INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 18, Number 3, Pages 399–425

A POSITIVITY-PRESERVING AND CONVERGENT NUMERICAL SCHEME FOR THE BINARY FLUID-SURFACTANT SYSTEM

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Abstract. In this paper, we develop a first order (in time) numerical scheme for the binary fluid surfactant phase field model. The free energy contains a double-well potential, a nonlinear coupling entropy and a Flory-Huggins potential. The resulting coupled system consists of two Cahn-Hilliard type equations. This system is solved numerically by finite difference spatial approximation, in combination with convex splitting temporal discretization. We prove the proposed scheme is unique solvable, positivity-preserving and unconditionally energy stable. In addition, an optimal rate convergence analysis is provided for the proposed numerical scheme, which will be the first such result for the binary fluid-surfactant system. Newton iteration is used to solve the discrete system. Some numerical experiments are performed to validate the accuracy and energy stability of the proposed scheme.

Key words. Binary fluid-surfactant system, convex splitting, positivity-preserving, unconditional energy stability, Newton iteration

1. Introduction

Two important characteristics of surfactants in binary fluid is that they can move towards the fluid interface due to their amphiphilic structure and they can reduce the interfacial tension and system energy [37]. Therefore, surfactants have various applications in many fields such as biotechnology and industry because of their features [2, 35]. In the past two decades, there have been a number of excellent studies related to models with surfactants [17, 27, 29, 53, 61, 63]. Often, there are two different ideas to model the interfacial dynamics with surfactants. One is the sharp interface model which has a long history dated back to one century ago [19, 48], and this kind of model has been adopted in [24, 26]. In fact, sharp interface models have made great progresses in explaining kinetics of diffusional phase transformations and simulating multiphase systems with surfactants at one time. However, there are some difficulties stemming from the interface interactions with various complex processes during the course of phase transformations [35]. The other approach method is the known phase-field method [16, 28, 18, 54]. This approach makes use of an appropriate free energy functional to character the interfacial dynamics, and it has been adopted to investigate the interfacial dynamics with surfactants in [17, 29, 49, 51, 52]. In particular, phase-field method was used to in [29] to study the phase transition behaviors of the monolayer microemulsion system, formed by surfactant molecules. Generally, the free energy of binary fluid-surfactant model consists of the following two parts: the first part is the classical Ginzburg-Landau double well potential, which is used to describe a binary mixture, and the other part, called nonlinear coupling entropy term, has a historical evolution process, and is used to account for the influence of the surfactant in boosting the formation of interfaces. Laradji et al. in the pioneering work [29] introduced

Received by the editors October 5, 2020 and, in revised form, January 25, 2021.
2000 *Mathematics Subject Classification.* 35K30, 35K55, 49J40, 65M06, 65M12.
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two phase field variables to represent the local densities of the fluids, as well as the local concentration of the surfactant, respectively. As mentioned in [27], an extra diffusion term was added to prevent the model from becoming unbounded and a Ginzburg-Landau type potential for the concentration variable to allow the coexistence of the two bulk states. In order to restrict the range of the concentration variable, the authors added the logarithmic Flory-Huggins potential in [53], based on the nonlinear coupling entropy similar to [27, 29]. In consideration of penalizing the concentration to accumulate along the fluid interface, the authors changed the nonlinear coupled entropy slightly in [17]. In addition, a further modified model was considered in [50] by adding the Flory-Huggins potential for the local concentration variable as well, in comparison with the model in [17].

In this paper, we focus on constructing unconditionally energy stable numerical schemes for the binary fluid-surfactant model in [50]. There have been some works about numerical approximation to multi-phase models [7, 25]. Owing to the stiff nonlinear terms originated from the thin interface thickness parameter, there are a lot of subtle difficulties to construct numerical schemes with unconditional energy stability, especially for the second order accurate (in time) scheme. Lots of efforts have been made to solve these problems [7, 59, 66], etc. Since a simple fully implicit or explicit type discretization brings extremely severe time step size constraint on the interfacial width [1, 15, 47], a semi-implicit method was adopted in [50]. However, the author mentioned that it suffers from a small CFL conditional number. Recently, Gu et al. in [20] constructed an energy stable finite difference scheme for the binary fluid-surfactant system, which is based on the convex splitting approach [13, 43, 56, 58]: implicit treatment for the convex part and explicit treatment for the concave part. Meanwhile, it is observed that, the convexity analysis for one mixed term has not been theoretically justified in [20], due to the multi variables involved in the system. In addition, the positivity-preserving property has not been theoretically proved, so that the well-defined nature of the numerical scheme is not available. More recently, Yang et al. constructed the linear and stable schemes for the binary fluid-surfactant system with constant mobility in [63], using the invariant energy quadratization (IEQ) technique [6, 21, 23, 60, 62, 64, 65, 68]. In this approach, the free energy is transformed into an equivalent quadratic form by introducing appropriate auxiliary variables, and all nonlinear terms in this system are treated semi-explicitly [63]. The energy stability has been derived for the IEQ method, while such a stability has to be based on an alternate energy functional (involved with auxiliary variables), not for the original energy functional, as always in the IEQ approach. Moreover, the positivity-preserving property is not available to the IEQ-based numerical method, because of the explicit treatment for the nonlinear logarithmic term. In addition to the IEQ idea, Zhu et al. proposed the scalar auxiliary variable (SAV) method to the surfactant model in [69], following similar ideas in [46, 45]. The SAV approach introduces a constant-coefficient linear equation to solve at each time step, and the energy stability could be derived for an alternate energy involved with a scalar variable. The convergence and error estimate for the SAV approach, for the typical Cahn-Hilliard equation with double-well potential, has also been established in recent works [33, 44]. However, an application of the SAV approach to the surfactant model could not overcome the difficulty to theoretically justify the positivity-preserving property, due to the explicit treatment of the logarithmic term. In turn, the Flory-Huggins energy potential has to be re-defined and extended around and beyond the singular phase