



An energy stable algorithm for a quasi-incompressible hydrodynamic phase-field model of viscous fluid mixtures with variable densities and viscosities

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ABSTRACT

A quasi-incompressible hydrodynamic phase field model for flows of fluid mixtures of two incompressible viscous fluids of distinct densities and viscosities is derived by using the generalized Onsager principle, which warrants the variational structure, the mass conservation and energy dissipation law. We recast the model in an equivalent form and discretize the equivalent system in space firstly to arrive at a time-dependent ordinary differential and algebraic equation (DAE) system, which preserves the mass conservation and energy dissipation law at the semi-discrete level. Then, we develop a temporal discretization scheme for the DAE system, where the mass conservation and the energy dissipation law are once again preserved at the fully discretized level. We prove that the fully discretized algorithm is unconditionally energy stable. Several numerical examples, including drop dynamics of viscous fluid drops immersed in another viscous fluid matrix and mixing dynamics of binary polymeric solutions, are presented to show the convergence property as well as the accuracy and efficiency of the new scheme.

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1. Introduction

Fluid mixtures are abundant in nature as well as in industrial settings. A mixture of immiscible fluids tends to form a multiphase fluid mixture with a well-separated phases, while a mixture of miscible fluids indeed yields a new well-mixed fluid. Hydrodynamic theories employing both the sharp interface formulation and the diffuse interface formulation have been developed to describe hydrodynamics in the complex fluid flow of immiscible multiphase fluid mixtures. For immiscible multiphase fluid flows, sharp interface models assume that there exist infinitely thin interfacial material surfaces separating different phases in the mixture [1–3]. On the other hand, diffuse interface models have been used to describe not only immiscible fluid flows but also flows of miscible fluid mixtures [4–7]. The diffuse interface model is commonly called the phase field model today. The phase field approach yields a method to solve interfacial problems, where instead of tracking the interface, a smooth phase variable is introduced [8], whose spatially varying transitional layer represents the interface. Due to its simple numerical implementation compared with the one of sharp interface methods, the phase field method has gained tremendous popularity recently in applications in life sciences [5,9–12], cell biology [12–17], biofilms [5–7], cell adhesion and motility [12,14,18–21], cell membrane [22–26], tumor growth [10], materials science [27–29], fluid dynamics [2,30,31], image processing [32–34], etc.

When phase field models are used to describe hydrodynamics of multiphase fluid flows, one has to couple the phase variable with the fluid flow to derive hydrodynamic phase field models. When the hydrodynamic phase field model is derived through a variational principle coupled with the generalized Onsager principle [35–37], the governing hydrodynamic phase field system obeys an energy dissipation law, i.e., the model is dissipative. As a result, the models are usually well-posed. The derivation procedure often serves as a guide for developing energy stable numerical algorithms, where the numerical schemes preserve or at least respect the energy dissipation property in the discrete (or semi-discrete) level.

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Here, we give a brief overview of the hydrodynamic phase field model for binary viscous fluid mixtures. For a binary fluid with components A and B , we introduce a phase variable $\phi \in [0, 1]$ with ϕ the volume fraction of component A . The volume fraction of component B is given by $1 - \phi$. $0 < \phi < 1$ denotes the interfacial region between the two pure phases: A and B . Consider a smooth domain $\Omega \in \mathbb{R}^2$, the free energy of the mixture system is given by

$$F[\phi] = \int_{\Omega} \left(\frac{\gamma_1}{2} |\nabla \phi|^2 + f(\phi) \right) d\mathbf{x}, \quad (1.1)$$

where γ_1 is a parameter measuring the strength of the conformational entropy and $f(\phi)$ is the bulk energy density. For example, for immiscible binary fluids, one choice of the bulk energy density is given by a double well repulsive potential

$$f(\phi) = \gamma_2 \phi^2 (1 - \phi)^2, \quad (1.2)$$

where γ_2 measures the strength of the repulsive potential. In order to control numerically $\phi \in (-\epsilon, 1 + \epsilon)$ for small positive number ϵ , we modify the above bulk energy density (1.2) as

$$f(\phi) = \gamma_2 (\phi^2 (1 - \phi)^2 + f_1(\phi)), \quad (1.3)$$

where

$$f_1(\phi) = \begin{cases} 0, & \phi \in [0, 1], \\ N\phi^4(1 - \phi)^4, & \text{otherwise,} \end{cases} \quad (1.4)$$

and here N is a large enough positive number. This potential has up to third order continuous derivatives.

For miscible binary polymeric blends, $f(\phi)$ is given by the Flory–Huggins free energy density

$$f(\phi) = \gamma_2 \left(\frac{\phi}{N_1} \ln \phi + \frac{(1 - \phi)}{N_2} \ln(1 - \phi) + \chi \phi(1 - \phi) \right), \quad (1.5)$$

where N_1 and N_2 are the polymerization index for the A and B phases, respectively, χ is the mixing parameter, and γ_2 measures the strength of the bulk potential.

For a fluid mixture of two incompressible viscous fluids, we have derived the governing system of equations of the binary fluid mixture in a hydrodynamic binary fluid model as follows using the generalized Onsager principle [38]

$$\rho(\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} - \phi \nabla \mu, \quad (1.6a)$$

$$\nabla \cdot \mathbf{v} = \frac{\lambda_1 \lambda_2 (\rho_2 - \rho_1)^2}{\lambda_1 \rho_1^2 + \lambda_2 \rho_2^2} \Delta p + \frac{\lambda_1 \lambda_2 \rho_2 (\rho_2 - \rho_1)}{\lambda_1 \rho_1^2 + \lambda_2 \rho_2^2} \Delta \mu, \quad (1.6b)$$

$$\partial_t \phi + \nabla \cdot (\phi \mathbf{v}) = \frac{\lambda_1 \lambda_2 \rho_2 (\rho_2 - \rho_1)}{\lambda_1 \rho_1^2 + \lambda_2 \rho_2^2} \Delta p + \frac{\lambda_1 \lambda_2 \rho_2^2}{\lambda_1 \rho_1^2 + \lambda_2 \rho_2^2} \Delta \mu, \quad (1.6c)$$

where $\rho_{1,2}$ and $\lambda_{1,2}$ are constant mass density and mobility coefficient of components A and B , respectively, $\rho = \rho_1 \phi + \rho_2 (1 - \phi)$ is the total mass density, $\mathbf{v}$ is the mass-average velocity, p is the hydrostatic pressure,

$$\boldsymbol{\tau} = 2\eta \mathbf{D} + \left(\nu - \frac{2\eta}{3} \right) \text{tr}(\mathbf{D}) \mathbf{I} \quad (1.7)$$

is the viscous stress tensor with the shear viscosity $\eta = \eta_1 \phi + \eta_2 (1 - \phi)$ and the bulk viscosity $\nu = \nu_1 \phi + \nu_2 (1 - \phi)$, $\mathbf{D} = \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^T)$ is the rate of strain tensor, $\mu = \frac{\delta F}{\delta \phi}$ is the chemical potential given by $\mu = f'(\phi) - \gamma_1 \Delta \phi$. To ensure energy dissipation, $\eta, \nu - 2\eta/3 \geq 0$. With suitable boundary conditions, the system (1.6) satisfies an energy dissipation law (see Section 2). This hydrodynamic phase field model respects the mass conservation and the momentum conservation. The second equation does not yield $\nabla \cdot \mathbf{v} = 0$ if $\rho_1 \neq \rho_2$. So, the model is quasi-incompressible [30,39,40], in which the material density and the viscosity are variables depending on the phase variable ϕ . The model is incompressible only when $\rho_1 = \rho_2$. An analogous model was derived for mass fractions [30]. We remark that most of the hydrodynamic phase field models analyzed and computed so far either corresponding to the case $\rho_1 = \rho_2$ so that the model is incompressible or given by some ad hoc models in which $\nabla \cdot \mathbf{v} = 0$ is assumed [41].

Given the dissipative property of the governing system of equations, one would like to have the numerical solver developed for the system to possess an analogous energy dissipation law at the discrete level. A numerical scheme of this property is known as the energy stable scheme. There have been quite a number of papers in the literature today discussing how to develop energy stable schemes for phase field models when the models are dissipative. Here, we briefly recall some well-known strategies. The authors in [42–46] extended the convex splitting technique originally proposed by [47] to several phase field models, where they split the energy into a difference of two convex functions, allowing them to prove energy stability for some schemes and the uniqueness of weak solutions. This strategy has since been applied to the epitaxial model and crystal growth model etc. However, even though they can prove the scheme is uniquely solvable, the scheme ends up with a fully nonlinear systems to solve, where one has to use Newton iterations or other nonlinear solvers to solve it. On the other hand, the authors in [48,49] used the stabilizer approach to derive energy stable schemes for some phase field models and later hydrodynamic phase field models [48,50–53], where they introduced an extra stabilizing term in the same order of accuracy as the scheme, then they can prove energy stability for the schemes. The resultant schemes obtained this way are good in term of its linearity, however, the coefficient for the stabilizer has to be determined empirically, which may lead to a large error. Recently, an energy quadratization approach has been applied to develop linear energy stable schemes for a class of (hydrodynamic) phase field models [54–61].

Another strategy for developing energy stable schemes for hydrodynamic phase field models is to develop spatial discretization to preserve energy stability at the semi-discrete level in space first. Then, one applies conservative numerical schemes developed for time-dependent ODEs to arrive at fully discretized schemes that preserve energy dissipation. We have developed such a second order scheme

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