooling of surfaces, crop spraying, spray coating, etc.), MCL problem has always been an appealing and challenging topic for mathematical modeling and simulations. Different to hydrodynamics of one simple fluid, the no-slip boundary condition for Navier–Stokes equations is not applicable for multi-fluid MCL problems because a non-physical velocity discontinuity will occur at the MCLs (cf. [9,10,33]). To understand the hydrodynamical behavior near the MCLs, several methods have been developed including MD simulations [27,28,53], microscopic–macroscopic hybrid simulations [20,39], the level set method [52,56,57], the VOF method [24,40], the front tracking method [22], and the phase-field approach [12,25,34,35,37,41,51] considered in this paper.

Among aforementioned models/numerical methods, the phase-field (or diffuse interface) approach is now popular and widely used to simulate the interfacial dynamics due to its versatility in modeling as well as simulations (cf. [4,19,23,26, 29,31,43,60], and the references therein). Its idea can actually be dated back to the ancient work of Rayleigh [38] and van der Waals [54] one century ago. Such a method considers the fluid–fluid interface as a continuous, but steep change of some physical properties of two fluids, e.g., density or viscosity, etc. An order parameter (or called phase field variable) is introduced to label the two fluid components, thus the fluid–fluid interface is then represented by a thin but smooth

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transition layer that can remove the singularities in practice. The model is then derived from the energy-based variational formalisms, thus the interfacial dynamics and the complex rheology are incorporated to an unified theoretical framework that allows the dynamical model for each component to be combined in a single model. Therefore, the developed governing system is normally well-posed and satisfies a thermodynamically consistent energy dissipation law (or called energy stable), that makes it possible to implement corresponding mathematical analysis or design efficient numerical methods.

We recall that a series of pioneering works about the macroscopic phase field modeling for the MCL problem, as well as their analysis and numerical simulations had been carried out by Qian et al. in [35–37]. The governing system consists of the Navier–Stokes equations with the general Navier boundary condition (GNBC), and the Cahn–Hilliard equation with the dynamic contact line condition (DCLC). From the numerical point of view, it is quite a challenging topic to develop efficient time marching schemes, in particular, the energy stable schemes to solve such a complex dynamical system. The difficulties include (i) the small interfacial width that introduces stiffness into the system; (ii) the nonlinear coupling between the phase variable and the velocity due to nonlinear convections and stresses; (iii) the nonlinear couplings between the velocity and the phase variable on the MCL boundaries; and (iv) the coupling between the density, the viscosity, the velocity and the pressure in the fluid momentum equation. Recently, several attempts were made to improve the numerical stability and efficiency of schemes for solving MCL problems including the work of He et al. [21], Gao and Wang [12,13], Salgado et al. [41], Aland and Chen [3], Dong [7], Dong and Shen [8], and Shen et al. [51], etc. However, for the variable density and/or viscosity case, those schemes are either nonlinearly coupled [12,13,41] that requires some efficient iterative solvers and need relatively high computational cost, or linearly decoupled but unable to provide the energy stability in theory [7,8].

Therefore, in this paper, we aim to construct some effective and efficient numerical schemes to solve the phase-field MCL model for the case of variable densities and viscosities. More precisely, the schemes are expected to be unconditionally energy stable, satisfy an energy law in the discrete level, and lead to linear, decoupled, or coupled elliptic equations to solve at each time step.

The rest of the paper is organized as follows. In Section 2, we introduce the hydrodynamics coupled phase-field model with MCLs in the presence of non-matched densities and viscosities, and derive its associated PDE energy dissipation law. In Section 3, we present the numerical schemes, and prove their discrete energy dissipation law rigorously. In Section 4, we present the spatial discretization method using the Galerkin approach. In section 5, we present various numerical examples to illustrate the accuracy and efficiency of the proposed schemes. Some concluding remarks are given in Section 6.

2. The PDE system and its energy law

We now describe the phase-field model for a mixture of two immiscible, incompressible fluids in a confined domain $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ with densities ρ_1, ρ_2 and viscosities μ_1, μ_2, respectively.

We introduce a phase field variable (macroscopic labeling function) $\phi(\boldsymbol{x}, t)$ such that

$$\phi(\boldsymbol{x}, t) = \begin{cases} 1, & \text{fluid I}, \\ -1, & \text{fluid II}, \end{cases} \tag{2.1}$$

with a thin, smooth transition region of width $O(\epsilon)$, and consider the following Ginzburg–Landau type of Helmholtz free energy functional:

$$E_{mix} = \lambda \int_\Omega \Big(\frac{\epsilon}{2} |\nabla \phi|^2 + F(\phi) \Big) d\boldsymbol{x}, \tag{2.2}$$

where λ denotes rescaled characteristic strength of phase mixing energy. The first term in E_{mix} contributes to the hydrophilic type (tendency of mixing) of interactions between the materials and the second part, the double well bulk energy $F(\phi) = \frac{1}{4\epsilon}(\phi^2 - 1)^2$, represents the hydro-phobic type (tendency of separation) of interactions. As the consequence of the competition between the two types of interactions, the equilibrium configuration will include a diffusive interface with a thickness proportional to the parameter ϵ (cf., for instance, [60]).

The total energy of the hydrodynamic system is a sum of the kinetic energy E_k together with the mixing energy E_{mix}:

$$E = E_k + E_{mix} = \int_\Omega \Big(\frac{\rho}{2} |\mathbf{u}|^2 + \lambda \big(\frac{\epsilon}{2} |\nabla \phi|^2 + F(\phi) \big) \Big) d\boldsymbol{x}, \tag{2.3}$$

where $\mathbf{u}$ is the fluid velocity field and ρ is the density.

The evolution of the phase function is governed by the Cahn–Hilliard phase equation in the conserved form.

$$\phi_t + \nabla \cdot (\mathbf{u}\phi) = M \Delta \mu, \tag{2.4}$$

$$\mu = \lambda(-\epsilon \Delta \phi + f(\phi)), \tag{2.5}$$

where μ is the chemical potential and M is a mobility parameter related to the relaxation time scale, and $f(\phi) = F'(\phi) = \frac{1}{\epsilon}\phi(\phi^2 - 1)$.