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A Fully Decoupled Linear Second-Order Energy Stable Numerical Scheme for the Moving Contact Line Problem

Min Gao[1] and Yi Shi[2,3,*]

[1]*Division of Foundational Teaching, Guangzhou College of Technology and Business, Guangzhou 510850, P.R. China.*
[2]*School of Mathematics, Shandong University, Jinan 250100, P.R. China.*
[3]*Shandong National Center for Applied Mathematics, Jinan 250100, P.R. China.*

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Abstract. A decoupled linear second-order accurate unconditionally energy stable scheme for a phase-field model of the moving contact line (MCL) problem is proposed. The model consists of coupled Cahn-Hilliard and Navier-Stokes equations with the generalized Navier boundary condition. The scheme proposed introduces three scalar auxiliary variables to decouple nonlinear coupling terms while retaining stability and accuracy. Two of these variables represent the bulk and boundary energy, and one captures the "zero-energy-contribution" property between convection and surface tension terms. All related terms are decoupled by applying semi-explicit treatments while preserving stability and accuracy. Further coupling between velocity and pressure is removed by adopting a projection method. The overall scheme is second-order accurate, and the unconditional stability of energy is rigorously proved. Numerical results demonstrate the accuracy, efficiency, and stability of the method for the MCL problem. Besides, a consistent implementation of the contact angle hysteresis (CAH) is conducted to model important CAH phenomena.

AMS subject classifications: 65M06, 65M12, 76T06, 35Q35

Key words: Moving contact line, phase-field model, fully decoupled, second-order, unconditional energy stability.

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 [15, 18, 19]. It is well-known that classical hydrodynamic models with no-slip boundary conditions lead to nonphysical singularity in the vicinity of the contact line [17]. The recent discovery of the generalized Navier boundary condition (GNBC) [16, 17] has resolved this issue for immiscible flows

*Corresponding author. *Email addresses:* `gaomin@gzgs.edu.cn` (M. Gao), `shiyi@sdu.edu.cn` (Y. Shi)

over flat surfaces. A phase-field model with the GNBC was proposed in [17], involving a coupled system of the Cahn-Hilliard (CH) equation and the Navier-Stokes (NS) equations. Numerical results based on the GNBC have been shown to quantitatively reproduce the results from the molecular dynamics simulations, indicating that the new hydrodynamic model can accurately describe the behavior near the contact line.

Thereafter, developing efficient numerical schemes for the phase-field model has attracted many researchers [2, 6, 7, 11, 14, 22, 24, 25, 29, 31, 33, 35, 37]. However, it remains a challenging task because of the high complexity of the coupled system. The Cahn-Hilliard equation introduces severe stability constraints on the time step because of its high-order (fourth) derivatives and strong nonlinearity. Additionally, the coupling between velocity and pressure results in saddle point problems after discretization. Extra complexity arises in the moving contact line model because of the generalized Navier boundary condition. Further coupling introduced by the convection term and surface tension remains unresolved in the sense that these terms have yet to be effectively decoupled while maintaining stability. In the previous works [6, 7], we applied convex splitting to handle the CH equation and boundary conditions, and a pressure correction method to decouple velocity and pressure. An efficient, energy stable scheme was obtained, but unconditional stability was achieved only for the first-order version, and the resulting system remained coupled due to surface tension and convection terms. Shen *et al.* [22] proposed first-order accurate, linear, coupled and decoupled energy stable schemes. The stabilization approach was used for the CH equation to obtain a linear scheme, while the decoupled scheme was achieved by adding a stabilizing term to the convective velocity of the CH equation [3]. Energy stability was proved for both schemes; however, for the decoupled scheme, stability held only under static contact line conditions. The time step constraint of the decoupled scheme was investigated in detail with respect to the capillary number and boundary relaxation coefficient. Yu and Yang [33] further extended these ideas [22] to variable densities and viscosities, while ensuring strictly energy stability. Based on the invariant energy quadratization (IEQ) approach, Yang and Yu [31] first developed a second-order, energy stable scheme for the phase-field MCL model. The IEQ approach introduces an auxiliary variable to transform the nonlinear potentials in the CH equation and boundary conditions into a quadratic form of a new variable, allowing all nonlinear terms to be treated semi-explicitly. Thus, two second-order accurate, weakly coupled through stress, energy stable schemes were proposed, resulting in a linear system with variable coefficients. Later, combining with the scalar auxiliary variable (SAV) method, Zhu *et al.* [37] proposed a first-order, energy stable scheme that is linear with constant coefficients, and energy stability was proved for the fully discrete scheme. More recently, Yang [29, 30] noted that the advection and surface tension terms satisfy a “zero-energy-contribution” feature and rewrote the PDE system by introducing a nonlocal variable. The authors then proposed a completely decoupled scheme for the binary surfactant model with simple boundary conditions while still preserving second-order accuracy and energy stability. The introduction of the nonlocal variable enabled the decomposition of discrete coupled equations into four sub-equations with constant coefficients, which could be solved independently and efficiently. Later, this method was applied to phase-field models in various applications [27, 28, 32, 36].