Journal of Computational Physics 231 (2012) 1372–1386

Contents lists available at SciVerse ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

A gradient stable scheme for a phase field model for the moving contact line problem

Min Gao, Xiao-Ping Wang *

Department of Mathematics, The Hong Kong University of Science and Technology Clear Water Bay, Kowloon, Hong Kong, China

ARTICLE INFO

Article history:
Received 13 December 2010
Received in revised form 13 August 2011
Accepted 12 October 2011
Available online 23 October 2011

Keywords:
Navier–Stokes equations
Cahn–Hilliard equation
Phase field
Moving contact line
Convex splitting

ABSTRACT

In this paper, an efficient numerical scheme is designed for a phase field model for the moving contact line problem, which consists of a coupled system of the Cahn–Hilliard and Navier–Stokes equations with the generalized Navier boundary condition [1,2,4]. The nonlinear version of the scheme is semi-implicit in time and is based on a convex splitting of the Cahn–Hilliard free energy (including the boundary energy) together with a projection method for the Navier–Stokes equations. We show, under certain conditions, the scheme has the total energy decaying property and is unconditionally stable. The linearized scheme is easy to implement and introduces only mild CFL time constraint. Numerical tests are carried out to verify the accuracy and stability of the scheme. The behavior of the solution near the contact line is examined. It is verified that, when the interface intersects with the boundary, the consistent splitting scheme [21,22] for the Navier Stokes equations has the better accuracy for pressure.

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 leads to nonphysical singularity in the vicinity of the contact line [3]. The recent discovery of the generalized Navier boundary condition (GNBC) [1,2] has resolved this issue with respect to the immiscible flow over flat surfaces. A phase field model with generalized Navier boundary condition is proposed in [1] which involves a coupled system of the Cahn–Hilliard equation and the Navier–Stokes equations. 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.

There have been many work on developing efficient numerical schemes for the Cahn–Hilliard (or Allen–Cahn) Navier–Stokes system for two-phase flow [13–15,17,18,24]. 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 complicated generalized Navier boundary condition. For the Navier–Stokes equations, a class of efficient solvers of projection type have been developed in recent years (see the review article [22]). There are also a lot of work on the numerical methods for the Cahn–Hilliard equation and its non-conservative, lower order version, the Allen–Cahn equation [5–12]. In particular, attention has been paid to how to construct stable, energy decreasing scheme. An innovative idea, proposed by Eyre [9,10], leads to an unconditionally gradient

* Corresponding author. Tel.: +852 2358 7438; fax: +852 2358 1643.
E-mail addresses: gaomin@ust.hk (M. Gao), mawang@ust.hk (X.-P. Wang).

0021-9991/$ - see front matter
doi:10.1016/j.jcp.2011.10.015

stable, uniquely solvable one-step scheme based on a convex splitting of total free energy functional into contractive and expansive parts. The idea has also been extended to solve other systems [8,16,19,20].

In this paper, we develop an unconditionally gradient stable scheme for the coupled Cahn–Hilliard Navier–Stokes equations with the generalized Navier boundary condition. The scheme is based on a convex splitting of both the bulk free energy functional and the surface energy. We show, under certain condition, the scheme has the total energy decaying property and is unconditionally stable. Numerical tests are carried out to verify the stability and accuracy of the scheme. We also compared the performances of two types of Navier–Stokes solvers. It is verified that, when the interface intersects with the boundary, the consistent splitting scheme with accurate boundary condition [21,22] has the better accuracy for pressure.

The rest of the paper is organized as follows. In Section 2, we briefly describe the phase field model with GNBC. In Section 3, we derive the energy law for the PDE system. The Numerical scheme and discrete energy law are derived in Section 4. Numerical tests are performed and the results are analyzed in Section 5. The paper concludes in Section 6 with a few remarks.

2. The phase field model with the generalized Navier boundary condition

A phase field model with generalized Navier boundary condition is proposed in [1] to model the moving contact line problem. The system includes a coupled system of Cahn–Hilliard Navier–Stokes equations,

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = M \Delta \mu \tag{2.1}$$

$$\rho \left[\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] = -\nabla p + \nabla \cdot \boldsymbol{\sigma}^{v} + \mu \nabla \phi + \rho \mathbf{g}_{ext} \tag{2.2}$$

$$\nabla \cdot \mathbf{v} = 0 \tag{2.3}$$

Here p is the pressure, $\boldsymbol{\sigma}^{v} = \eta(\nabla \mathbf{v} + \nabla \mathbf{v}^{T})$ denotes the viscous part of the stress tensor, ρ, η are the fluid mass density and viscosity, which are assumed to be constant in this paper, $\rho \mathbf{g}_{ext}$ is the external body force density, and M is the phenomenological mobility coefficient; $\mu = -K\Delta\phi - r\phi + u\phi^3$ is the chemical potential, and $\mu\nabla\phi$ is the capillary force; K, r, u are the parameters that are related to the interface profile thickness $\xi = \sqrt{K/r}$, the interfacial tension $\gamma = 2\sqrt{2}r^2\xi/3u$, and the two homogeneous equilibrium phases $\phi_{\pm} = \pm\sqrt{r/u}$ (=±1 in our case).

We will consider a two-phase Couette flow confined in a channel as in Fig. 1. To describe the system, Eq. (2.2) is supplemented with the generalized Navier boundary condition (GNBC),

$$\beta v_x^{slip} = -\eta \partial_n v_x + L(\phi) \partial_x \phi \tag{2.4}$$

Here $L(\phi) = K\partial_n\phi + \partial\gamma_{wf}(\phi)/\partial\phi$, and $\gamma_{wf}(\phi) = -\frac{1}{2}\gamma \cos\theta_s^{surf} \sin\left(\frac{\pi}{2}\phi\right)$, θ_s^{surf} is the static contact angle, β is the slip coefficient. The velocity field is denoted by $\mathbf{v} = (v_x, v_z)$, where v_x is velocity along x direction, v_z is velocity along z direction. $(\mathbf{n}, \tau)$ denote normal and tangential directions to the boundary. In addition, a dynamic boundary condition is imposed on the phase field variable ϕ at the top and bottom boundaries,

$$\frac{\partial \phi}{\partial t} + v_x \partial_x \phi = -\Gamma[L(\phi)] \tag{2.5}$$

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

$$v_z = 0, \quad \partial_n \mu = 0 \tag{2.6}$$

To obtain dimensionless equations as in [1], we scale length by some length scale L, ϕ by $\sqrt{r/u}$ (=1, in this paper), velocity by the wall speed V, time by L/V, and pressure by $\eta V/L$. Then the equations become

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = \mathcal{L}_d \Delta \mu \tag{2.7}$$

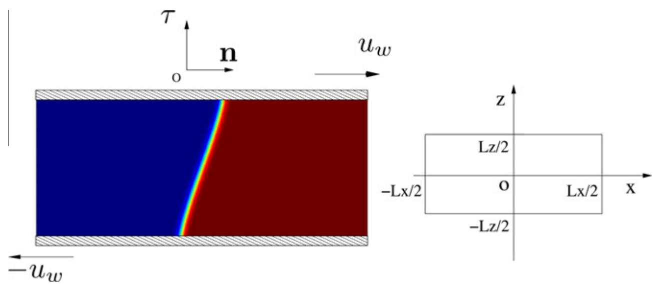

Fig. 1. Two-phase Couette flow with wall speed u_w.