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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A B S T R A C T

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.

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 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 multiphasic 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 transition 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 multiphasic 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.
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 $\phi$ 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 $\Omega \subset \mathbb{R}^2$, the free energy of the mixture system is given by

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

where $\gamma_1$ 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

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

where $\gamma_2$ measures the strength of the repulsive potential. In order to control numerically $\phi \in (-\epsilon, 1 + \epsilon)$ for small positive number $\epsilon$, we modify the above bulk energy density (1.2) as

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

where

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

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

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

where $N_1$ and $N_2$ are the polymerization index for the $A$ and $B$ phases, respectively, $\chi$ is the mixing parameter, and $\gamma_2$ 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]

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

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

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

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,

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

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 $\phi$. 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.
for a general hydrodynamic phase field model with an arbitrary bulk energy density [62]. Schemes developed following this strategy are usually nonlinear, requiring iterative solvers.

We note that in all the above numerical treatment of hydrodynamic phase field models, the models are incompressible, i.e., the divergence free condition $\nabla \cdot \mathbf{v} = 0$ is adopted. For fluid mixtures of different densities and viscosities, the physically appropriate hydrodynamic phase field model is the quasi-incompressible model as alluded to above [30, 38, 40]. In [40], a comparative investigation was made between the incompressible hydrodynamic phase field model and the quasi-incompressible hydrodynamic phase field model using a linear numerical scheme, which is not energy stable. The study showed that the two models predict different dynamics at the fluid interfaces and in the regions where fluids are highly mixed. For thermodynamical consistency and preservation of physical conservation laws, the quasi-incompressible should be used. In [63], an energy stable scheme is developed for a quasi-incompressible model for binary viscous fluid flows formulated using mass fractions based on a finite element spatial discretization. This fully discrete numerical scheme is nonlinear so that a Newton iteration had to be employed. Recently, in [64], the authors propose some mass conservative, energy stable finite difference methods to solve the quasi-incompressible model proposed in [65]. In this paper, we take a new approach to develop a novel second order both in time and space energy stable numerical scheme for the quasi-incompressible model derived in [38]. We also present a set of numerical examples to show its convergence and efficiency. In order to populate the quasi-incompressible hydrodynamic phase field model for fluid mixtures, we believe that more high order and stable numerical algorithms are necessary.

The rest of the paper is organized as follows. In Section 2, the quasi-incompressible hydrodynamic phase field model is reformulated and its energy dissipation property is discussed. In Section 3, the spatially discretized structure-preserving scheme is presented. The time discretization is given in Section 4. The numerical convergence test and several numerical examples are presented in Section 5. A concluding remark is given in the Section 6.

2. Model reformulation and energy dissipation

Using the identity
\[
\nabla \cdot (\rho \mathbf{v} \mathbf{v}) = \rho \mathbf{v} \cdot \nabla \mathbf{v} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}),
\]
we rewrite the hydrodynamic phase field model in system (1.6) as follows:
\[
\begin{align*}
\rho a_t \mathbf{v} &+ \frac{1}{2} (\mathbf{v} \cdot \nabla \mathbf{v} + \nabla \cdot (\rho \mathbf{v} \mathbf{v})) - \frac{1}{2} \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot \tau - \phi \nabla \mu, \\
\nabla \cdot \mathbf{v} &= a_1 \Delta \rho + a_2 \Delta \mu, \\
\phi_t + \nabla \cdot (\rho \mathbf{v}) &= a_2 \Delta p + a_3 \Delta \mu,
\end{align*}
\]
where $a_1 = \frac{1+3 \| \mathbf{v} \|_2^2}{\gamma \| \mathbf{v} \|^2}$, $a_2 = \frac{1+3 \| \mathbf{v} \|_2^2}{\| \mathbf{v} \|^2}$, and $a_3 = \frac{1+3 \| \mathbf{v} \|_2^2}{\| \mathbf{v} \|^2}$. Note that the constants $a_i (i = 1, 2, 3)$ satisfy
\[
\begin{align*}
rho_2 a_1 + (\rho_1 - \rho_2) a_2 &= 0, \\
rho_2 a_2 + (\rho_1 - \rho_2) a_3 &= 0, \\
a_1 a_3 &= a_2^2.
\end{align*}
\]
When $\rho_1 \neq \rho_2$, the transport equation for $\phi$ can be rewritten as
\[
\phi_t + \nabla \cdot \left[ \phi \left( \frac{\rho_2}{\rho_2 - \rho_1} \right) + \nabla \left( \left( \frac{\rho_2}{\rho_2 - \rho_1} \right) \mathbf{v} \right) \right] = 0.
\]
This is equivalent to the mass conservation equation. For simplicity, we adopt the periodic boundary conditions in this study. The effect of various boundary conditions on the numerical scheme warrants a completely new consideration and treatment, which we will comment in a remark below.

We define the inner product $(\cdot, \cdot)$ and norm $\| \cdot \|$ for matrix functions as follows:
\[
\langle F, G \rangle = \sum_{m,n} \int_{\Omega} F_{m,n} G_{m,n} d\mathbf{x}, \quad \| F \| = (\langle F, F \rangle)^{1/2},
\]
where $\Omega$ is the domain of the fluid flow, $\mathbf{F}$ and $\mathbf{G}$ are matrix functions or 2nd order tensor functions defined in $\Omega$. For scalar and vector functions, the inner product can be defined analogously. With the periodic boundary conditions, we have the following integration-by-parts formulae:
\[
\begin{align*}
(f, a_x g) + (a_y f, g) &= 0, \quad \alpha = x \mathrm{or} y, \\
(f, \nabla \cdot \mathbf{v}) + (\nabla f, \mathbf{v}) &= 0,
\end{align*}
\]
and
\[
\begin{align*}
(\mathbf{v}, \nabla \cdot \mathbf{F}) + (\nabla \mathbf{v}, \mathbf{F}) &= 0.
\end{align*}
\]
By a simple calculation, it is readily shown that
\[
\langle \mathbf{u}, \mathbf{F} \cdot \mathbf{v} \rangle = (\mathbf{u} \cdot \mathbf{v}) (\mathbf{F}),
\]
where $\mathbf{u}$, $\mathbf{v}$ are vector-valued functions and $\mathbf{F}$ is a matrix-valued function.
Theorem 2.1. With the periodic boundary conditions, the solution of system (1.6) satisfies the following energy dissipation law
\[
\frac{dE}{dt} + \|\sqrt{a_1}\nabla p + \text{sign}(a_2)\sqrt{a_1}\nabla \mu\|^2 + 2\langle \eta, |D|^2 \rangle + \left( v - \frac{2\eta}{3}, \nabla \cdot v \right)^2 = 0,
\] (2.11)
where \( E \) is the total energy of (1.6) defined as
\[
E = \frac{1}{2} \langle \rho, |v|^2 \rangle + \frac{\gamma}{2} \|\nabla \phi\|^2 + \langle f(\phi), 1 \rangle.
\] (2.12)

Proof. Multiplying (2.1b) and (2.1c) by \( \rho_2 \) and \( \rho_1 - \rho_2 \), respectively, then adding the results, we obtain the mass conservation
\[
\partial_t \rho + \nabla \cdot (\rho v) = 0.
\] (2.13)
According to (2.9) and (2.10), we have
\[
\langle \mathbf{v}, \rho \mathbf{v} \cdot \nabla \mathbf{v} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) \rangle = \langle \rho \mathbf{v} \mathbf{v}, \nabla \mathbf{v} \rangle + \langle \mathbf{v}, \nabla \cdot (\rho \mathbf{v} \mathbf{v}) \rangle = 0,
\] (2.14)
and
\[
\langle \mathbf{v}, \nabla \cdot \mathbf{\tau} \rangle = -\langle \nabla \mathbf{v}, \mathbf{\tau} \rangle = -2\langle \eta, |D|^2 \rangle - \left( v - \frac{2\eta}{3}, \nabla \cdot v \right)^2.
\] (2.15)
Computing the inner product of (2.1a) with \( \mathbf{v} \), then using (2.1b), (2.8), (2.13) and (2.14), we have
\[
\langle \mathbf{v}, \rho \partial_t \mathbf{v} \rangle + \frac{1}{2} \langle \partial_t \rho, |v|^2 \rangle = \langle \mathbf{v}, -\nabla p + \nabla \cdot \mathbf{\tau} - \phi \nabla \mu \rangle
\]
\[
= \langle \nabla \cdot \mathbf{v}, p \rangle + \langle \mathbf{v}, \nabla \cdot \mathbf{\tau} \rangle - \langle \phi \nabla \mu, \nabla \mu \rangle
\]
\[
= (a_1 \Delta p + a_2 \Delta \mu, p) + \langle \nabla \cdot (\phi \nabla \mu), \mu \rangle
\]
\[
= -a_1 \|\nabla p\|^2 - a_2 (\nabla \mu \cdot \nabla p) + \langle \mathbf{v}, \nabla \cdot \mathbf{\tau} \rangle + \langle \nabla \cdot (\phi \nabla \mu), \mu \rangle.
\] (2.16)
Computing the inner product of (2.1c) with \( \mu \), we obtain
\[
\langle \mu, \partial_t \phi \rangle + \langle \mu, \nabla \cdot (\phi \mathbf{v}) \rangle = -a_2 (\nabla \mu \cdot \nabla p) - a_3 \|\nabla \mu\|^2,
\] (2.17)
where (2.8) is used. Adding (2.16) and (2.17), we have
\[
\langle \mathbf{v}, \rho \partial_t \mathbf{v} \rangle + \frac{1}{2} \langle \partial_t \rho, |v|^2 \rangle + \langle \mu, \partial_t \phi \rangle = -\|\sqrt{a_1}\nabla p + \text{sign}(a_2)\sqrt{a_1}\nabla \mu\|^2 + \langle \mathbf{v}, \nabla \cdot \mathbf{\tau} \rangle,
\] (2.18)
where (2.4) is used. Combining (2.15) and (2.18), we obtain
\[
\frac{dE}{dt} = \frac{1}{2} \langle \rho, |v|^2 \rangle + \langle \rho, \mathbf{v} \cdot \mathbf{v} \rangle + \gamma_1 \langle \nabla \phi, \nabla \phi \rangle + \langle f(\phi), \phi \rangle
\]
\[
= \frac{1}{2} \langle \rho, |v|^2 \rangle + \langle \mathbf{v}, \rho \mathbf{v} \rangle + \langle \mu, \phi \rangle
\]
\[
= -\|\sqrt{a_1}\nabla p + \text{sign}(a_2)\sqrt{a_1}\nabla \mu\|^2 - 2\langle \eta, |D|^2 \rangle - \left( v - \frac{2\eta}{3}, \nabla \cdot v \right)^2,
\]
which leads to (2.11). \( \square \)

Remark 2.1. The theorem also holds for the following physical boundary conditions:
\[
\mathbf{v}|_{\partial \Omega} = 0, \quad \nabla \phi \cdot \mathbf{n}|_{\partial \Omega} = 0, \quad \nabla \left( \frac{\rho_2 - \rho_1}{\rho_2} p + \mu \right) \cdot \mathbf{n}|_{\partial \Omega} = 0.
\] (2.19)
Throughout this paper, the results are proved with the periodic boundary conditions; but they are valid equally well with the above physical boundary conditions subject to a special spatial treatment.

In the proof of Theorem 2.1, the integration-by-parts formulae are essential for deducing the energy dissipation law. Thus, to construct energy dissipation preserving algorithm, spatial discretization should preserve the corresponding discrete integral-by-parts formulae, i.e., the summation-by-parts formulae presented in next section.

3. Structure preserving spatial discretization

In this section, we devise a semi-discrete, spatial, finite difference method for the two dimensional hydrodynamic system (2.1) with the periodic boundary condition in a rectangular domain \( \Omega = [0, L_x] \times [0, L_y] \). The scheme preserves the discrete inner product and thereby the mass conservation and the discrete energy dissipation law. Note that we present the numerical scheme in 2-dimensional space; it can be readily extended to 3D.

Let \( N_x, N_y \) be two positive integers. The domain \( \Omega = [0, L_x] \times [0, L_y] \) is uniformly partitioned with mesh size \( h_x = L_x/N_x, \ h_y = L_y/N_y \) and
\[
\Omega_h = \{ (x_j, y_k) | x_j = jh_x, \ y_k = kh_y, \ 0 \leq j \leq N_x, \ 0 \leq k \leq N_y \}. 
\]
To approximate the periodic boundary condition, let \( x_{-1} = -h_x, y_{-1} = -h_y \). A grid function \( f \) is called periodic if

\[
(x\text{-periodic})f_{-1,k} = f_{N_x,-1,k}, \quad f_{0,k} = f_{N_x,k}; \quad (y\text{-periodic})f_{j,-1} = f_{j,-N_y}, \quad f_{j,0} = f_{j,N_y}.
\]

For convenience, we define the following discrete difference operators

\[
\delta_x^+ f_{j,k} = \frac{f_{j+1,k} - f_{j,k}}{h_x}, \quad \delta_x^- f_{j,k} = \frac{f_{j,k} - f_{j-1,k}}{h_x}, \quad \delta_y^+ f_{j,k} = \frac{f_{j,k+1} - f_{j,k}}{h_y}, \quad \delta_y^- f_{j,k} = \frac{f_{j,k} - f_{j,k-1}}{h_y},
\]

\[
\nabla_h^+ = \left( \frac{\delta_x^+}{\delta_y^+} \right), \quad \nabla_h^- = \left( \frac{\delta_x^-}{\delta_y^-} \right),
\]

\[
\nabla_h = \frac{\nabla_h^+ + \nabla_h^-}{2}, \quad \Delta_h = \delta_x^+ \delta_y ^+ + \delta_x^- \delta_y ^-.
\]

The discrete inner product and norm (e.g. for matrix functions) are defined respectively as follows

\[
(F, G)_h = \sum_{m,n} \sum_{j=0}^{N_x-1} \sum_{k=0}^{N_y-1} (F_{m,n,j,k} G_{m,n,j,k} h_x h_y), \quad ||F||_h = (F, F)_h^{1/2}.
\]

The following summation-by-parts formulae are analogous to the integration-by-parts formulae (2.7)–(2.9)

\[
\begin{align*}
(f, \delta_x g)_h + (\delta_x^+ f, g)_h &= 0, \\
(f, \delta_y g)_h + (\delta_y^+ f, g)_h &= 0, \\
(f, \nabla_h^+ \cdot v)_h + (\nabla_h^+ f, v)_h &= 0, \\
(f, \nabla_h^- \cdot v)_h + (\nabla_h^- f, v)_h &= 0, \\
(v, \nabla_h^+ F)_h + (\nabla_h^+ v, F)_h &= 0, \\
(v, \nabla_h^- F)_h + (\nabla_h^- v, F)_h &= 0, \\
(v, \nabla_h F)_h + (\nabla_h v, F)_h &= 0,
\end{align*}
\]

where \( \alpha = x \) or \( y \). In addition, we have

\[
(u, F \cdot v)_h = (uv, F)_h.
\]

Applying the central difference scheme in space to the hydrodynamic system (2.1), we obtain

\[
\begin{align*}
\rho_j k \frac{d}{dt} v_{j,k} + \frac{1}{2} \left( \rho_j k v_{j,k} \cdot \nabla_h v_{j,k} + \nabla_h \cdot (\rho_j k v_{j,k} v_{j,k}) - \frac{1}{2} \nabla_h \cdot (\rho_j k v_{j,k} v_{j,k}) \right) &= - \nabla_h \cdot (\rho_j k v_{j,k} v_{j,k}) - \nabla_h \cdot (\rho_j k v_{j,k} v_{j,k}) - \mu_j k \nabla_h \mu_j k, \\
\frac{d}{dt} \phi_{j,k} + \nabla_h \cdot (\phi_{j,k} v_{j,k}) &= \mu_j k \Delta_h \mu_j k, \quad \mu_j k = \frac{1}{2} \nabla_h \mu_j k + \frac{1}{2} \frac{(v_1 - v_2)}{3} \text{tr} (D_j k),
\end{align*}
\]

where

\[
\rho_j k = (\rho_1 - \rho_2) \phi_{j,k} + \rho_2, \quad \eta_j k = (\eta_1 - \eta_2) \phi_{j,k} + \eta_2, \quad \nu_j k = (v_1 - v_2) \phi_{j,k} + v_2,
\]

\[
D_j k = \frac{1}{2} (\nabla h \nu j k + \nabla h \nu j k), \quad \tau_{j,k} = 2 \eta_j k D_j k + (v_1 - v_2) \frac{2 \eta_j k}{3} \text{tr} (D_j k),
\]

and \( j = 0, 1, \ldots, N_x - 1, k = 0, 1, \ldots, N_y - 1 \).

**Theorem 3.1.** The scheme given by (3.10) preserves the following semi-discrete energy dissipation law

\[
\frac{dE_h}{dt} + ||\sqrt{\mu} \nabla h p + \text{sign}(a_2) \sqrt{\mu} \nabla h \mu_h^2 ||_h^2 + 2(\eta, |D|^2)_h + (v - \frac{2\eta}{3}, |\nabla_h v|^2)_h = 0, \quad (3.11)
\]

where \( E_h \) is the semi-discrete energy functional defined as

\[
E_h = \frac{1}{2} (\rho, |v|^2)_h + \frac{\nu_1}{2} ||\nabla_h \phi||_h^2 + (f(\phi), 1)_h.
\]

**Proof.** Multiplying the last two equations of (3.10) by \( \rho_2 \) and \( \rho_1 - \rho_2 \), respectively, then adding the results, we obtain the semi-discrete mass conservation law

\[
\frac{d}{dt} \rho_j k + \nabla_h \cdot (\rho_j k v_{j,k}) = 0, \quad (3.12)
\]
From (3.8) and (3.9), we have
\[
(\mathbf{v}, \rho \mathbf{v} \cdot \nabla_h \mathbf{v} + \nabla_h \cdot (\rho \mathbf{v} \mathbf{v}))_h = (\rho \mathbf{v} \mathbf{v}, \nabla_h \mathbf{v})_h + (\mathbf{v}, \nabla_h \cdot (\rho \mathbf{v} \mathbf{v}))_h = 0,
\]
(3.13)
and
\[
(\mathbf{v}, \nabla_h \cdot \tau)_h = - (\nabla_h \mathbf{v}, \tau)_h = - 2(\eta, |D|^2)_h - \left( v - \frac{2\eta}{3}, |\nabla_h \cdot \mathbf{v}|^2 \right)_h.
\]
(3.14)
Computing the discrete inner product of the first equation of (3.10) with $$\mathbf{v}$$, then using (3.3), (3.5), (3.10), (3.12) and (3.13), we obtain
\[
(\mathbf{v}, \rho \frac{d}{dt} \mathbf{v})_h + \frac{1}{2} \left( \frac{d}{dt} \rho \cdot |\mathbf{v}|^2 \right)_h = - a_1 \| \nabla_h^+ \mathbf{p} \|_h^2 - a_2 (\nabla_h^+ \mu, \nabla_h^+ \mathbf{p})_h + (\mathbf{v}, \nabla_h \cdot \tau)_h + \left( \nabla_h \cdot (\rho \mathbf{v} \mathbf{v}), \mu \right)_h.
\]
(3.15)
Computing the discrete inner product of the last equation of (3.10) with $$\mu$$, we obtain
\[
\left( \frac{d}{dt} \rho \phi \right)_h + (\mu, \nabla_h \cdot (\rho \mathbf{v} \phi))_h = - a_2 (\nabla_h^+ \mu, \nabla_h^+ \mathbf{p})_h - a_3 \| \nabla_h^+ \mu \|^2_h,
\]
(3.16)
where (3.3) is used. Adding (3.15) and (3.16) leads to
\[
(\mathbf{v}, \rho \frac{d}{dt} \mathbf{v})_h + \frac{1}{2} \left( \frac{d}{dt} \rho \cdot |\mathbf{v}|^2 \right)_h + \left( \frac{d}{dt} \rho \phi \right)_h = - \| \sqrt{\alpha} \nabla_h^+ \mathbf{p} + \text{sign}(a_2) \sqrt{\alpha} \nabla_h^+ \mu \|^2_h - 2(\eta, |D|^2)_h - \left( v - \frac{2\eta}{3}, |\nabla_h \cdot \mathbf{v}|^2 \right)_h,
\]
(3.17)
According to (3.3), (3.14) and (3.17), we have
\[
\frac{dE_h}{dt} \leq \frac{1}{2} \left( \frac{d}{dt} \rho \cdot |\mathbf{v}|^2 \right)_h + \left( \frac{d}{dt} \rho \phi \right)_h + \gamma_1 \left( \nabla_h^+ \phi \cdot \nabla_h^+ \frac{d}{dt} \phi \right)_h + \left( f(\phi), \frac{d}{dt} \phi \right)_h
\]
\[
= - \| \sqrt{\alpha} \nabla_h^+ \mathbf{p} + \text{sign}(a_2) \sqrt{\alpha} \nabla_h^+ \mu \|^2_h - 2(\eta, |D|^2)_h - \left( v - \frac{2\eta}{3}, |\nabla_h \cdot \mathbf{v}|^2 \right)_h,
\]
which directly leads to (3.11). □

4. Structure preserving temporal discretization

In this section, we propose a special temporal discretization for the semi-discrete system (3.10), where the mass conservation and the energy dissipation law are preserved at the fully discretized level.

For a positive integer $$N$$, we define time-step $$\Delta t = T/N$$, $$t_n = n \Delta t$$, $$0 \leq n \leq N$$. We denote
\[
\delta^n T = \frac{t^{n+1} - t^n}{\Delta t}, \quad \delta^n \| = \frac{f^{n+1} - f^n}{2}.
\]

Our numerical scheme is summarized as follows.

Algorithm:
Given the initial conditions $$\mathbf{v}^0$$ and $$\phi^0$$, we compute $$(\mathbf{v}^{n+1}, \phi^{n+1}, \mathbf{v}^{n+1})$$ for $$n \geq 0$$.

Step 1:
\[
\begin{cases}
\rho^n_{j+k}^{n+1/2} - \rho^n_{j,k} = \frac{1}{2} \left( \rho^n_{j,k}^{n+1/2}, \nabla_h \mathbf{v}^{n+1}_{j,k} + \nabla_h \cdot (\rho^n_{j,k}^{n+1/2} \mathbf{v}^{n+1}_{j,k}) \right) - \frac{1}{2} \nabla_h \cdot (\rho^n_{j,k}^{n+1/2} \mathbf{v}^{n+1}_{j,k}), \\
\sqrt{\alpha} \mathbf{v}^{n+1}_{j,k} = \sqrt{\alpha} \mathbf{v}^{n}_{j,k} + \delta^n \mathbf{v}^{n+1}_{j,k}, \quad \mathbf{v}^{n+1}_{j,k} = \frac{1}{2} \left( \mathbf{v}^{n+1}_{j,k} + (\mathbf{v}^{n+1}_{j,k} + \nabla_h \mathbf{v}^{n+1}_{j,k}) \right), \\
\mathbf{D}^{n+1}_{j,k} = \frac{1}{2} \left( \nabla_h \mathbf{v}^{n+1}_{j,k} + (\nabla_h \mathbf{v}^{n+1}_{j,k})^T \right), \\
\gamma_1 \Delta h \mathbf{p}^{n+1}_{j,k} + \mathbf{a}_2 \Delta h \mu^{n+1}_{j,k} = \mathbf{a}_1 \Delta h \mathbf{p}^{n+1/2}_{j,k} + \mathbf{a}_2 \Delta h \mu^{n+1/2}_{j,k}, \\
\Delta h \mathbf{v}^{n+1}_{j,k} = \mathbf{a}_1 \Delta h \mathbf{p}^{n+1}_{j,k} + \mathbf{a}_2 \Delta h \mu^{n+1}_{j,k}, \\
\mathbf{g}^{n+1}_{j,k} = (\mathbf{g}^{n+1}_{j,k}), \quad \mathbf{s}^{n+1}_{j,k} = (\mathbf{s}^{n+1}_{j,k}), \\
\delta^n \phi^{n+1}_{j,k} = \delta^n \phi^{n+1}_{j,k} - \gamma_1 \Delta h \phi^{n+1/2}_{j,k}, \quad \delta^n \phi^{n+1}_{j,k} = \frac{f(a) - f(b)}{a - b}, \quad \text{if } a \neq b,
\end{cases}
\]
(4.1)

where
\[
\begin{align*}
\mathbf{v}^{n+1}_{j,k} &= \frac{1}{2} \left( \mathbf{v}^{n+1}_{j,k} + (\mathbf{v}^{n+1}_{j,k} + \nabla_h \mathbf{v}^{n+1}_{j,k}) \right), \\
\mathbf{D}^{n+1}_{j,k} &= \frac{1}{2} \left( \nabla_h \mathbf{v}^{n+1}_{j,k} + (\nabla_h \mathbf{v}^{n+1}_{j,k})^T \right), \\
\mathbf{g}^{n+1}_{j,k} &= (\mathbf{g}^{n+1}_{j,k}), \quad \mathbf{s}^{n+1}_{j,k} = (\mathbf{s}^{n+1}_{j,k}), \\
\delta^n \phi^{n+1}_{j,k} &= \delta^n \phi^{n+1}_{j,k} - \gamma_1 \Delta h \phi^{n+1/2}_{j,k}, \quad \delta^n \phi^{n+1}_{j,k} = \frac{f(a) - f(b)}{a - b}, \quad \text{if } a \neq b,
\end{align*}
\]
Step 2:

\[ v_{ij,k}^{n+1} = \begin{cases} 
\tilde{v}_{ij,k}^{n+1}, & \text{if } \tilde{v}_{ij,k}^{n+1} + v_{ij,k}^n \neq 0, \\
\sqrt{\frac{\rho_{ij,k}^n}{\rho_{ij,k}^{n+1}} v_{ij,k}^{n+1}}, & \text{if } \tilde{v}_{ij,k}^{n+1} + v_{ij,k}^n = 0,
\end{cases} \quad i = 1, 2. \tag{4.2} \]

**Theorem 4.1.** The fully discretized scheme (4.1)–(4.2) preserves the discrete energy dissipation law

\[ \delta_t^E E_h^n + \| \sqrt{\alpha} v_h^n \rho^{n+1/2} + \text{sign}(a_2) \sqrt{\alpha} v_h^n \mu_{n,n+1}^2/2 + 2\eta v^{n+1/2} + |D|^{n+1/2} \|^2_h + \left( v^{n+1/2} - \frac{2\eta^{n+1/2}}{3} , \nabla \cdot v_h^{n+1} \right)_h = 0, \tag{4.3} \]

where

\[ E_h^n = \frac{1}{2} (\rho^n, |v^n|^2)_h + \frac{\gamma_f}{2} \| v_h^n \phi^n \|^2_h + (f(\phi^n), 1)_h. \]

**Proof.** Analogous to the proof of Theorem 3.1, we have

\[ \delta_t^E \rho_{ij,k}^n + \nabla_h \cdot (\rho_{ij,k}^{n+1/2} v_{ij,k}^{n+1}) = 0, \tag{4.4} \]

\[ (v_h^{n+1}, \rho^{n+1/2} v_{ij,k}^{n+1} , \nabla_h v_h^{n+1} + \nabla_h \cdot (\rho^{n+1/2} v_{ij,k}^{n+1} v_{ij,k}^{n+1}))_h = 0, \tag{4.5} \]

and

\[ (v_h^{n+1}, \nabla_h \cdot \tau_{n,n+1})_h = -2(\eta^{n+1/2}, |D|^{n+1/2} |^2_h - \left( v^{n+1/2} - \frac{2\eta^{n+1/2}}{3}, \nabla_h \cdot v_h^{n+1} \right)_h. \tag{4.6} \]

Let

\[ q_{ij,k}^{n+1} = \begin{cases} 
\frac{(\tilde{v}_{ij,k}^{n+1})^2 + (v_{ij,k}^n)^2}{2}, & \text{if } \tilde{v}_{ij,k}^{n+1} + v_{ij,k}^n \neq 0, \ i = 1, 2. \\
0, & \text{if } \tilde{v}_{ij,k}^{n+1} + v_{ij,k}^n = 0. \tag{4.7} \end{cases} \]

Computing the discrete inner product of the first equation of (4.1) with \( \tilde{v}^{n+1} \), then using (3.3), (3.5), (4.1), (4.4) and (4.5), we have

\[ \left( v_h^{n+1}, \rho^{n+1/2} (v_h^{n+1} - v^n) \right)_h + \frac{1}{2} \rho^2 \delta_t^E q_{ij,k}^{n+1} + q_{ij,k}^{n+1} + q_{ij,k}^{n+1} = -a_1 \| \nabla_h p^{n+1/2} \|^2_h - a_2 (\nabla_h \mu^{n,n+1}, \nabla_h p^{n+1/2})_h + (\nabla^{n+1} h, \nabla \cdot \tau^{n+1})_h + (\nabla h, (\phi^{n+1/2} v_h^{n+1}), \mu^{n,n+1})_h. \tag{4.8} \]

Computing the discrete inner product of the last equation of (4.1) with \( \mu^{n,n+1} \), we obtain

\[ (\mu^{n,n+1}, \delta_t^E \phi^n_h + \mu^{n,n+1}, \nabla_h \cdot (\phi^{n+1/2} v_h^{n+1}))_h = -a_2 (\nabla_h \mu^{n,n+1}, \nabla_h p^{n+1/2})_h - a_3 \| \nabla_h \mu^{n,n+1} \|^2_h. \tag{4.9} \]

Adding (4.8) and (4.9), we deduce

\[ \left( v_h^{n+1}, \rho^{n+1/2} (v_h^{n+1} - v^n) \right)_h + \frac{1}{2} \rho^2 \delta_t^E q_{ij,k}^{n+1} + q_{ij,k}^{n+1} + q_{ij,k}^{n+1} + (\mu^{n,n+1}, \delta_t^E \phi^n)_h \\
= -a_1 \| \nabla_h p^{n+1/2} \|^2_h + \text{sign}(a_2) \sqrt{\alpha} v_h^n \mu_{n,n+1}^2/2 + (\nabla^{n+1} h, \nabla \cdot \tau^{n+1})_h. \tag{4.10} \]

According to (4.2) and the identity \( ab - cd = \frac{1}{2}(a-c)(b+d) + \frac{1}{2}(a+c)(b-d) \), we have

\[ \rho_{ij,k}^{n+1} (v_{ij,k}^n)^2 = \rho_{ij,k}^{n+1} (\tilde{v}_{ij,k}^{n+1})^2 - \rho_{ij,k}^{n+1} (v_{ij,k}^n)^2, \quad \text{if } \tilde{v}_{ij,k}^{n+1} + v_{ij,k}^n \neq 0, \]

\[ = \rho_{ij,k}^{n+1} (\tilde{v}_{ij,k}^{n+1} + v_{ij,k}^n) (\tilde{v}_{ij,k}^{n+1} - v_{ij,k}^n), \quad \text{if } \tilde{v}_{ij,k}^{n+1} + v_{ij,k}^n = 0, \]

which leads to

\[ \frac{1}{2} \delta_t^E (\rho_{ij,k}^{n+1} v_{ij,k}^n)^2 = \frac{1}{2} \delta_t^E \rho_{ij,k}^{n+1} (\tilde{v}_{ij,k}^{n+1} + v_{ij,k}^n) + \rho_{ij,k}^{n+1} v_{ij,k}^{n+1} \frac{\tilde{v}_{ij,k}^{n+1} - v_{ij,k}^n}{\Delta t}. \tag{4.11} \]

Using (3.3), (4.6), (4.10), (4.11) and the following identity

\[ \delta_t^E (u^n \cdot v^n) = \delta_t^E u^n \cdot v^{n+1/2} + u^{n+1/2} \cdot \delta_t^E v^n, \]
Fig. 5.1. The effect of density variation on coalescing dynamics. We observe the dynamics slows down when either the drop or the solvent is heavier. The pseudocolor of $\phi$ is plotted. Fluid 1 is the drop and fluid 2 is the ambient fluid matrix.

Table 5.1
Mesh refinement test of the proposed schemes (4.1)–(4.2) for $v_1$ (or $v_2$).

<table>
<thead>
<tr>
<th>$r$</th>
<th>$N$</th>
<th>Error $L^\infty$</th>
<th>Error $L^2$</th>
<th>Order $L^\infty$</th>
<th>Order $L^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/10</td>
<td>11</td>
<td>6.271e−02</td>
<td>1.691e−01</td>
<td>1.2749</td>
<td>2.1227</td>
</tr>
<tr>
<td>1/30</td>
<td>33</td>
<td>5.151e−03</td>
<td>1.642e−02</td>
<td>2.2749</td>
<td>2.2749</td>
</tr>
<tr>
<td>1/90</td>
<td>99</td>
<td>5.725e−04</td>
<td>1.817e−03</td>
<td>1.9998</td>
<td>2.0041</td>
</tr>
<tr>
<td>1/270</td>
<td>297</td>
<td>6.352e−05</td>
<td>2.015e−04</td>
<td>2.0013</td>
<td>2.0015</td>
</tr>
</tbody>
</table>

Table 5.2
Mesh refinement test of the proposed schemes (4.1)–(4.2) for $\phi$.

<table>
<thead>
<tr>
<th>$r$</th>
<th>$N$</th>
<th>Error $L^\infty$</th>
<th>Error $L^2$</th>
<th>Order $L^\infty$</th>
<th>Order $L^2$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>2.502e−01</td>
<td>1.2749</td>
<td>2.1227</td>
</tr>
<tr>
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<td>2.939e−02</td>
<td>1.5861</td>
<td>1.9494</td>
</tr>
<tr>
<td>1/90</td>
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<td>2.447e−03</td>
<td>3.293e−03</td>
<td>1.9382</td>
<td>1.9923</td>
</tr>
<tr>
<td>1/270</td>
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<td>2.805e−04</td>
<td>3.739e−04</td>
<td>1.9716</td>
<td>1.9802</td>
</tr>
</tbody>
</table>

we obtain

$$\delta^t_i E_h^n = \frac{1}{2} (\delta^t_i (\rho^n |\nabla \phi^n|^2), 1)_h + \gamma_1 (\nabla \phi^n \delta^t_i \phi^n)_h + (\delta^t_i f(\phi^n), 1)_h$$

$$= \frac{1}{2} (\delta^t_i \rho^n, q_1^{n, n+1} + q_2^{n, n+1})_h + \left(\nabla \phi^{n+1} - \nabla \phi^n \Delta t\right)^2 + (\mu^{n, n+1}, \delta^t_i \phi^n)_h$$

$$= \| \sqrt{\alpha_1} \nabla \phi^{n+1} + \text{sign}(\alpha_2) \sqrt{\alpha_2} \nabla \mu^{n, n+1} \|_h^2 - 2(\eta^{n+1/2}, |Dv^{n, n+1}|^2)_h$$

This completes the proof. □
Fig. 5.2. (a) Energy plot at different time for the solutions in Fig. 5.1; (b) the total volume change $\int_\Omega \phi(t) - \phi(0)dx$; (c) the divergence of $v$ (i.e. $\nabla \cdot v$) for each case in Fig. 5.1 at $t = 10$; (d) the velocity field $v$ for each case in Fig. 5.1 at $t = 10$, where the length of the arrow represents the magnitude of the velocity with the maximum value at 0.004743, 0.005992, 0.004846, respectively. When the fluid is heavier outside, the four vortices in the velocity field seem to be weaker than the other two cases.

**Remark 4.1.** According to (4.4), it is readily shown that the total mass in the fluid domain is conserved as well, i.e.,

$$\sum_{j=0}^{N_x-1} \sum_{k=0}^{N_y-1} \rho_{j,k}^1 h_x h_y = \sum_{j=0}^{N_x-1} \sum_{k=0}^{N_y-1} \rho_{j,k}^2 h_x h_y.$$

(4.12)

5. Numerical results

To test the performance of the proposed method, we solve nonlinear system (4.1) by using a simple fixed-point iteration method proposed in [62]. We first eliminate the pressure $p$ and then apply the FFT algorithm in the numerical calculation. In the $k$th fixed-point iteration step, the linear terms involving the unknowns are labeled at the $k$th level while the nonlinear terms are labeled at the $k - 1$th level.
\( \rho_1 = 1, \rho_2 = 10, \lambda_1 = \lambda_2 = 10^{-7}, t = 0, 10, 20, 50. \)

\( \rho_1 = 1, \rho_2 = 10, \lambda_1 = 5 \times 10^{-8}, \lambda_2 = 2 \times 10^{-7}, t = 0, 10, 20, 50. \)

\( \rho_1 = 1, \rho_2 = 10, \lambda_1 = 2 \times 10^{-7}, \lambda_2 = 5 \times 10^{-8}, t = 0, 10, 20, 50. \)

**Fig. 5.3.** The effect of motility on drop coalescing dynamics. The pseudocolor of \( \phi \) is plotted. We observe the coalescing speed is an increasing function of \( \frac{\lambda_1}{\lambda_2} \).

**Fig. 5.4.** Energy dissipation and mass conservation. (a) Energy plot at different time for the solutions in Fig. 5.3; (b) total volume change \( \int_\Omega \phi(t) - \phi(0) dx \).

### 5.1 Convergence rate test

In order to test the convergence rate, we consider problem (1.6) with the double-well free energy (1.2) in a rectangular domain \( \Omega = [0, 2\pi] \times [0, 2\pi] \). We make the following functions exact solutions of the system modified by some appropriate forcing functions

\[
\begin{align*}
 v_1(x, y, t) &= \sin(x) \cos(y) \sin(t), \\
v_2(x, y, t) &= \cos(x) \sin(y) \sin(t), \\
\phi(x, y, t) &= \cos(x) \cos(y) \cos(t), \\
p(x, y, t) &= \sin(x) \sin(y) \sin(t).
\end{align*}
\] (5.1)
The parameter values are chosen as $\rho_1 = 1$, $\rho_2 = 3$, $\eta = 1$, $\nu = 2/3$, $\gamma_1 = 0.01$, $\gamma_2 = 1$, $\lambda_1 = \lambda_2 = 2.0 \times 10^{-7}$. We choose the number of spatial grids as $N_x = N_y = N$ and compute the solution of the discrete nonlinear algebraic system using the fixed-point iteration. In Tables 5.1–5.2, we compare the numerical solution with the exact solution at $t = 1$, and compute the $L_2$ and $L_\infty$ errors of velocity $v_1$ and phase variable $\phi$ by varying the grid size in space and time, respectively. From Tables 5.1–5.2, we observe that the proposed scheme is second-order accurate in both time and space for all variables.

Next, we consider dynamics of binary fluid mixtures of immiscible and miscible viscous fluids, respectively.

5.2. Dynamics of immiscible binary fluid mixtures

We consider a mixture of two immiscible incompressible viscous fluids. We adopt the double well potential in this study. Through numerical experiments, we observe that dynamics of quasi-incompressible fluid mixtures of different densities (i.e. $\rho_1 \neq \rho_2$) exhibits quite different behavior when compared with the incompressible fluid mixture with the same density (i.e. $\rho_1 = \rho_2$).

First of all, we study coalescing dynamics of two fluid drops. Given $L_x = L_y = 1$, define

$$R_1 = \sqrt{(x - 0.25)^2 + (y - 0.5)^2}, \quad R_2 = \sqrt{(x - 0.75)^2 + (y - 0.5)^2}$$

and the initial condition of the drops

$$\phi(x, t) = \frac{1}{4} \left( \tanh \frac{R - R_1}{\varepsilon} + 1 \right) \left( \tanh \frac{R - R_2}{\varepsilon} + 1 \right), \quad v = 0.$$

First of all, we study the effect of the density ratio on the dynamics. We fix all the other parameter values except that we vary the two densities as follows: (i) $\rho_1 = \rho_2 = 1$; (ii) $\rho_1 = 1$, $\rho_2 = 10$; (iii) $\rho_1 = 10$, $\rho_2 = 1$, respectively. The numerical results are summarized

![Fig. 5.5. The effect of the density ratio on coarsening dynamics. The pseudocolor of $\phi$ is plotted at different times for varying density ratios: (a) $\rho_1 = 1$, $\rho_2 = 10$; (b) $\rho_1 = 10$, $\rho_2 = 1$; (c) $\rho_1 = \rho_2 = 1$; (d) $\rho_1 = \rho_2 = 10$. We observe that fluid mixtures with a larger density contrast are more likely to form two-phase fluids with the heavier fluid forming circular shaped drops. Whereas, fluid mixtures with an equal density ratio tend to form two-phase fluids of banded or stripe patterns. This separates the predictions made with a quasi-incompressible model from those of the incompressible one.](image-url)
(a) $\eta_1 = 1$, $\eta_2 = 10$, $\phi$ at $t = 0, 5, 10, 50, 100$.  

(b) $\eta_1 = 10$, $\eta_2 = 1$, $\phi$ at $t = 0, 5, 10, 50, 100$.  

(c) $\eta_1 = 1$, $\eta_2 = 1$, $\phi$ at $t = 0, 5, 10, 50, 100$.  

**Fig. 5.6.** Effect of different viscosities on coalescing dynamics. Here, we keep all the other parameters the same and $\rho_1 = \rho_2 = 1$, except (a) $\eta_1 = 1$, $\eta_2 = 10$; (b) $\eta_1 = 10$, $\eta_2 = 1$; (c) $\eta_1 = \eta_2 = 1$. The contour plots for $\phi$ at time $t = 0, 5, 10, 50, 100$ are shown in (a–b) and (c–d), respectively. When the viscosity of the ambient matrix is higher than the drops, the two drops eventually break up. In the other two cases, the two drops merge to form a single drop. However, the coalescing dynamics of the case with two distinct viscosities takes place more slowly than the case with the same viscosity.

**Fig. 5.7.** Energy plot vs. time for the simulations in Fig. 5.6.

in Fig. 5.1. The energy change with respect to time, the velocity field and its divergence at a selected moment are shown in Fig. 5.2. One prominent phenomenon we observe is that the coalescing dynamics slows down whenever there exists a difference in the densities. In addition, the more viscous drop coalesces more slowly early on than the less viscous drop when compared with the ambient fluid. This behavior reverses as time goes by. This phenomenon is manifested in the energy curve shown in Fig. 5.2. Among the three cases, the total energy decays the fastest when the two densities are equal. We also plot the velocity field together with $\nabla \cdot \mathbf{v}$ for the three cases investigated. We see that the fluid mixture is divergence free in the case of the equal density. While for the mixture of different densities, fluid compression/expansion at the interface between the two different fluids is visible in Fig. 5.2.

Next, we study the effect of the motility parameters on coalescing dynamics of lighter viscous fluid drops immersed in a heavier viscous fluid matrix. Specifically, three numerical simulations are conducted, where we use the same parameter values except (a) $\lambda_1 = \lambda_2 = 10^{-7}$; (b) $\lambda_1 = 5 \times 10^{-3}$, $\lambda_2 = 2 \times 10^{-7}$; (c) $\lambda_1 = 2 \times 10^{-7}$, $\lambda_2 = 5 \times 10^{-8}$, respectively. The numerical results are summarized in Fig. 5.3, and the energy curves vs. time are shown in Fig. 5.4. From the numerical simulations, we observe that the energy dissipation rate is a decreasing function of the mobility parameter ratio $\frac{\lambda_1}{\lambda_2}$. As a result, coalescing dynamics is faster in the case where $\frac{\lambda_1}{\lambda_2}$ is larger. So, the mobility in the transport equation for the viscous fluid matrix can facilitate the coalescing dynamics. In addition, from Fig. 5.4(b), our numerical scheme preserves the total volume well. As we alluded to earlier this implies that the total mass of the fluid mixture is conserved.

Then, we conduct another set of simulations on coarsening dynamics of the model with the initial condition

$$\phi(x, y)|_{t=0} = 0.5 + 0.45 \sin(4\pi x) \sin(4\pi y),$$  

(5.4)

where $L_x = L_y = 1$. Here, we focus on the effect of the density ratio. Three numerical examples with different density combinations, namely (a) $\rho_1 = 1$, $\rho_2 = 10$; (b) $\rho_1 = 10$, $\rho_2 = 1$; (c) $\rho_1 = 1$, $\rho_2 = 1$; (d) $\rho_1 = 10$, $\rho_2 = 10$ are shown respectively in Fig. 5.5. Notice that
the total volume of fluid 1 ( ϕ ) and fluid 2 ( 1 − ϕ ) are equal. Then the governing system preserves this property during the time evolution. Interestingly, we observe that the fluid of a larger density is more likely to form a drop than the one with a smaller density as shown in Fig. 5.5(a–b). When the two fluids have the same density, they retain the symmetry by forming a band structure, shown in Fig. 5.5(c–d). We remark that this numerical example highlights the necessity to study fluid mixtures using the quasi-incompressible fluid model. It indicates that for a fluid mixture of different densities, you simply cannot treat it as an incompressible fluid! A systematic parameter study will be desirable, but it will not be the objective of the current paper. We therefore omit it here.

Then we switch to study the effect of fluid viscosities on coalescing dynamics. We consider a test case where initially, there are two circular drops with radius \( r = 0.15 \) connected by a thin bridge. The profiles of \( \phi \) at different times of the simulation are shown in Fig. 5.6. The corresponding energies at different time are shown in Fig. 5.7. We observe that different choices of viscosity values can have quite dramatic effects on drop dynamics. For the case \( \eta_1 = 1, \eta_2 = 10 \), where the fluid in the drop is less viscous than the ambient fluid matrix, two drops are formed due to the capillary instability at the end of the simulation; whereas, for the case \( \eta_1 = \eta_2 = 10, \eta_1 = 1, \eta_2 = 1 \), the two drops merge into a single, large drop. From the energy plot, we observe that energies for the cases with different viscosities decay much slower than the case of the same viscosities \( \eta_1 = \eta_2 = 1 \).

5.3. Coarsening dynamics in miscible binary polymeric fluids

In this section, we study mixing dynamics of two miscible, viscous polymeric fluids governed by the Flory–Huggins mixing free energy given in (1.5). Given a random initial condition, we use the set of parameter values

\[
\eta = 1, \nu = 2/3, \gamma_1 = 0.01, \gamma_2 = 1, \lambda_1 = \lambda_2 = 10^{-7}, N_1 = 1, N_2 = 2,
\]  

and discuss the effect of the density ratio on coarsening dynamics. We note that the polymerization index of fluid 1 is smaller than that of fluid 2.

Here we conduct three simulations with the density ratios: (i) \( \rho_1 = \rho_2 = 1 \); (ii) \( \rho_1 = 1, \rho_2 = 10 \); (iii) \( \rho_1 = 10, \rho_2 = 1 \), respectively. The numerical results are summarized in Fig. 5.8. The total energy plots at different time for all three cases are summarized in Fig. 5.9(a). The divergence of velocity field \( \nabla \cdot \mathbf{v} \) is shown in Fig. 5.9(b) and the velocity field at a time slot is summarized in Fig. 5.9(c). The simulation shows that our scheme preserves the incompressibility property for the fluids with the same densities and captures accurately the mixture fluid flow of variable density as well. The fluid of a smaller polymerization index tends to form droplets while the one with a larger
Fig. 5.9. (a) Energy plot at different time for the simulations depicted in Fig. 5.8. (b) Divergence of the velocity at $t = 300$ for the solution shown in Fig. 5.8. The plots from the left to right correspond to the case a through c in Fig. 5.8. (c) The velocity field at $t = 300$ for the solution in Fig. 5.8, where the length of the arrow represents the magnitude of the velocity with maximum values 0.000407, 0.000307, 0.000576, respectively. From the left to the right, the plots correspond to case (a) through (c) in Fig. 5.8. The velocity fields are different in the three different cases.

6. Concluding remarks

A new second order numerical algorithm for solving a quasi-incompressible hydrodynamic fluid mixture model of two viscous fluids is presented. The scheme is shown both analytically and numerically second order accurate and unconditionally energy stable. It conserves the total density as well. Several numerical examples are given with respect to the fluid mixture of immiscible viscous fluids (the double-well potential) and miscible fluids (the Flory–Huggins potential), respectively, to explore coarsening dynamics and drop coalescing dynamics of various type of fluid mixtures. We demonstrate in the numerical study that a quasi-incompressible model is necessary for the fluid mixture with variable densities as well as viscosities. This numerical scheme provides us with the necessary tool to resolve the solution of the quasi-incompressible hydrodynamic mixture model accurately and efficiently. Although periodic boundary conditions are assumed in this paper, the numerical algorithm for the same model subject to the physical boundary conditions can be developed and shown to be energy stable when staggered-grids are adopted in the discretization of the velocity field.
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