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DECOUPLED, ENERGY STABLE SCHEME FOR HYDRODYNAMIC ALLEN-CAHN PHASE FIELD MOVING CONTACT LINE MODEL*

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Abstract

In this paper, we present an efficient energy stable scheme to solve a phase field model incorporating contact line condition. Instead of the usually used Cahn-Hilliard type phase equation, we adopt the Allen-Cahn type phase field model with the static contact line boundary condition that coupled with incompressible Navier-Stokes equations with Navier boundary condition. The projection method is used to deal with the Navier-Stokes equations and an auxiliary function is introduced for the non-convex Ginzburg-Landau bulk potential. We show that the scheme is linear, decoupled and energy stable. Moreover, we prove that fully discrete scheme is also energy stable. An efficient finite element spatial discretization method is implemented to verify the accuracy and efficiency of proposed schemes. Numerical results show that the proposed scheme is very efficient and accurate.

Mathematics subject classification: 65N06, 65B99.
Key words: Moving contact line, Phase-field, Navier-Stokes equations, Allen-Cahn equation, Finite element, Energy stable scheme, Linear element.

1. Introduction

Two phase immiscible flows are common in our lives, such as the air bubble in the water, and droplet of oil in the water, and cells in the blood, etc.. When the air bubble rises to the edge of glass, the interface will change its geometry. Then it will form a moving contact line (MCL) problem. Moving contact line, where the fluid-fluid interface touches the solid wall, has been widely investigated by the researcher theoretically and experimentally. People are interested in the topic that how the contact line evolves when the solid wall moves. In this situation, the no-slip boundary condition for the flow is not applicable again. From this viewpoint, Qian et al. [28, 29] proposed the generalized Navier boundary condition (GNBC) according to the molecular dynamics theory. To investigate the complex behavior at MCLs, plenty of models are studied by the researchers. For example, molecular dynamical (MD) simulations are studied by Koplik et al. [15, 16] and Qian et al. [28, 29]. Microscopic-macroscopic hybrid simulations

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had been carried out by Hadjiconstantinou [8], Ren and E [30] etc. Although this approach is powerful, the computational cost is very expensive for macroscopic applications.

There are a lot of methods to study the MCL problem, such as the immersed interface method [17], the volume of fluid method [31], a hybrid atomistic-continuum method [8], and phase field method [41] etc. In the recent years, phase field method has been used widely on the interfacial phenomena, and has been applied to simulate many dynamical processes successfully in many fields [2,4,11–14,18–20,22,25,27,35,36,38–43,46–49,51,52,56,61,63,64]. In a phase field model, a continuous phase field function is used to denote the two immiscible fluids where the fluid-fluid interface has a thickness. In the framework of phase field approach, the governing system is usually obtained from the gradient flow, which is a variational formalism from the total free energy. Thus, there is usually a physical energy law associated with the phase field model [29]. This energy law will help us to carry out mathematical analysis and further design efficient numerical scheme. Thus, from the numerical point view, we are interested in constructing a simple and efficient (linear and decoupled) scheme which satisfies the discrete energy law.

Qian et al. [29] have proposed a Navier-Stokes Cahn-Hilliard (NSCH) system to study the MCL problem, where the GNBC is used for Navier-Stokes equation and the dynamic contact line condition (DCLC) is applied on the Cahn-Hilliard equation. As we all know, the Cahn-Hilliard equation is a four-order equation with volume fraction being conserved, but it needs more time to carry out than Allen-Cahn (second-order) equation on numerical computation. Though Allen-Cahn equation is not conserved on volume fraction, it can keep conserved with the introduction of a Lagrangian multiplier. Thus in this paper we use Allen-Cahn equation to replace the Cahn-Hilliard equation.

The purpose of our paper is to construct a linear, decoupled, fully discrete, first-order, and unconditionally energy stable scheme for the Navier-Stokes Allen-Cahn (NSAC) system. We know that the NSAC system is a coupled system, which includes the coupling between the phase field variable and the velocity in the convection and the stress, and the coupling between the velocity and the pressure in the momentum equation. There are several methods to design the energy stable scheme, such as the operator-splitting on the time-discretization [10], a convex splitting scheme in [1,33], and the stabilization approach in [21,22,24,36–39]. Although these schemes are energy stable, they still have some disadvantages. Firstly, the operator-splitting scheme and the convex splitting scheme are usually coupled and nonlinear due to the couplings in the system, which take much time on iterations to carry out the numerical results. Secondly, it is difficult to prove the unconditional solvability for these nonlinear schemes. At last, although the stabilizing approach is linear and decoupled, the truncation error is introduced in the scheme, which requires the double well potential to be bounded form the viewpoint of mathematics. Thus, in this paper, we shall overcome these difficulties to construct a fully discrete, linear and decoupled energy stable scheme using the recently developed "Invariant Energy Quadratization" approach [5,9,50,53–55,57,58,60,62]. In our previous paper [24,59], we developed some decoupled, energy stable numerical schemes to solve the hydrodynamics coupled Allen-Cahn MCL phase field model by adding the extra stabilizing terms for phase field equation. In this paper we adopt a novel skill to construct a linear, decoupled, and unconditionally energy stable scheme without using the stabilizing approach for the phase field equation.

The rest of the paper is organized as follows. In the next section, we present the phase field model of moving contact line condition and show the energy dissipation law for the system. In