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An energy-stable finite-difference scheme for the binary fluid-surfactant system

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ABSTRACT

We present an unconditionally energy stable finite-difference scheme for the binary fluid-surfactant system. The proposed method is based on the convex splitting of the energy functional with two variables. Here are two distinct features: (i) the convex splitting energy method is applied to energy functional with two variables, and (ii) the stability issue is related to the decay of the corresponding energy. The full discrete scheme leads to a decoupled system including a linear sub-system and a nonlinear sub-system. Algebraic multigrid and Newton-multigrid methods are adopted to solve the linear and nonlinear systems, respectively. Numerical experiments are shown to verify the stability of such a scheme.

1. Introduction

There has been a large amount of research studies about the surfactant adsorption on the binary fluid interface due to the amphophilic nature and many applications of the surfactant molecules. For instance, surfactant molecules can reduce the risk from bubbles formed in blood due to rapid decompression [1], facilitate the break up of large droplets into smaller ones [8,11] and prevent the coalescence of smaller droplets [11].

Various methods have been developed to model the evolution behavior of the binary fluid and the mass transportation of surfactant in fluids. In [12,19], the macroscopic approach specifying a mixing energy law is adopted to model the role of surfactant in fluids and provides a mechanism of the adsorption of surfactant on binary fluid interfaces. In [3,17,18], the fluid mixture is described by the Cahn–Hilliard type of energy. In this paper, the equilibrium and dynamical behaviors of the binary fluid surfactant system (BFS) are investigated through a phase field model. The total free energy of the phase field system is defined as [20]:

$$G(u,\rho)=\int_{\Omega}\frac{f(u)}{\epsilon}+\frac{\epsilon}{2}|\nabla u|^2+\frac{\alpha}{2}\big(\rho-|\nabla u|\big)^2+\beta H(\rho)\,d\mathbf{x}, \tag{1.1}$$

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where

$$f(u) = \frac{1}{4}u^2(1-u)^2, \quad H(\rho) = \rho\ln\rho + (1-\rho)\ln(1-\rho),$$

$\Omega \subseteq \mathbf{R}^2$ or $\mathbf{R}^3$, $u : \Omega \to \mathbf{R}$ is an order parameter in which $u = 1$ and $u = 0$ represent two different fluid phases, and $\rho : \Omega \to \mathbf{R}$ is the surfactant concentration. ϵ, α and β are small positive parameters. Here we choose both α and β to be $\mathcal{O}(\epsilon)$ to ensure the equally competing effect.

The above energy consists of three parts [20]:

(1) The Cahn–Hilliard free energy, $f(u)/\epsilon + \epsilon|\nabla u|^2/2$, describing the behavior of the binary fluid and leading to the coarsening of separated phase domains.
(2) The surfactant-interface coupling energy, $(\rho - |\nabla u|)^2$, describing the adsorption behavior of the surfactant near the binary fluid interfaces.
(3) An entropy term $H(\rho)$ specifying the ideal mixing manner of surfactant in fluids. This term restricts the value of ρ to be in the range $(0, 1)$. ρ will reach it's upper bound if the interface is fully saturated with surfactant [19].

The time evolutional equations of u and ρ are assumed to obey the generalized Fich law and are of the Cahn–Hilliard type as follows [2]:

$$\frac{\partial u}{\partial t} = \nabla\cdot(\nabla\bar{\mu}), \tag{1.2}$$

$$\frac{\partial \rho}{\partial t} = \nabla\cdot\left(M_\rho(\rho)\nabla\tilde{\mu}\right), \tag{1.3}$$

where $\bar{\mu} = \frac{\delta G}{\delta u}(u,\rho)$ and $\tilde{\mu} = \frac{\delta G}{\delta \rho}(u,\rho)$ are the corresponding chemical potentials of u and ρ, respectively. We assume that $\bar{\mu}$ and $\tilde{\mu}$ are periodic on Ω. $M_\rho(\rho) = \rho(1-\rho)$ is the mobility chosen to obtain a Ficikan equation for ρ [15]. Eqs. (1.2) and (1.3) are subject to the periodic boundary conditions and suitable initial data.

In [21], local-in-time error estimates were presented to ensure the convergence of the scheme based on convex splitting method. In [20], the time-dependent solutions of the system were studied by numerical computations based on pseudo-spectral Fourier method. In [14], two nonlinear diffusion equations for thin film epitaxy are studied and initial-boundary-value problems for equations are proven to be well-posed. In this work, we construct such a finite difference scheme that guarantees energy stability and mass conservation. The both properties are verified theoretically and numerically.

There have been many numerical studies based on energy stability. In [13], the author reviewed the recent development of phase-field models and their numerical methods for multi-component fluid flows with interfacial phenomena. In [22], an implicit–explicit scheme was proposed for solving the molecular beam epitaxial growth models. The unconditionally energy stability was guaranteed by adding some linear terms consistent with the truncation errors. The disadvantage of this method is that the artificial term depends on the unknown numerical solutions. An improved larger time step strategy was then proposed in [9]. The similar technique was used by Zhu, Chen, and Tikare [23] in the simulation of the Cahn–Hilliard equation. An energy stable spectral are developed to the anisotropic Cahn–Hilliard systems in [4]. Two semi-implicit finite difference schemes were proposed for the molecular beam epitaxy growth model[16]. One deals with the diffusion term explicitly using the known previous data, and the other scheme uses the Crank–Nicolson (C–N) type implicit approximation. The both resulting schemes are proved unconditionally energy stable. Numerically, the Newton-multigrid iterative method is applied to solve the nonlinear system.

In this paper, the convex splitting of the energy functional is adopted to prove energy stability and we construct the difference scheme directly based on the splitting of the functional instead of partial differential equations. Such a method has been used in [21,5] for a full discrete scheme of the phase field crystal (PFC) model which corresponds to a single variable energy functional. It is reasonable to extend this method to the energy functional of two variables such as (1.1), which is the novelty of this paper. Numerical computation is also carried out to illustrate energy stability. In our computation, based on convex splitting method at the discrete-time level, the fully discrete form is obtained by further adopting the central difference schemes. Also, the fully discrete schemes lead to a decoupled system containing a linear sub-system and a nonlinear sub-system. We choose algebraic multigrid method to solve the linear system and combine Newton-iteration method with algebraic multigrid method to solve the nonlinear system efficiently. We provide the evolution of energy with time which is agreement with the theoretical result. Moreover, the numerical solution u and ρ are observed to match well with the ones in the referenced papers.

The rest of the paper is organized as follows. In Section 2, we first prove the existence of a convex splitting energy and present a time-discrete, space-continuous scheme. The energy property is proved. In Section 3, we construct a finite difference scheme and prove the energy stability and mass conservation in discrete sense. Numerical experiments and discussions with two different initial conditions are provided in Section 4 followed by some conclusions in Section 5.