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Fully Decoupled, Linear and Unconditionally Energy Stable Schemes for the Binary Fluid-Surfactant Model

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Abstract. Here, we develop a first and a second order time stepping schemes for a binary fluid-surfactant phase field model by using the scalar auxiliary variable approach. The free energy contains a double-well potential, a nonlinear coupling entropy and a Flory-Huggins potential. The resulting coupled system consists of a Cahn-Hilliard type equation and a Wasserstein type equation which leads to a degenerate problem. By introducing only one scalar auxiliary variable, the system is transformed into an equivalent form so that the nonlinear terms can be treated semi-explicitly. Both the schemes are linear and decoupled, thus they can be solved efficiently. We further prove that these semi-discretized schemes in time are unconditionally energy stable. Some numerical experiments are performed to validate the accuracy and energy stability of the proposed schemes.

AMS subject classifications: 35K35, 35K55, 65M12, 65M22

Key words: Binary fluid-surfactant, scalar auxiliary variable approach, unconditional energy stability, linear scheme, decoupled.

1 Introduction

Surfactants in binary fluid move towards the fluid interface due to their amphiphilic structure which contains hydrophile and hydrophobe groups. Therefore, they can reduce the interfacial tension and system energy [35]. Because of this property, surfactants have a number of applications in many fields. Examples are that in biotechnology surfactants

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can reduce the risk from bubbles formed in blood due to rapid decompression [4], and in industry surfactants can improve food and shampoo processing and enhance oil recovery [34].

In the past two decades, there are numerous studies related to surfactants [17, 28, 30, 47, 53, 56]. Actually, there are two basic ways to simulate the interfacial dynamics with surfactants. One is the sharp interface model which has a long history dated back to one century ago [19, 42]. This kind of model is 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 [34]. The other is the phase-field model [16, 18, 29, 48]. The phase-field model makes use of an appropriate free energy functional to character the interfacial dynamics. This kind of method is adopted to investigate the interfacial dynamics with surfactants in [17, 30, 43, 45, 46]. And in [30], the phase-field method was used 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. The other is the nonlinear coupling entropy term to account for the influence of the surfactant in boosting the formation of interfaces. It has a historical evolution process about this part of energy. Laradji et al. in the pioneering work [30] introduced 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 [28], the authors added an extra diffusion term 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 in [47] added the logarithmic Flory-Huggins potential based on the nonlinear coupling entropy which is similar in [28, 30]. In consideration of penalizing the concentration to accumulate along the fluid interface, the author changed the nonlinear coupled entropy slightly in [17]. In [44] the authors further modified the model in [17] by adding the Flory-Huggins potential for the local concentration variable as well.

In this paper, we focus on constructing unconditional energy stable numerical schemes for the multi-phase model in [44]. There have been some works about numerical approximation to multi-phase models [11, 25]. Owing to the stiff nonlinear terms which originate from the thin interface thickness parameter, there are a lot of difficulties to construct numerical schemes with unconditional energy stability, especially for the second order scheme. Lots of efforts have been made to solve these problems [11, 51, 59]. The simple fully implicit or explicit type discretization brings extremely severe time step size constraint on the interfacial width [3, 15, 41]. The semi-implicit method is adopted in [44]. However, the author mentioned that it suffers from a small CFL conditional number. Recently, Gu et al. in [20] had constructed an energy stable finite difference scheme for the