Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2016-0008

Vol. **21**, No. 3, pp. 867-889
March 2017

Numerical Approximations for Allen-Cahn Type Phase Field Model of Two-Phase Incompressible Fluids with Moving Contact Lines

Lina Ma[1], Rui Chen[2], Xiaofeng Yang[3,*] and Hui Zhang[4]

[1] *Department of Mathematics, Penn State University, State College, PA 16802, USA.*
[2] *Institute of Applied Physics and Computational Mathematics, Beijing, 100088, P.R. China.*
[3] *Department of Mathematics, University of South Carolina, Columbia, SC 29208, USA; Beijing Institute for Scientific and Engineering Computing, Beijing University of Technology, Beijing, 100124, P.R. China.*
[4] *Shool of Mathematical Sciences, Beijing Normal University, Laboratory of Mathematics and Complex Systems, Ministry of Education, Beijing, 100875, P.R. China.*

Received 15 January 2016; Accepted (in revised version) 28 July 2016

Abstract. In this paper, we present some efficient numerical schemes to solve a two-phase hydrodynamics coupled phase field model with moving contact line boundary conditions. The model is a nonlinear coupling system, which consists the Navier-Stokes equations with the general Navier Boundary conditions or degenerated Navier Boundary conditions, and the Allen-Cahn type phase field equations with dynamical contact line boundary condition or static contact line boundary condition. The proposed schemes are linear and unconditionally energy stable, where the energy stabilities are proved rigorously. Various numerical tests are performed to show the accuracy and efficiency thereafter.

AMS subject classifications: 65M12, 65M70, 65P99

Key words: Phase-field, two-phase flow, Navier-Stokes, contact lines, stability.

1 Introduction

Phase field (or diffuse interface) methods have been used widely and successfully to simulate a variety of interfacial phenomena, and have become one of the major tools to study the interfacial dynamics in many science and engineering fields (cf. [4–6, 8, 9, 12, 13, 15, 16,

*Corresponding author. *Email addresses:* `linama@psu.edu` (L. Ma), `ruichenbnu@gmail.com` (R. Chen), `xfyang@math.sc.edu` (X. Yang), `hzhang@bnu.edu.cn` (H. Zhang)

25] and the references therein). The starting point of the phase-field approach is that the interface between multiple material components is viewed as a transition layer, where the two components are assumed to mix to a certain degree. Hence, the dynamics of the interface can be determined by the competition between the kinetic energy and the "elastic" mixing energy. Based on the variational formalism, the derived phase field model usually follows the thermodynamically consistent (or called energy stable) energy dissipation law, making it possible to carry out mathematical analysis, to develop efficient numerical schemes, and further to perform reliable numerical simulations.

In typical phase field models, there are mainly two categories of system equations: the Allen-Cahn equation (Bray [2]) and the Cahn-Hilliard equation (Cahn and Hilliard [3]), based on choices of diffusion rates. From the numerical point of view, the Allen-Cahn equation is a second-order equation, which is easier to solve numerically but does not conserve the volume fraction, while the Cahn-Hilliard equation is a fourth-order equation which conserves the volume fraction but is relatively harder to solve numerically. Since the PDE of either system usually follows the energy law, people are particularly interested in developing efficient numerical schemes that can satisfy a thermo-consistent energy law in the discrete level. Moreover, it is specifically desirable to develop some "easy-to-implement" (linear or decoupled) schemes in order to avoid expensive computational cost spent on the iterations needed by the nonlinear schemes.

In [18–21], the authors developed an efficient phase field model to simulate the so called "moving contact line" (MCL) problem, where the fluid-fluid interface may touch the solid wall. For such situation, the simple no-slip boundary conditions implying that the position of the contact line does not move, are not applicable since there may exist quite a few molecules near the surface that they "bounce along" down the surface. Thus the phase field model derived in [18–21] consists of Navier-Stokes equations with the general Navier boundary condition (GNBC), and the equations for the phase field variable with the so-called dynamical contact line boundary condition (DCLBC). Due to the considerations of volume conservation, the dynamics of the phase field variable is governed by the fourth order Cahn-Hilliard equation. We recall that a nonlinear, energy stable numerical scheme was proposed in [10], where the convective term was treated semi-implicitly, and the double well potential was handled by the convex splitting approach. Such a scheme requires solving a coupled nonlinear system that usually is not convenient for the computations.

Therefore, in this paper, we aim to develop some efficient numerical schemes to solve the phase field model with MCLs. To avoid the difficulties to solve the fourth order Cahn-Hilliard equation, we adopt the second order Allen-Cahn equation by assuming that the relaxation of the phase variable is governed by the L^2 gradient flow. To overcome non-conservation of the volume fraction, an extra term is added in the free energy to penalize the volume, which is one of the common practices in the framework of phase field models [8, 26]. We develop two numerical schemes, one for the static contact line boundary condition (SCLBC) and the other for the DCLBC. Both schemes are linear and unconditionally energy stable. Moreover, the computations of the phase variable are