On the energy stability of linear numerical schemes for polymer-solvent phase field models

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Abstract

We present new linear energy stable numerical schemes for numerical simulation of complex polymer-solvent mixtures. The mathematical model proposed by Zhou, Zhang and E *Physical Review E 73 (2006)* consists of the Cahn-Hilliard equation which describes dynamics of the interface that separates polymer and solvent and the Oldroyd-B equations for the hydrodynamics of polymeric mixtures. The model is thermodynamically consistent and dissipates free energy. Our main goal in this paper is to derive numerical schemes for the polymer-solvent mixture model that are energy dissipative and efficient in time. To this end we will propose several problem-suited time discretizations yielding linear schemes and discuss their properties.

1 Introduction

Phase separation in binary fluids is a fundamental process in condensed-matter physics. For Newtonian fluids the phenomenon of spinodal decomposition is reasonably well understood in terms of the so-called "model H" [16, 3, 23], where the hydrodynamic equations of motion for mass and momentum conservation are coupled to a convection-diffusion equation for the concentration (or in general the "phase field" variable ϕ), and the thermodynamics, which is described by a (free) energy functional $E(\phi)$, gives rise to a driving force, see, e.g., [1, 26, 15, 30]. In such "diffuse interface" or "phase field" models, the interface between two phases is a thin layer of finite thickness, across which ϕ varies continuously.

A big advantage of such models is that interfaces are defined implicitly and do not need to be tracked. Similarly, topological changes of the interface structure are automatically described correctly. The physics (and therefore also the mathematics and numerics) becomes more involved if one component — or both — is a macromolecular compound. In this case, the large molecular relaxation time gives rise to a dynamic coupling between intra-molecular processes and the unmixing on experimentally relevant time scales, with interesting new phenomena, for which the term "viscoelastic phase separation" [24] has been coined. Here the construction of physically sound dynamic equations with suitable constitutive relations to describe the viscoelasticity is already a challenge in itself. *Tanaka* [24] made the first attempt in this direction; however, *Zhou et al.* [30] showed later that this dynamics violates the second law of thermodynamics and provided a corrected set of equations that satisfy it. We thus study the diffuse-interface viscoelastic equations put forward in [30] for the case of the unmixing process of a polymer-solvent system.

Typically the interfacial region separating the two fluids is very narrow, and a high spatial resolution is required to accurately capture the interface dynamics. In fact, the underlying problem is stiff, which necessitates an implicit time discretization. Moreover, the solution admits several

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time scales over which it evolves, cf. [19]. In the literature one can find already several numerical methods that have been used for the numerical approximation of diffuse interface models, see, e.g., [5, 15, 19, 20, 26] and the references therein.

In order to describe the dynamics of a complex polymer-solvent mixture, the Cahn-Hilliard equations for the phase field evolution are coupled with the Oldroyd-B equations, which consist of the momentum equation for the velocity field, the continuity equation, and the rheological equation for time evolution of the elastic stress tensor. We note in passing that there is quite a large number of analytical as well as numerical results available in the literature for the Oldroyd-B system, see, e.g., [2, 10, 11, 22]. The main challenge in this field is to obtain a stable approximate numerical solution for large Weissenberg numbers. The dimensionless Weissenberg number represents elastic effects; it is large when the molecular relaxation time is comparable to the time scale of the flow, or even exceeds it significantly. In the present work we consider the non-critical regime of Weissenberg numbers. Applying the techniques from [10, 22], a further generalization using the log-transformation of the elastic stress tensor and the Lagrange-type approximation of the convective term is possible. We would like to mention that a preliminary subset of the results presented here including introduction to the problem has already been published in proceeding paper [21].

The paper is organized in the following way. In Section 2 we present a mathematical model for the polymer-solvent mixture consisting of the Cahn-Hilliard equation for the interface dynamics and the Oldroyd-B equations for the hydrodynamics. We also introduce a simplified model modelling only interface dynamics of the polymer-solvent mixture without any hydrodynamic effects. Section 3 is devoted to problem-suited numerical methods for both models. We present first and second order schemes that are linear and energy dissipative. We start with the simplified model and continue with the full model for polymer-solvent mixture. For the latter we propose two types of linear, free energy dissipative schemes, fully coupled schemes in Subsection 3.2 and the splitting scheme in Subsection 3.3. Numerical experiments presented in Section 4 confirm the schemes robustness and reliability to simulate viscoelastic phase separation.

2 Mathematical models

A classical approach to model interface problems is the diffuse interface theory that describes the dynamics of the interfaces by layers of small thickness whose structure is determined by a balance of molecular forces. Here the tendencies for mixing and de-mixing are in competition through a non-local mixing energy. Diffuse interface models are able to treat topological changes of the interface in a natural way. The surface motion is governed by the Cahn-Hilliard equation that can be derived as the gradient flow of a phase-field free energy functional

$$E_{mix}(\phi) = \int_\Omega \left(\frac{C_0}{2} |\nabla \phi|^2 + F(\phi) \right). \tag{2.1}$$

Here ϕ denotes the phase-field function that is used to express two phases of the system: $\phi = 1$ is one phase and $\phi = 0$ the other one. The phase-field function varies smoothly over the interfacial regions. Further, Ω is a computational domain with Lipschitz continuous boundary, C_0 is a positive constant controlling the interface width and $F(\phi)$ denotes a double-well potential that represents the tendency of a system to have two different stable phases.

In order to model polymer-solvent mixtures we use the Flory-Huggins potential, see [12, 18],

$$F_{log}(\phi) = \frac{1}{n_p} \phi \ln \phi + \frac{1}{n_s} (1 - \phi) \ln(1 - \phi) + \frac{\chi_0}{T} \phi(1 - \phi), \tag{2.2}$$

with n_p and n_s the molecular weights of the two components, χ_0 a positive constant and T the constant temperature.

Note that in literature the phase-field function often expresses the two phases by $\phi = 1$ and $\phi = -1$. In this case the Flory-Huggins potential reads

$$\tilde{F}_{log}(\phi) = \frac{1}{n_p} (1 + \phi) \ln(1 + \phi) + \frac{1}{n_s} (1 - \phi) \ln(1 - \phi) + \frac{\chi_0}{T} (1 - \phi^2). \tag{2.3}$$

Since the Flory-Huggins potential likely interferes with the energy stability of numerical schemes, a polynomial potential, the so called Ginzburg-Landau double-well potential, is mostly used in the literature, see, e.g., *Elliot, Zheng* [9], *Elliot, Garcke* [7, 8],

$$F_{pol}(\phi) = \frac{1}{4}(\phi^2 - 1)^2 \,. \tag{2.4}$$

This is a polynomial reconstruction of fourth order of the Flory-Huggins potential (2.3). We will discuss this topic in more detail in Remark 3.1.

The Cahn-Hilliard equation, see [4], can be derived from the mass balance law

$$\frac{\partial \phi}{\partial t} = -\nabla \cdot J \,,$$

where the mass flux J is defined as

$$J = -m(\phi)\nabla\mu \,.$$

Here

$$m(\phi) = M \left(\phi(1 - \phi) \right)^n$$

denotes the mobility function with M a positive constant, $n \in \mathbb{N}_0$ and μ denotes the chemical potential such that

$$\mu := \frac{\delta E_{mix}}{\delta \phi} = -C_0 \Delta \phi + f(\phi) \,.$$

Here $\frac{\delta E_{mix}}{\delta \phi}$ is the variational derivative of the mixing energy and $f(\phi) = F'(\phi)$.

Gathering this equations yields the Cahn-Hilliard equation

$$\frac{\partial \phi}{\partial t} = \nabla \cdot \left\{ M \left(\phi(1 - \phi) \right)^n \nabla \left[-C_0 \Delta \phi + f(\phi) \right] \right\} \,. \tag{2.5}$$

Dynamics of Newtonian two-phase mixtures is usually described as the gradient flow of the free energy consisting of the mixing energy E_{mix} and the kinetic energy E_{kin}. This leads to a coupled Cahn-Hilliard-Navier-Stokes system. In order to include the influence of polymers in such a system we extend it to a viscoelastic phase field model. This has been done at first by *Tanaka* [24] by adding viscoelastic energy due to the bulk and shear stress, here the separation of the total stress tensor into a bulk and a shear part was motivated by *Tanaka and Araki* [25]. This model violates the second law of thermodynamics, i.e. it is not free energy dissipative. In the recent paper [30] *Zhou, Zhang and E* propose an improved model for the viscoelastic phase separation that is thermodynamically consistent.

The total free energy E is given as

$$E_{tot}(\phi, q, \boldsymbol{\sigma}, \boldsymbol{u}) = E_{mix}(\phi) + E_{kin}(\boldsymbol{u}) + E_{conf}(q) + E_{el}(\boldsymbol{\sigma})$$

$$= \int_\Omega \left(\frac{C_0}{2} |\nabla \phi|^2 + F(\phi) \right) + \int_\Omega \frac{1}{2} |\boldsymbol{u}|^2 + \int_\Omega \frac{1}{2} |q|^2 + \int_\Omega \frac{1}{2} \mathrm{tr}(\boldsymbol{\sigma}) \,, \tag{2.6}$$

where $\boldsymbol{u}$ is the averaged velocity field of the two components, q the scalar bulk stress with E_{conf} the corresponding chain conformational entropy of the polymer molecules and $\boldsymbol{\sigma}$ the shear stress tensor with E_{el} the corresponding elastic energy of the polymer molecules. Using the Flory-Huggins potential (2.2) we obtain by the variational principle of the free energy minimization following the

standard procedures of nonequilibrium thermodynamics, see [30],

$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = \nabla \cdot \left\{ \phi(1-\phi)\, M \left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\, q) \right] \right\},$$

$$\frac{\partial q}{\partial t} + \boldsymbol{u} \cdot \nabla q = -\frac{1}{\tau_b(\phi)} q - A_1(\phi)\, \nabla \cdot \left\{ M \left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\, q) \right] \right\},$$

$$\frac{\partial \boldsymbol{\sigma}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{\sigma} = (\nabla\boldsymbol{u}) \cdot \boldsymbol{\sigma} + \boldsymbol{\sigma} \cdot (\nabla\boldsymbol{u})^T - \frac{1}{\tau_s(\phi)}\boldsymbol{\sigma} + B_2(\phi)\left[\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T \right], \qquad (2.7)$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\nabla p + \nabla \cdot \left\{ \eta(\phi)\left[\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T \right] \right\} - \nabla \cdot (C_0 \nabla\phi \otimes \nabla\phi) + \nabla \cdot \boldsymbol{\sigma},$$

$$\nabla \cdot \boldsymbol{u} = 0,$$

where $\mu = -C_0 \Delta\phi + f(\phi)$, $\tau_b(\phi) = \tau_b^0 \, \phi^2$ and $\tau_s(\phi) = \tau_s^0 \, \phi^2$ are the relaxation times, $B_2(\phi) = m_s^0 \, \phi^2$ is the relaxation modulus, and τ_b^0, τ_s^0 and m_s^0 are positive constants. $A_1(\phi)$ is the bulk modulus. The precise definition will be given in Section 4. Further, $\eta(\phi) = 1 - \tau_s(\phi)B_2(\phi)$ is the viscosity which is dependant on the relaxation and p is the pressure. For the aforementioned mobility the quartic function $m(\phi) = M\left(\phi(1-\phi)\right)^2$ is used.

Zhou et al. [30] also considered the special case of model (2.7) without hydrodynamic transport, i.e. $\boldsymbol{u} = 0$. Note, that we use the same symbol 0 for a scalar, a vector or a matrix. The resulting simplified model reads

$$\frac{\partial \phi}{\partial t} = \nabla \cdot \left\{ \phi(1-\phi)M\left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\, q) \right] \right\},$$
$$\frac{\partial q}{\partial t} = -\frac{1}{\tau_b(\phi)} q - A_1(\phi)\nabla \cdot \left\{ M\left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\, q) \right] \right\}. \qquad (2.8)$$

In literature we can find already several well-established numerical methods for the Cahn-Hilliard equation (2.5), see, e.g., [5, 15, 19, 20, 26]. In the following subsection we start by discussing the simplified model (2.8).

2.1 Simplified model without hydrodynamics

In a special case when the hydrodynamics effects are neglected, i.e. $\boldsymbol{u} = 0$, the total energy of the system consists of the mixing energy and the chain conformational energy

$$E_{tot}(\phi, q) = E_{mix}(\phi) + E_{conf}(q) = \int_\Omega \left(\frac{C_0}{2} |\nabla\phi|^2 + F(\phi) \right) + \int_\Omega \frac{1}{2} |q|^2. \qquad (2.9)$$

The minimization principle yields the model (2.8).

Theorem 2.1 *The problem* (2.8) *satisfies the following energy law*

$$\frac{dE_{tot}(\phi, q)}{dt} = -\frac{1}{\tau_b^0} \left\| \frac{q}{\phi} \right\|_{L^2(\Omega)}^2 - \int_\Omega M\left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\, q) \right]^2. \qquad (2.10)$$

Proof. Multiplying $(2.8)_1$ by μ and integrating over the computational domain Ω, assuming suitable boundary conditions (e.g. periodic boundary conditions), and applying integration by parts we obtain

$$\int_\Omega \frac{\partial \phi}{\partial t}\mu - \int_\Omega \nabla \cdot \left\{ \phi(1-\phi)M\left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\, q) \right] \right\} \mu$$
$$= \int_\Omega \frac{\partial \phi}{\partial t}\frac{\delta E_{mix}(\phi)}{\delta\phi} + \int_\Omega \left\{ \phi(1-\phi)M\left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\, q) \right] \right\} \nabla\mu$$
$$= \frac{dE_{mix}(\phi)}{dt} + \int_\Omega M\left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\, q) \right]\left[\phi(1-\phi)\nabla\mu \right] = 0.$$

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Further, multiplying $(2.8)_2$ by q and integrating over Ω with suitable boundary conditions yields

$$\int_\Omega \frac{\partial q}{\partial t} q + \int_\Omega \frac{1}{\tau_b(\phi)} q^2 + \int_\Omega A_1(\phi) \nabla \cdot \left\{ M\left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\,q)\right]\right\} q$$

$$= \int_\Omega \frac{1}{2}\frac{\partial q^2}{\partial t} + \int_\Omega \frac{1}{\tau_b^0 \phi^2} q^2 + \int_\Omega \nabla \cdot M\left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\,q)\right] A_1(\phi)\,q$$

$$= \frac{d}{dt}\left(\int_\Omega \frac{1}{2}q^2\right) + \frac{1}{\tau_b^0}\int_\Omega \left(\frac{q}{\phi}\right)^2 - \int_\Omega M\left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\,q)\right]\nabla(A_1(\phi)\,q)$$

$$= \frac{dE_{conf}(q)}{dt} + \frac{1}{\tau_b^0}\left\|\frac{q}{\phi}\right\|_{L^2(\Omega)}^2 + \int_\Omega M\left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\,q)\right]\left[-\nabla(A_1(\phi)\,q)\right] = 0\,.$$

Then, adding both relations we obtain

$$\frac{dE_{mix}(\phi)}{dt} + \frac{dE_{conf}(q)}{dt} + \frac{1}{\tau_b^0}\left\|\frac{q}{\phi}\right\|_{L^2(\Omega)}^2 + \int_\Omega M\left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\,q)\right]\left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\,q)\right] = 0\,,$$

which is the desired energy law (2.10). ∎

2.2 Two-phase model for viscoelastic flow

In this subsection we consider the full two-phase model for viscoelastic phase separation (2.7). The total free energy of the system consists of the mixing energy, the conformation energy, the elastic energy and the kinetic energy

$$E_{tot}(\phi, q, \boldsymbol{\sigma}, \boldsymbol{u}) = E_{mix}(\phi) + E_{conf}(q) + E_{el}(\boldsymbol{\sigma}) + E_{kin}(\boldsymbol{u})$$

$$= \int_\Omega \left(\frac{C_0}{2}|\nabla\phi|^2 + F(\phi)\right) + \int_\Omega \frac{1}{2}|q|^2 + \int_\Omega \frac{1}{2}\mathrm{tr}(\boldsymbol{\sigma}) + \int_\Omega \frac{1}{2}|\boldsymbol{u}|^2\,. \quad (2.11)$$

In order to prove that a solution of (2.7) dissipates the total free energy in time we need the following lemma.

Lemma 2.1 *The following relation holds*

$$\nabla \cdot (C_0 \nabla\phi \otimes \nabla\phi) = -\mu\nabla\phi + \nabla\left(\frac{C_0}{2}|\nabla\phi|^2 + F(\phi)\right)\,. \quad (2.12)$$

Proof. For e_i the i-th unit vector and d the spatial dimension the following relation holds

$$\nabla \cdot (C_0 \nabla\phi \otimes \nabla\phi) = C_0 \sum_{j=1}^d \frac{\partial}{\partial x_j}\left(\sum_{i=1}^d \frac{\partial\phi}{\partial x_i}e_i \cdot \sum_{j=1}^d \frac{\partial\phi}{\partial x_j}e_j^T\right)$$

$$= C_0 \sum_{i,j=1}^d \frac{\partial}{\partial x_j}\left(\frac{\partial\phi}{\partial x_i}\frac{\partial\phi}{\partial x_j}\right)e_i = C_0 \sum_{i,j=1}^d \left(\frac{\partial\phi}{\partial x_i}\frac{\partial^2\phi}{\partial x_j^2} + \frac{\partial^2\phi}{\partial x_i\partial x_j}\frac{\partial\phi}{\partial x_j}\right)e_i$$

$$= C_0 \sum_{j=1}^d \frac{\partial^2\phi}{\partial x_j^2} \cdot \sum_{i=1}^d \frac{\partial\phi}{\partial x_i}e_i + \frac{C_0}{2}\sum_{i=1}^d \frac{\partial}{\partial x_i}\sum_{j=1}^d \left(\frac{\partial\phi}{\partial x_j}\right)^2 e_i$$

$$= C_0 \sum_{j=1}^d \frac{\partial^2\phi}{\partial x_j^2} \cdot \sum_{i=1}^d \frac{\partial\phi}{\partial x_i}e_i + \frac{C_0}{2}\sum_{i=1}^d \frac{\partial}{\partial x_i}\sum_{j=1}^d \left(\frac{\partial\phi}{\partial x_j}\right)^2 e_i - f(\phi)\frac{\partial\phi}{\partial x_i}e_i + \frac{\partial F(\phi)}{\partial\phi}\frac{\partial\phi}{\partial x_i}e_i$$

$$= \left(C_0 \sum_{j=1}^{d} \frac{\partial^2 \phi}{\partial x_j^2} - f(\phi) \right) \sum_{i=1}^{d} \frac{\partial \phi}{\partial x_i} e_i + \sum_{i=1}^{d} \frac{\partial}{\partial x_i} e_i \left(\frac{C_0}{2} \sum_{j=1}^{d} \left(\frac{\partial \phi}{\partial x_j} \right)^2 + F(\phi) \right)$$

$$= \left(C_0 \Delta \phi - f(\phi) \right) \nabla \phi + \nabla \left(\frac{C_0}{2} |\nabla \phi|^2 + F(\phi) \right)$$

$$= -\mu \nabla \phi + \nabla \left(\frac{C_0}{2} |\nabla \phi|^2 + F(\phi) \right).$$

■

Now, we introduce the new pressure term $\tilde{p} = p + \frac{C_0}{2} |\nabla \phi|^2 + F(\phi)$. Together with equation (2.12) this allows us to rewrite system (2.7) as follows

$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi - \nabla \cdot \left\{ \phi(1 - \phi) M \left[\phi(1 - \phi) \nabla \mu - \nabla(A_1(\phi) q) \right] \right\} = 0,$$

$$\frac{\partial q}{\partial t} + \boldsymbol{u} \cdot \nabla q + \frac{1}{\tau_b(\phi)} q + A_1(\phi) \nabla \cdot \left\{ M \left[\phi(1 - \phi) \nabla \mu - \nabla(A_1(\phi) q) \right] \right\} = 0,$$

$$\frac{\partial \boldsymbol{\sigma}}{\partial t} + (\boldsymbol{u} \cdot \nabla) \boldsymbol{\sigma} - (\nabla \boldsymbol{u}) \cdot \boldsymbol{\sigma} - \boldsymbol{\sigma} \cdot (\nabla \boldsymbol{u})^T + \frac{1}{\tau_s(\phi)} \boldsymbol{\sigma} - B_2(\phi) \left[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T \right] = 0, \qquad (2.13)$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla) \boldsymbol{u} - \nabla \cdot \left\{ \eta(\phi) \left[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T \right] \right\} + \nabla \tilde{p} - \mu \nabla \phi - \nabla \cdot \boldsymbol{\sigma} = 0,$$

$$\nabla \cdot \boldsymbol{u} = 0.$$

Theorem 2.2 *System (2.13) obeys the following energy law*

$$\frac{dE_{tot}(\phi, q, \boldsymbol{\sigma}, \boldsymbol{u})}{dt} = -\frac{1}{\tau_b^0} \left\| \frac{q}{\phi} \right\|_{L^2(\Omega)}^2 - \int_\Omega M \left[\phi(1 - \phi) \nabla \mu - \nabla(A_1(\phi) q) \right]^2$$

$$- \int_\Omega \frac{1}{2\,\tau_s(\phi)} \mathrm{tr}(\boldsymbol{\sigma}) - \int_\Omega \frac{\eta(\phi)}{2} \sum_{i,j=1}^{d} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)^2. \qquad (2.14)$$

Proof. Analogously to the derivation of the energy law (2.10), $(2.13)_1$ is multiplied by μ and $(2.13)_2$ by q and both are integrated. Assuming suitable boundary conditions we obtain

$$\frac{dE_{mix}(\phi)}{dt} + \frac{dE_{conf}(q)}{dt} + \frac{1}{\tau_b^0} \left\| \frac{q}{\phi} \right\|_{L^2(\Omega)}^2 + \int_\Omega M \left[\phi(1 - \phi) \nabla \mu - \nabla(A_1(\phi) q) \right]^2 + \int_\Omega \boldsymbol{u} \cdot \nabla \phi \mu = 0.$$

Further, we multiply $(2.13)_3$ by $\frac{1}{2}\mathbb{1}$, where $\mathbb{1}$ is the unit matrix, and integrate over Ω. Taking into account that for all $\mathbf{A} \in \mathbb{R}^{n \times n}, n \in \mathbb{N}, \mathbf{A} : \mathbb{1} = \mathrm{tr}(\mathbf{A} \cdot \mathbb{1}) = \mathrm{tr}(\mathbf{A})$ we get

$$\int_\Omega \frac{1}{2} \mathrm{tr} \left(\frac{\partial \boldsymbol{\sigma}}{\partial t} \right) + \int_\Omega \frac{1}{2} \mathrm{tr} \left((\boldsymbol{u} \cdot \nabla) \boldsymbol{\sigma} \right) - \int_\Omega \frac{1}{2} \left(\nabla \boldsymbol{u} : \boldsymbol{\sigma}^T + \boldsymbol{\sigma} : \nabla \boldsymbol{u} \right) - \int_\Omega \frac{1}{2\,\tau_s(\phi)} \mathrm{tr}(\boldsymbol{\sigma}) + B_2(\phi) \mathrm{tr}(\nabla \boldsymbol{u})$$

$$= \int_\Omega \frac{1}{2} \frac{\partial\,\mathrm{tr}(\boldsymbol{\sigma})}{\partial t} - \int_\Omega \frac{1}{2} \mathrm{tr} \left((\nabla \cdot \boldsymbol{u}) \boldsymbol{\sigma} \right) - \int_\Omega \boldsymbol{\sigma} : \nabla \boldsymbol{u} + \int_\Omega \frac{1}{2\,\tau_s(\phi)} \mathrm{tr}(\boldsymbol{\sigma}) + \int_\Omega B_2(\phi)(\nabla \cdot \boldsymbol{u})$$

$$= \frac{d}{dt} \int_\Omega \frac{1}{2} \mathrm{tr}(\boldsymbol{\sigma}) - \int_\Omega \boldsymbol{\sigma} : \nabla \boldsymbol{u} + \int_\Omega \frac{1}{2\,\tau_s(\phi)} \mathrm{tr}(\boldsymbol{\sigma}) = 0.$$

Multiplying $(2.13)_4$ by $\boldsymbol{u}$ and integrating over Ω yields

$$\int_\Omega \frac{\partial \boldsymbol{u}}{\partial t} \cdot \boldsymbol{u} + \int_\Omega (\boldsymbol{u} \cdot \nabla)|\boldsymbol{u}|^2 + \int_\Omega \left\{ \eta(\phi)\left[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T \right] \right\} : \nabla \boldsymbol{u} - \int_\Omega \tilde{p}(\nabla \cdot \boldsymbol{u}) - \mu \nabla \phi \cdot \boldsymbol{u} + \nabla \cdot \boldsymbol{\sigma} \cdot \boldsymbol{u}$$

$$= \int_\Omega \frac{1}{2}\frac{\partial |\boldsymbol{u}|^2}{\partial t} - \int_\Omega (\nabla \cdot \boldsymbol{u})|\boldsymbol{u}|^2 + \int_\Omega \left\{ \eta(\phi)\left[|\nabla \boldsymbol{u}|^2 + Tr\left((\nabla \boldsymbol{u})^2 \right) \right] \right\} - \int_\Omega \boldsymbol{u} \cdot \nabla \phi \mu + \int_\Omega \boldsymbol{\sigma} : \nabla \boldsymbol{u}$$

$$= \frac{d}{dt}\int_\Omega \frac{1}{2}|\boldsymbol{u}|^2 + \int_\Omega \frac{\eta(\phi)}{2} \sum_{i,j=1}^d \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)^2 - \int_\Omega \boldsymbol{u} \cdot \nabla \phi \mu + \int_\Omega \boldsymbol{\sigma} : \nabla \boldsymbol{u} = 0 \,.$$

Summing up the above relations we obtain the energy law (2.14). ■

Remark 2.1 *We should point out that the elastic stress tensor $\boldsymbol{\sigma}$ does not necessarily need to be positive definite. Thus, $tr(\boldsymbol{\sigma})$ in the energy law (2.14) is not necessarily positive and could therefore interfere with the energy dissipation. To control this we introduce the so-called conformation tensor $\boldsymbol{c}$, $\boldsymbol{c} := \frac{1}{B_2(\phi)}\boldsymbol{\sigma} + \mathbb{1}$, where $\mathbb{1}$ is the identity matrix. By its definition the conformation tensor $\boldsymbol{c}$ is positive definite. In [17] Hu & Lelièvre studied the classical Oldroyd-B model with $B_2(\phi) =$const. and $\tau_s(\phi) =$const. They were able to prove that if the determinant of the initial conformation tensor is greater than one, then $\text{tr}(\boldsymbol{\sigma}) > 0$ for all times. This result indicates that it is important to control the initial data for the elastic stress $\boldsymbol{\sigma}$ in such a way that the determinant of $\boldsymbol{c}$ is enough large in order to get an elastic stress tensor which remains positive definite as well.*

Remark 2.2 *In Subsection 3.3 we will present a new splitting scheme. To this end we have to introduce a new pressure term $\hat{p} = \tilde{p} - \phi\mu$ which allows us to rewrite system (2.13) as follows*

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\boldsymbol{u}\phi) - \nabla \cdot \left\{ \phi(1-\phi)M\left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\,q) \right] \right\} = 0 \,,$$

$$\frac{\partial q}{\partial t} + \boldsymbol{u} \cdot \nabla q + \frac{1}{\tau_b(\phi)}q + A_1(\phi)\nabla \cdot \left\{ M\left[\phi(1-\phi)\nabla\mu - \nabla(A_1(\phi)\,q) \right] \right\} = 0 \,,$$

$$\frac{\partial \boldsymbol{\sigma}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{\sigma} - (\nabla \boldsymbol{u}) \cdot \boldsymbol{\sigma} - \boldsymbol{\sigma} \cdot (\nabla \boldsymbol{u})^T + \frac{1}{\tau_s(\phi)}\boldsymbol{\sigma} - B_2(\phi)\left[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T \right] = 0 \,, \tag{2.15}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} - \nabla \cdot \left\{ \eta(\phi)\left[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T \right] \right\} + \nabla\hat{p} + \phi\nabla\mu - \nabla \cdot \boldsymbol{\sigma} = 0 \,,$$

$$\nabla \cdot \boldsymbol{u} = 0 \,.$$

Note that for the advection term of the Cahn-Hilliard equation $(2.15)_1$ it holds $\nabla \cdot (\boldsymbol{u}\phi) = \boldsymbol{u} \cdot \nabla\phi + \phi\nabla \cdot \boldsymbol{u} = \boldsymbol{u} \cdot \nabla\phi$, thanks the incompressibility condition $(2.15)_5$.

In what follows we will write for the sake of simplicity p instead of $\tilde{p}$ and $\hat{p}$.

3 Numerical schemes

3.1 Schemes for the simplified model

We start this subsection proposing the one step numerical scheme for the simplified model (2.8). We consider an uniform partition of the time interval $[0, T]$ with a constant time step Δt. Given (ϕ^n, q^n) from the previous time step we compute (ϕ^{n+1}, q^{n+1}) such that

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} - \nabla \cdot \left\{ \phi^n(1-\phi^n)M\left[\phi^n(1-\phi^n)\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^n)\,q^{n+\frac{1}{2}}) \right] \right\} = 0 \,,$$

$$\mu^{n+\frac{1}{2}} = -C_0\Delta\phi^{n+\frac{1}{2}} + f(\phi^{n+1}, \phi^n) \,, \tag{3.1}$$

$$\frac{q^{n+1} - q^n}{\Delta t} + \frac{1}{\tau_b(\phi^n)}q^{n+\frac{1}{2}} + A_1(\phi^n)\nabla \cdot \left\{ M\left[\phi^n(1-\phi^n)\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^n)\,q^{n+\frac{1}{2}}) \right] \right\} = 0 \,.$$

Here we use the notations $\phi^{n+\frac{1}{2}} := \frac{\phi^{n+1}+\phi^n}{2}$ and $q^{n+\frac{1}{2}} := \frac{q^{n+1}+q^n}{2}$ that are the Crank-Nicolson-type approximations.

Theorem 3.1 *Let $f(\phi^{n+1}, \phi^n)$ represents a suitable linearized approximation of $f(\phi) = F'(\phi)$. Then the resulting numerical scheme* (3.1) *is linear and satisfies the following discrete version of the energy law* (2.10)

$$\frac{E_{tot}(\phi^{n+1}, q^{n+1}) - E_{tot}(\phi^n, q^n)}{\Delta t} = -ND_{phobic}^{n+1}$$

$$- \frac{1}{\tau_b^0} \left\| \frac{q^{n+\frac{1}{2}}}{\phi^n} \right\|_{L^2(\Omega)}^2 - \int_\Omega M \left[\phi^n(1-\phi^n)\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^n)\,q^{n+\frac{1}{2}}) \right]^2 , \quad (3.2)$$

where

$$ND_{phobic}^{n+1} := \int_\Omega f(\phi^{n+1}, \phi^n)\frac{\phi^{n+1} - \phi^n}{\Delta t} - \int_\Omega \frac{F(\phi^{n+1}) - F(\phi^n)}{\Delta t} .$$

Depending on the approximation considered for $f(\phi^{n+1}, \phi^n)$, we obtain different numerical schemes with different discrete energy laws, see Remark 3.1.

Proof. It is clear that the proposed scheme is linear. The discrete mixing and conformation energy can be derived following the same calculations presented in the proof of Theorem 2.1. Multiplying $(3.1)_1$ by $\mu^{n+\frac{1}{2}}$, integrating over Ω and applying suitable boundary conditions yields

$$\frac{E_{mix}(\phi^{n+1}) - E_{mix}(\phi^n)}{\Delta t} + ND_{phobic}^{n+1}$$

$$+ \int_\Omega M \left[\phi^n(1-\phi^n)\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^n)\,q^{n+\frac{1}{2}}) \right] \left[\phi^n(1-\phi^n)\nabla\mu^{n+\frac{1}{2}} \right] = 0 .$$

Analogously, multiplying $(3.1)_3$ by $q^{n+\frac{1}{2}}$, integrating over Ω while assuming suitable boundary conditions implies

$$\frac{E_{conf}(q^{n+1}) - E_{conf}(q^n)}{\Delta t} + \frac{1}{\tau_b^0} \left\| \frac{q^{n+\frac{1}{2}}}{\phi^n} \right\|_{L^2(\Omega)}^2$$

$$+ \int_\Omega M \left[\phi^n(1-\phi^n)\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^n)\,q^{n+\frac{1}{2}}) \right] \left[-\nabla(A_1(\phi^n)q^{n+\frac{1}{2}}) \right] = 0 .$$

Summing up both relations leads to the discrete energy conservation law (3.2)

$$\frac{E_{tot}(\phi^{n+1}, q^{n+1}) - E_{tot}(\phi^n, q^n)}{\Delta t} + ND_{phobic}^{n+1} + \frac{1}{\tau_b^0} \left\| \frac{q^{n+\frac{1}{2}}}{\phi^n} \right\|_{L^2(\Omega)}^2$$

$$+ \int_\Omega M \left[\phi^n(1-\phi^n)\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^n)\,q^{n+\frac{1}{2}}) \right] \left[\phi^n(1-\phi^n)\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^n)\,q^{n+\frac{1}{2}}) \right] = 0 .$$

$\blacksquare$

The numerical scheme (3.1) is linear and first order in time. We propose a linear second order numerical scheme by using a second order extrapolation for the explicit terms, arriving at a two-step numerical scheme, obeying an analogous discrete energy law as scheme (3.1). The proposed

linear second order numerical scheme reads

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} - \nabla \cdot \left\{ \phi^{n-\frac{1}{2}} (1 - \phi^{n-\frac{1}{2}}) M(\phi^{n-\frac{1}{2}}) \left[\phi^{n-\frac{1}{2}} (1 - \phi^{n-\frac{1}{2}}) \nabla \mu^{n+\frac{1}{2}} - \nabla (A_1(\phi^{n-\frac{1}{2}}) q^{n+\frac{1}{2}}) \right] \right\} = 0 \,,$$

$$\mu^{n+\frac{1}{2}} = -C_0 \Delta \phi^{n+\frac{1}{2}} + f(\phi^{n+1}, \phi^n) \,,$$

$$\frac{q^{n+1} - q^n}{\Delta t} + \frac{1}{\tau_b(\phi^{n-\frac{1}{2}})} q^{n+\frac{1}{2}}$$
$$+ A_1(\phi^{n-\frac{1}{2}}) \nabla \cdot \left\{ M(\phi^{n-\frac{1}{2}}) \left[\phi^{n-\frac{1}{2}} (1 - \phi^{n-\frac{1}{2}}) \nabla \mu^{n+\frac{1}{2}} - \nabla (A_1(\phi^{n-\frac{1}{2}}) q^{n+\frac{1}{2}}) \right] \right\} = 0 \,,$$
$$(3.3)$$

where

$$\phi^{n-\frac{1}{2}} := \frac{3\phi^n - \phi^{n-1}}{2}$$

is the second order extrapolation at the intermediate old time level $t_{n-1/2}$. In order to compute the pair (ϕ^1, q^1) from (ϕ^0, q^0) a second order one-step nonlinear scheme could be considered. We overcome this by setting $\phi^{-1} := \phi^0$ and thus solving the first order scheme in the first time step. As long as the initial data is sufficiently smooth, the influence is usually negligable for $T \gg 0$, see the experimental order of convergence (EOC) presented in Section 4, Table 4.1.

Definition 3.1 *A numerical scheme is called energy stable if for any $n \in \mathbb{N}$*

$$E_{tot}(w^{n+1}) \leq E_{tot}(w^n) \,,$$

where w^{n+1} and w^n are the solution vectors at times t_{n+1} and t_n, respectively.

Remark 3.1 *The choice of the approximation for $f(\phi^{n+1}, \phi^n)$ is highly dependant on a given potential $f(\phi)$. Anyway, in order to obtain an energy stable numerical scheme it is necessary that it holds $ND_{phobic}^{n+1} \geq 0$, i.e.*

$$\int_\Omega f(\phi^{n+1}, \phi^n) \frac{\phi^{n+1} - \phi^n}{\Delta t} \geq \int_\Omega \frac{F(\phi^{n+1}) - F(\phi^n)}{\Delta t} \,.$$

In literature the Ginzburg-Landau potential F_{pol} (2.4) is often used. For the Ginzburg-Landau potential we propose following [14] the linear first order approximation

$$f_{pol}^1(\phi^{n+1}, \phi^n) = f_{pol}(\phi^n) + \frac{1}{2} \|f_{pol}'\|_{L^\infty(-1,1)} (\phi^{n+1} - \phi^n) = f_{pol}(\phi^n) + \phi^{n+1} - \phi^n \,, \qquad (3.4)$$

which satisfies $ND_{phobic}^{n+1} \geq 0$ if F is bounded outside $[-1, 1]$, see Guillén-González et al. [14].

For the linear second order approximation we suggest to use the convex-concave splitting of the potential, which has been proposed by Wu, van Zwieten and van der Zee [28]. The corresponding approximation for $f_{pol}(\phi^{n+1}, \phi^n)$ consists of two second order Taylor approximations and reads

$$f_{pol}^2(\phi^{n+1}, \phi^n) = f_{vex}(\phi^{n+1}) - \frac{\phi^{n+1} - \phi^n}{2} f_{vex}'(\phi^{n+1}) + f_{cave}(\phi^n) + \frac{\phi^{n+1} - \phi^n}{2} f_{cave}'(\phi^n) \,. \quad (3.5)$$

Since the convex part $f_{vex} = 2\phi$, (3.5) is linear. Note that the derivative of the concave part, $f_{cave} = \phi^3 - 3\phi$, is nonlinear and thus calculated explicitly. Further, to achieve energy stability by using approximation (3.5) the chemical potential has to be modified in the following way

$$\mu^{n+\frac{1}{2}} = -C_0 \Delta \phi^{n+\frac{1}{2}} + f_{pol}^2(\phi^{n+1}, \phi^n) - \Delta t \frac{\left(\|f_{vex}'\|_{L^\infty(-1,1)} + \| -f_{cave}'\|_{L^\infty(-1,1)} \right)^2}{16} \Delta \phi^{n+\frac{1}{2}} \,. \quad (3.6)$$

We note that the Flory-Huggins potential F_{log} is logarithmic and its derivatives are unbounded. Consequently, the choice of linear approximations for $f_{log}(\phi^{n+1}, \phi^n)$ is severely limited. To ensure energy dissipation without modifying the potential, it is necessary to use a nonlinear approximation

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for $f_{log}(\phi^{n+1}, \phi^n)$. Since we are focussing on linear schemes we propose to use the second order Taylor approximation

$$f_{log}(\phi^{n+1}, \phi^n) = f_{log}(\phi^n) + \frac{\phi^{n+1} - \phi^n}{2} f'_{log}(\phi^n) \,. \tag{3.7}$$

This is called the "optimal dissipation 2" (OD2) approximation, see [15], because it leads to $ND^{n+1}_{phobic} = \mathcal{O}(\Delta t^2)$. However, using this approximation it is not possible to control the sign of ND^{n+1}_{phobic}. Nevertheless, our numerical simulations presented in Section 4 suggest that the dissipation of the total energy is not violated.

In the recent work [29] Yang and Zhao have proposed a modification of F_{log} introducing a suitable cut off function close to the boundaries in order to achieve the boundedness of the derivatives. Consequently, we can, e.g., use the above mentioned convex-concave splitting (3.5) with a modified chemical potential (3.6). We may thus achieve a linear, second order and provably energy stable numerical scheme, using a modified Flory-Huggins potential. Verification of this question is left for a future work.

3.2 Coupled schemes for two-phase viscoelastic flows

In this subsection we present fully coupled linear energy dissipative schemes for the full two-phase viscoelastic model (2.7). Given $(\phi^n, q^n, \boldsymbol{\sigma}^n, \boldsymbol{u}^n)$ from the previous time step we compute $(\phi^{n+1}, q^{n+1}, \boldsymbol{\sigma}^{n+1}, \boldsymbol{u}^{n+1}, p^{n+1})$ such that

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} + \boldsymbol{u}^{n+1} \cdot \nabla \phi^n - \nabla \cdot \left\{ \phi^n(1-\phi^n)M\left[\phi^n(1-\phi^n)\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^n)\,q^{n+\frac{1}{2}})\right]\right\} = 0\,,$$

$$\mu^{n+\frac{1}{2}} = -C_0\Delta\phi^{n+\frac{1}{2}} + f(\phi^{n+1}, \phi^n)\,,$$

$$\frac{q^{n+1} - q^n}{\Delta t} + \boldsymbol{u}^n \cdot \nabla q^{n+\frac{1}{2}} + \frac{1}{\tau_b(\phi^n)}q^{n+\frac{1}{2}} + A_1(\phi^n)\nabla \cdot \left\{ M\left[\phi^n(1-\phi^n)\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^n)\,q^{n+\frac{1}{2}})\right]\right\} = 0\,,$$

$$\frac{\boldsymbol{\sigma}^{n+1} - \boldsymbol{\sigma}^n}{\Delta t} + (\boldsymbol{u}^n \cdot \nabla)\boldsymbol{\sigma}^n - (\nabla\boldsymbol{u}^{n+1})\cdot\boldsymbol{\sigma}^n - \boldsymbol{\sigma}^n \cdot \left(\nabla\boldsymbol{u}^{n+1}\right)^T + \frac{1}{\tau_s(\phi^{n+\frac{1}{2}})}\boldsymbol{\sigma}^n - B_2(\phi^{n+\frac{1}{2}})2D(\boldsymbol{u}^{n+1}) = 0\,,$$

$$\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t} + (\boldsymbol{u}^n \cdot \nabla)\boldsymbol{u}^{n+1} - \nabla \cdot \left\{\eta(\phi^n)2D(\boldsymbol{u}^{n+1})\right\} + \nabla p^{n+1} - \mu^{n+\frac{1}{2}}\nabla\phi^n - \nabla \cdot \boldsymbol{\sigma}^n = 0\,,$$

$$\nabla \cdot \boldsymbol{u}^{n+1} = 0\,,$$

$$\tag{3.8}$$

where

$$D(\boldsymbol{u}^{n+1}) = \frac{1}{2}\left[\nabla\boldsymbol{u}^{n+1} + (\nabla\boldsymbol{u}^{n+1})^T\right]\,.$$

Theorem 3.2 The numerical scheme (3.8) is linear (up to the approximation considered for $f(\phi^{n+1}, \phi^n)$) and satisfies the discrete version of the energy law (2.14)

$$\frac{E_{tot}(\phi^{n+1}, q^{n+1}, \boldsymbol{\sigma}^{n+1}, \boldsymbol{u}^{n+1}) - E_{tot}(\phi^n, q^n, \boldsymbol{\sigma}^n, \boldsymbol{u}^n)}{\Delta t} = -ND^{n+1}_{phobic} - \frac{1}{\tau_b^0}\left\|\frac{q^{n+\frac{1}{2}}}{\phi^n}\right\|^2_{L^2(\Omega)}$$

$$- \int_\Omega M\left[\phi^n(1-\phi^n)\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^n)\,q^{n+\frac{1}{2}})\right]^2 - \int_\Omega \frac{1}{2\,\tau_s(\phi^{n+\frac{1}{2}})}\mathrm{tr}(\boldsymbol{\sigma}^n)$$

$$- \int_\Omega \frac{\eta(\phi^n)}{2}\sum_{i,j=1}^{d}\left(\frac{\partial u_i^{n+1}}{\partial x_j} + \frac{\partial u_j^{n+1}}{\partial x_i}\right)^2 - \frac{1}{2\Delta t}\|\boldsymbol{u}^{n+1} - \boldsymbol{u}^n\|^2_{L^2(\Omega)}\,, \quad (3.9)$$

where

$$ND^{n+1}_{phobic} := \int_\Omega f(\phi^{n+1}, \phi^n)\frac{\phi^{n+1} - \phi^n}{\Delta t} - \int_\Omega \frac{F(\phi^{n+1}) - F(\phi^n)}{\Delta t}\,.$$

Proof. Analogously to the derivation of the discrete energy law (3.2), $(3.8)_1$ is multiplied by $\mu^{n+\frac{1}{2}}$ and $(3.8)_3$ by $q^{n+\frac{1}{2}}$. Integrating both equations over Ω and summing them up we obtain

$$
\frac{E_{mix}(\phi^{n+1}) - E_{mix}(\phi^n)}{\Delta t} + \frac{E_{conf}(q^{n+1}) - E_{conf}(q^n)}{\Delta t} + ND_{phobic}^{n+1} + \frac{1}{\tau_b^0} \left\| \frac{q^{n+\frac{1}{2}}}{\phi^n} \right\|_{L^2(\Omega)}^2
$$

$$
+ \int_\Omega M\left[\phi^n(1-\phi^n)\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^n)\, q^{n+\frac{1}{2}})\right]^2 + \int_\Omega \boldsymbol{u}^{n+1}\cdot\nabla\phi^n\mu^{n+\frac{1}{2}} = 0\,.
$$

Further, we multiply $(3.8)_4$ by $\frac{1}{2}\mathbb{1}$ and apply analogous calculations as for the shear stress part of the continuous energy law (2.14)

$$
\frac{E_{el}(\boldsymbol{\sigma}^{n+1}) - E_{el}(\boldsymbol{\sigma}^n)}{\Delta t} - \int_\Omega \boldsymbol{\sigma}^n : \nabla\boldsymbol{u}^{n+1} + \int_\Omega \frac{1}{2\,\tau_s(\phi^{n+\frac{1}{2}})}\mathrm{tr}(\boldsymbol{\sigma}^n) = 0\,.
$$

Multiplying $(3.8)_5$ by $\boldsymbol{u}^{n+1}$ and integrating over Ω leads to

$$
\int_\Omega \frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t}\cdot\boldsymbol{u}^{n+1} + \int_\Omega \frac{\eta(\phi^n)}{2}\sum_{i,j=1}^d \left(\frac{\partial u_i^{n+1}}{\partial x_j} + \frac{\partial u_j^{n+1}}{\partial x_i}\right)^2
$$

$$
- \int_\Omega \boldsymbol{u}^{n+1}\cdot\nabla\phi^n\mu^{n+\frac{1}{2}} + \int_\Omega \boldsymbol{\sigma}^n : \nabla\boldsymbol{u}^{n+1} = 0\,,
$$

where

$$
\int_\Omega \frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t}\cdot\boldsymbol{u}^{n+1} = \frac{1}{\Delta t}\int_\Omega |\boldsymbol{u}^{n+1}|^2 - \boldsymbol{u}^n\cdot\boldsymbol{u}^{n+1}
$$

$$
= \frac{1}{2\,\Delta t}\int_\Omega |\boldsymbol{u}^{n+1} - \boldsymbol{u}^n|^2 + |\boldsymbol{u}^{n+1}|^2 - |\boldsymbol{u}^n|^2
$$

$$
= \frac{1}{2\,\Delta t}\|\boldsymbol{u}^{n+1} - \boldsymbol{u}^n\|_{L^2(\Omega)}^2 + \frac{E_{kin}(\boldsymbol{u}^{n+1}) - E_{kin}(\boldsymbol{u}^n)}{\Delta t}\,.
$$

The discrete energy law (3.9) by summing the above relations. ∎

Remark 3.2 *It is possible to eliminate the term $\frac{1}{2\,\Delta t}\|\boldsymbol{u}^{n+1} - \boldsymbol{u}^n\|_{L^2(\Omega)}^2$ from the energy law, considering the following linear one-step scheme.*

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} + \boldsymbol{u}^{n+\frac{1}{2}} \cdot \nabla\phi^n - \nabla \cdot \left\{ \phi^n(1-\phi^n)M\left[\phi^n(1-\phi^n)\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^n)\,q^{n+\frac{1}{2}})\right]\right\} = 0\,,$$

$$\mu^{n+\frac{1}{2}} = -C_0\Delta\phi^{n+\frac{1}{2}} + f(\phi^{n+1},\phi^n)\,,$$

$$\frac{q^{n+1} - q^n}{\Delta t} + \boldsymbol{u}^n \cdot \nabla q^{n+\frac{1}{2}} + \frac{1}{\tau_b(\phi^n)}q^{n+\frac{1}{2}}$$

$$+ A_1(\phi^n)\nabla \cdot \left\{ M\left[\phi^n(1-\phi^n)\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^n)\,q^{n+\frac{1}{2}})\right]\right\} = 0\,,$$

$$\frac{\boldsymbol{\sigma}^{n+1} - \boldsymbol{\sigma}^n}{\Delta t} + (\boldsymbol{u}^{n+\frac{1}{2}} \cdot \nabla)\boldsymbol{\sigma}^n - (\nabla\boldsymbol{u}^{n+\frac{1}{2}}) \cdot \boldsymbol{\sigma}^n - \boldsymbol{\sigma}^n \cdot \left(\nabla\boldsymbol{u}^{n+\frac{1}{2}}\right)^T$$

$$+ \frac{1}{\tau_s(\phi^{n+\frac{1}{2}})}\boldsymbol{\sigma}^n - B_2(\phi^{n+\frac{1}{2}})2D(\boldsymbol{u}^{n+\frac{1}{2}}) = 0\,,$$

$$\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t} + (\boldsymbol{u}^n \cdot \nabla)\boldsymbol{u}^{n+\frac{1}{2}} - \nabla \cdot \left\{\eta(\phi^n)2D(\boldsymbol{u}^{n+\frac{1}{2}})\right\} + \nabla p^{n+\frac{1}{2}} - \mu^{n+\frac{1}{2}}\nabla\phi^n - \nabla \cdot \boldsymbol{\sigma}^n = 0\,,$$

$$\nabla \cdot \boldsymbol{u}^{n+\frac{1}{2}} = 0\,,$$

$$(3.10)$$

where

$$D(\boldsymbol{u}^{n+\frac{1}{2}}) = \frac{1}{2}\left[\nabla\boldsymbol{u}^{n+\frac{1}{2}} + (\nabla\boldsymbol{u}^{n+\frac{1}{2}})^T\right]\,.$$

Analogous to scheme (3.3), using the second order extrapolation $z^{n-\frac{1}{2}} = \frac{3z^n - z^{n-1}}{2}, z \in \{\phi, \boldsymbol{u}, \boldsymbol{\sigma}\}$, for the explicit terms in scheme (3.10) yields the following linear and second order in time two-step numerical scheme

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} + \boldsymbol{u}^{n+\frac{1}{2}} \cdot \nabla\phi^{n-\frac{1}{2}}$$

$$- \nabla \cdot \left\{ \phi^{n-\frac{1}{2}}(1-\phi^{n-\frac{1}{2}})M\left[\phi^{n-\frac{1}{2}}(1-\phi^{n-\frac{1}{2}})\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^{n-\frac{1}{2}})\,q^{n+\frac{1}{2}})\right]\right\} = 0\,,$$

$$\mu^{n+\frac{1}{2}} = -C_0\Delta\phi^{n+\frac{1}{2}} + f(\phi^{n+1},\phi^n)\,,$$

$$\frac{q^{n+1} - q^n}{\Delta t} + \boldsymbol{u}^{n-\frac{1}{2}} \cdot \nabla q^{n+\frac{1}{2}} + \frac{1}{\tau_b(\phi^{n-\frac{1}{2}})}q^{n+\frac{1}{2}}$$

$$+ A_1(\phi^{n-\frac{1}{2}})\nabla \cdot \left\{ M\left[\phi^{n-\frac{1}{2}}(1-\phi^{n-\frac{1}{2}})\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^{n-\frac{1}{2}})\,q^{n+\frac{1}{2}})\right]\right\} = 0\,,$$

$$\frac{\boldsymbol{\sigma}^{n+1} - \boldsymbol{\sigma}^n}{\Delta t} + (\boldsymbol{u}^{n+\frac{1}{2}} \cdot \nabla)\boldsymbol{\sigma}^{n-\frac{1}{2}} - (\nabla\boldsymbol{u}^{n+\frac{1}{2}}) \cdot \boldsymbol{\sigma}^{n-\frac{1}{2}} - \boldsymbol{\sigma}^{n-\frac{1}{2}} \cdot \left(\nabla\boldsymbol{u}^{n+\frac{1}{2}}\right)^T$$

$$+ \frac{1}{\tau_s(\phi^{n+\frac{1}{2}})}\boldsymbol{\sigma}^{n-\frac{1}{2}} - B_2(\phi^{n+\frac{1}{2}})2D(\boldsymbol{u}^{n+\frac{1}{2}}) = 0\,,$$

$$\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t} + (\boldsymbol{u}^{n-\frac{1}{2}} \cdot \nabla)\boldsymbol{u}^{n+\frac{1}{2}}$$

$$- \nabla \cdot \left\{\eta(\phi^{n-\frac{1}{2}})2D(\boldsymbol{u}^{n+\frac{1}{2}})\right\} + \nabla p^{n+\frac{1}{2}} - \mu^{n+\frac{1}{2}}\nabla\phi^{n-\frac{1}{2}} - \nabla \cdot \boldsymbol{\sigma}^{n-\frac{1}{2}} = 0\,,$$

$$\nabla \cdot \boldsymbol{u}^{n+\frac{1}{2}} = 0\,.$$

$$(3.11)$$

Scheme (3.11) satisfies an analogous discrete energy law as scheme (3.10).

Remark 3.3 *Note that for small shear rates $D(u)$ and the Weissenberg numbers τ_s^0 that typically arise in our numerical experiments, the stiffness of the Oldroyd-B equation does not play a dominant*

role. If it is required the high Weissenberg problem can be treated by using additional techniques like the logarithmic transformation of the conformation tensor or considering the stress diffusion term in the evolution equation for $\boldsymbol{\sigma}$, for more details see, e.g., Lukáčová-Medviďová, Notsu, and She [22]. For large shear rates an implicit approximation of the elastic shear stress is suitable, but it hurts the linearity of a numerical scheme. The proposed modification of scheme (3.10) reads

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} + \boldsymbol{u}^{n+1} \cdot \nabla \phi^n - \nabla \cdot \left\{ \phi^n (1 - \phi^n) M \left[\phi^n (1 - \phi^n) \nabla \mu^{n+\frac{1}{2}} - \nabla (A_1(\phi^n) \, q^{n+\frac{1}{2}}) \right] \right\} = 0 \,,$$

$$\mu^{n+\frac{1}{2}} = -C_0 \Delta \phi^{n+\frac{1}{2}} + f(\phi^{n+1}, \phi^n) \,,$$

$$\frac{q^{n+1} - q^n}{\Delta t} + \boldsymbol{u}^n \cdot \nabla q^{n+\frac{1}{2}}$$
$$+ \frac{1}{\tau_b(\phi^n)} q^{n+\frac{1}{2}} + A_1(\phi^n) \nabla \cdot \left\{ M \left[\phi^n (1 - \phi^n) \nabla \mu^{n+\frac{1}{2}} - \nabla (A_1(\phi^n) \, q^{n+\frac{1}{2}}) \right] \right\} = 0 \,,$$

$$\frac{\boldsymbol{\sigma}^{n+1} - \boldsymbol{\sigma}^n}{\Delta t} + (\boldsymbol{u}^{n+\frac{1}{2}} \cdot \nabla) \boldsymbol{\sigma}^{n+1}$$
$$- (\nabla \boldsymbol{u}^{n+\frac{1}{2}}) \cdot \boldsymbol{\sigma}^{n+1} - \boldsymbol{\sigma}^{n+1} \cdot \left(\nabla \boldsymbol{u}^{n+\frac{1}{2}} \right)^T + \frac{1}{\tau_s(\phi^n)} \boldsymbol{\sigma}^{n+1} + B_2(\phi^{n+\frac{1}{2}}) 2D(\boldsymbol{u}^{n+\frac{1}{2}}) = 0 \,,$$

$$\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t} + (\boldsymbol{u}^n \cdot \nabla) \boldsymbol{u}^{n+\frac{1}{2}} - \nabla \cdot \left\{ \eta(\phi^n) \, 2D(\boldsymbol{u}^{n+\frac{1}{2}}) \right\} + \nabla p^{n+\frac{1}{2}} - \mu^{n+\frac{1}{2}} \nabla \phi^n - \nabla \cdot \boldsymbol{\sigma}^{n+1} = 0 \,,$$

$$\nabla \cdot \boldsymbol{u}^{n+\frac{1}{2}} = 0 \,.$$

$$(3.12)$$

Scheme (3.12) also satisfies an analogous discrete energy law as scheme (3.10).

Note that we can linearize scheme (3.12) by, e.g., using a fixed point iteration, see Remark 3.5. Further, using the idea presented in scheme 3.11 concerning the extrapolation of the explicit terms, while utilizing the Crank-Nicolson-type approximation $\boldsymbol{\sigma}^{n+\frac{1}{2}}$ for the implicit terms, we can obtain a second order two-step numerical scheme.

3.3 Splitting scheme for two-phase viscoelastic flows

In this subsection we present yet another possibility to discretize system (2.15). In order to save computational costs we split the computation into three different substeps. The first two steps are the interesting ones allowing us to decouple the calculation of the fluid part $(\boldsymbol{u}, p)$ from the phase field and bulk stress parts (ϕ, q). The third step is the calculation of the shear stress part $\boldsymbol{\sigma}$. In the first step we discretize the simplified model.

Step 1. Find (ϕ^{n+1}, q^{n+1}) such that

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} + \nabla \cdot (\boldsymbol{u}^* \phi^n) - \nabla \cdot \left\{ \phi^n (1 - \phi^n) M \left[\phi^n (1 - \phi^n) \nabla \mu^{n+\frac{1}{2}} - \nabla (A_1(\phi^n) \, q^{n+\frac{1}{2}}) \right] \right\} = 0 \,,$$

$$\mu^{n+\frac{1}{2}} = -C_0 \Delta \phi^{n+\frac{1}{2}} + f(\phi^{n+1}, \phi^n) \,,$$

$$\frac{q^{n+1} - q^n}{\Delta t} + \boldsymbol{u}^n \cdot \nabla q^{n+\frac{1}{2}} + \frac{1}{\tau_b(\phi^n)} q^{n+\frac{1}{2}}$$
$$+ A_1(\phi^n) \nabla \cdot \left\{ M \left[\phi^n (1 - \phi^n) \nabla \mu^{n+\frac{1}{2}} - \nabla (A_1(\phi^n) \, q^{n+\frac{1}{2}}) \right] \right\} = 0 \,,$$

$$(3.13)$$

where

$$\boldsymbol{u}^* := \boldsymbol{u}^n - \Delta t \, \phi^n \nabla \mu^{n+\frac{1}{2}} \,, \tag{3.14}$$

to split the phase field part from the hydrodynamic part. In the second step we discretize the fluid equations as follows.

Step 2. Find $(\boldsymbol{u}^{n+1}, p^{n+1})$ such that

$$\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^*}{\Delta t} + (\boldsymbol{u}^n \cdot \nabla)\boldsymbol{u}^{n+1} - \nabla \cdot \left\{ \eta(\phi^{n+\frac{1}{2}}) \, 2D(\boldsymbol{u}^{n+1}) \right\} + \nabla p^{n+1} - \nabla \cdot \boldsymbol{\sigma}^n = 0 \,,$$

$$\nabla \cdot \boldsymbol{u}^{n+1} = 0 \,. \tag{3.15}$$

Finally, in the third step we approximate the Oldroyd-B equation for the time evolution of the shear stress tensor $\boldsymbol{\sigma}$.

Step 3. Find $\boldsymbol{\sigma}^{n+1}$ such that

$$\frac{\boldsymbol{\sigma}^{n+1} - \boldsymbol{\sigma}^n}{\Delta t} + (\boldsymbol{u}^{n+1} \cdot \nabla)\boldsymbol{\sigma}^n - (\nabla \boldsymbol{u}^{n+1}) \cdot \boldsymbol{\sigma}^n + \boldsymbol{\sigma}^n \cdot \left(\nabla \boldsymbol{u}^{n+1} \right)^T$$

$$+ \frac{1}{\tau_s(\phi^{n+\frac{1}{2}})} \boldsymbol{\sigma}^n - B_2(\phi^{n+\frac{1}{2}}) \, 2D(\boldsymbol{u}^{n+1}) = 0 \,. \tag{3.16}$$

Theorem 3.3 *The numerical scheme* (3.13)-(3.16) *is linear and satisfies the discrete energy law*

$$\frac{E_{tot}(\phi^{n+1}, q^{n+1}, \boldsymbol{\sigma}^{n+1}, \boldsymbol{u}^{n+1}) - E_{tot}(\phi^n, q^n, \boldsymbol{\sigma}^n, \boldsymbol{u}^n)}{\Delta t} = -ND_{phobic}^{n+1} - ND_{split}^{n+1}$$

$$- \frac{1}{\tau_b^0} \left\| \frac{q^{n+\frac{1}{2}}}{\phi^n} \right\|_{L^2(\Omega)}^2 - \int_\Omega M \left[\phi^n(1-\phi^n)\nabla\mu^{n+\frac{1}{2}} - \nabla(A_1(\phi^n) \, q^{n+\frac{1}{2}}) \right]^2$$

$$- \int_\Omega \frac{1}{2\,\tau_s(\phi^{n+\frac{1}{2}})} \mathrm{tr}(\boldsymbol{\sigma}^n) - \int_\Omega \frac{\eta(\phi^{n+\frac{1}{2}})}{2} \sum_{i,j=1}^d \left(\frac{\partial u_i^{n+1}}{\partial x_j} + \frac{\partial u_j^{n+1}}{\partial x_i} \right)^2 \,, \tag{3.17}$$

where

$$ND_{split}^{n+1} := \frac{1}{2\,\Delta t} \left(\|\boldsymbol{u}^{n+1} - \boldsymbol{u}^*\|_{L^2(\Omega)}^2 + \|\boldsymbol{u}^* - \boldsymbol{u}^n\|_{L^2(\Omega)}^2 \right) \,.$$

Proof. Similar to the proof of the discrete energy law (3.9) we multiply (3.13)$_1$ by $\mu^{n+\frac{1}{2}}$, (3.13)$_3$ by $q^{n+\frac{1}{2}}$, (3.15)$_1$ by $\boldsymbol{u}^{n+1}$, and (3.16) by $\frac{1}{2}\mathbb{1}$, and integrate over Ω. Assuming suitable boundary conditions the derivations of the discrete elastic energies are analogous, while the calculation of the discrete mixing energy leads to the additional term $\int_\Omega \nabla \cdot (\boldsymbol{u}^*\phi^n)\mu^{n+\frac{1}{2}}$. The key idea of the splitting scheme lies in matching this term with $\int_\Omega \frac{1}{\Delta t}(\boldsymbol{u}^{n+1} - \boldsymbol{u}^*) \cdot \boldsymbol{u}^{n+1}$. This is possible by multiplying expression (3.14) by $\boldsymbol{u}^*$ and integrating over Ω, which yields

$$\|\boldsymbol{u}^*\|_{L^2(\Omega)}^2 = \int_\Omega \boldsymbol{u}^n \cdot \boldsymbol{u}^* + \int_\Omega \Delta t \, \phi^n \nabla\mu^{n+\frac{1}{2}} \cdot \boldsymbol{u}^*$$

$$= \int_\Omega \boldsymbol{u}^n \cdot \boldsymbol{u}^* + \int_\Omega \Delta t \, \nabla \cdot (\boldsymbol{u}^*\phi^n)\mu^{n+\frac{1}{2}} \,.$$

This can be rewritten as follows

$$\int_\Omega \nabla \cdot (\boldsymbol{u}^*\phi^n)\mu^{n+\frac{1}{2}} = \frac{1}{\Delta t} \left(\|\boldsymbol{u}^*\|_{L^2(\Omega)}^2 - \int_\Omega \boldsymbol{u}^n \cdot \boldsymbol{u}^* \right)$$

$$= \frac{1}{2\,\Delta t} \left(\|\boldsymbol{u}^*\|_{L^2(\Omega)}^2 - \|\boldsymbol{u}^n\|_{L^2(\Omega)}^2 + \|\boldsymbol{u}^* - \boldsymbol{u}^n\|_{L^2(\Omega)}^2 \right) \,.$$

Now, since

$$\int_\Omega \frac{1}{\Delta t}(\boldsymbol{u}^{n+1} - \boldsymbol{u}^*) \cdot \boldsymbol{u}^{n+1} = \frac{1}{2\,\Delta t} \left(\|\boldsymbol{u}^{n+1}\|_{L^2(\Omega)}^2 - \|\boldsymbol{u}^*\|_{L^2(\Omega)}^2 + \|\boldsymbol{u}^{n+1} - \boldsymbol{u}^*\|_{L^2(\Omega)}^2 \right) \,,$$

the additional terms $\pm\frac{1}{2\Delta t}\|\boldsymbol{u}^*\|_{L^2(\Omega)}^2$ are canceled and we obtain the desired discrete energy law (3.17). ∎

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Consequently,

$$E_{tot}(\phi^{n+1}, q^{n+1}, \boldsymbol{\sigma}^{n+1}, \boldsymbol{u}^{n+1}) \leq E_{tot}(\phi^n, q^n, \boldsymbol{\sigma}^n, \boldsymbol{u}^n), \tag{3.18}$$

provided that we control ND_{phobic}^{n+1}, since all other terms are non-negative. Indeed, even using the OD2 approximation (3.7), our numerical experiments in Chapter 4 suggest that the energy dissipation (3.18) holds, see Figure 4.2.

Remark 3.4 *To further reduce the computational costs of our splitting scheme in* **Step 2** *we propose to use Chorin's projection method, see Chorin [6]. This well-known algorithm allows to decouple computation of the velocity and the pressure of system* (3.15).
Step I. *Find* $\boldsymbol{u}^\dagger$ *such that*

$$\frac{\boldsymbol{u}^\dagger - \boldsymbol{u}^n}{\Delta t} + (\boldsymbol{u}^n \cdot \nabla)\boldsymbol{u}^\dagger - \nabla \cdot \left\{ \eta(\phi^n) \left[\nabla \boldsymbol{u}^\dagger + \left(\nabla \boldsymbol{u}^\dagger \right)^T \right] \right\} + \phi^n \nabla \mu^{n+\frac{1}{2}} - \nabla \cdot \boldsymbol{\sigma}^n = 0 \,,$$

and thus

$$\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^\dagger}{\Delta t} = \nabla p^{n+1} \,. \tag{3.19}$$

Step II. *Applying the divergence to* (3.19) *yields*

$$\frac{\nabla \cdot \boldsymbol{u}^{n+1} - \nabla \cdot \boldsymbol{u}^\dagger}{\Delta t} = \Delta p^{n+1} \,.$$

Consequently, due to the incompressibility condition $\nabla \cdot \boldsymbol{u}^{n+1} = 0$ *we find* p^{n+1} *such that*

$$\Delta p^{n+1} = -\frac{\nabla \cdot \boldsymbol{u}^\dagger}{\Delta t} \,.$$

Step III. *Since* $\boldsymbol{u}^\dagger$ *and* p^{n+1} *are now known, we find* $\boldsymbol{u}^{n+1}$ *by solving* (3.19).
In summary, instead of solving a coupled system for $(\boldsymbol{u}^{n+1}, p^{n+1})$, *we compute* $(\boldsymbol{u}^\dagger, p^{n+1}, \boldsymbol{u}^{n+1})$ *in a decoupled way.*

Remark 3.5 *For large shear rates* $D(u)$ *an implicit approximation of the shear stress would be suitable, but it would hurt the linearity of the numerical scheme, see also Remark 3.3. The proposed modification of* (3.15) *and* (3.16) *reads*
Step 2*. *Find* $(\boldsymbol{\sigma}^{n+1}, \boldsymbol{u}^{n+1}, p^{n+1})$ *such that*

$$\frac{\boldsymbol{\sigma}^{n+1} - \boldsymbol{\sigma}^n}{\Delta t} + (\boldsymbol{u}^{n+1} \cdot \nabla)\boldsymbol{\sigma}^{n+1} - (\nabla \boldsymbol{u}^{n+1}) \cdot \boldsymbol{\sigma}^{n+1} - \boldsymbol{\sigma}^{n+1} \cdot \left(\nabla \boldsymbol{u}^{n+1} \right)^T$$
$$+ \frac{1}{\tau_s(\phi^{n+\frac{1}{2}})}\boldsymbol{\sigma}^{n+1} + B_2(\phi^{n+\frac{1}{2}})2D(\boldsymbol{u}^{n+1}) = 0 \,,$$

$$\frac{\boldsymbol{u}^{n+1} - \boldsymbol{u}^n}{\Delta t} + (\boldsymbol{u}^n \cdot \nabla)\boldsymbol{u}^{n+1} - \nabla \cdot \left\{ \eta(\phi^{n+\frac{1}{2}})\,2D(\boldsymbol{u}^{n+1}) \right\} + \nabla p^{n+1} + \phi^n \nabla \mu^{n+\frac{1}{2}} - \nabla \cdot \boldsymbol{\sigma}^{n+1} = 0 \,,$$

$$\nabla \cdot \boldsymbol{u}^{n+1} = 0 \,.$$
$$\tag{3.20}$$

It is possible to linearize and split **Step 2*** *again by, e.g., using the following fixpoint iteration. Given* $(\boldsymbol{\sigma}^{n,0} = \boldsymbol{\sigma}^n, \boldsymbol{u}^{n,0} = \boldsymbol{u}^n)$ *from the previous time step, we repeat* **Step 2**† *and* **3**† *for* $l = 0, 1, ...,$ *until* $||z^{n,l+1} - z^{n,l}|| \leq \delta ||z^{n,l}||$, *for* $z \in \{\boldsymbol{\sigma}, \boldsymbol{u}, p\}$ *and* δ *sufficiently small.*
Step 2†**.** *Find* $(\boldsymbol{u}^{n,l+1}, p^{n,l+1})$ *such that*

$$\frac{\boldsymbol{u}^{n,l+1} - \boldsymbol{u}^n}{\Delta t} + (\boldsymbol{u}^n \cdot \nabla)\boldsymbol{u}^{n,l+1} - \nabla \cdot \left\{ \eta(\phi^{n+\frac{1}{2}})\,2D(\boldsymbol{u}^{n,l+1}) \right\} + \nabla p^{n,l+1} + \phi^n \nabla \mu^{n+\frac{1}{2}} - \nabla \cdot (\boldsymbol{\sigma}^{n,l}) = 0 \,,$$

$$\nabla \cdot \boldsymbol{u}^{n,l+1} = 0 \,,$$

$$\tag{3.21}$$

where

$$D(\boldsymbol{u}^{n,l+1}) = \frac{1}{2}\Big[\nabla\boldsymbol{u}^{n,l+1} + (\nabla\boldsymbol{u}^{n,l+1})^T\Big].$$

Step 3†. *Find $\boldsymbol{\sigma}^{n,l+1}$ such that*

$$\frac{\boldsymbol{\sigma}^{n,l+1} - \boldsymbol{\sigma}^n}{\Delta t} + (\boldsymbol{u}^{n,l+1}\cdot\nabla)\boldsymbol{\sigma}^{n,l+1} - (\nabla\boldsymbol{u}^{n,l+1})\cdot\boldsymbol{\sigma}^{n,l+1} - \boldsymbol{\sigma}^{n,l+1}\cdot\big(\nabla\boldsymbol{u}^{n,l+1}\big)^T$$

$$+ \frac{1}{\tau_s(\phi^{n+\frac{1}{2}})}\boldsymbol{\sigma}^{n,l+1} + B_2(\phi^{n+\frac{1}{2}})2D(\boldsymbol{u}^{n,l+1}) = 0. \quad (3.22)$$

Step 4†. *Update solution: $\boldsymbol{u}^{n+1} = \boldsymbol{u}^{n,l+1}, p^{n+1} = p^{n,l+1}, \boldsymbol{\sigma}^{n+1} = \boldsymbol{\sigma}^{n,l+1}$.*
Note that we can also use Chorin's projection method from Remark 3.4 in **Step 2**†.

Let us point out that we have proven energy dissipation for semi-discrete schemes. The proofs of the fully discrete schemes are analogous and our second order in space finite volume / finite difference scheme preserves this property as well, see *Lukáčová-Medviďová et al.* [22].

4 Numerical experiments

In this section we illustrate the behaviour of the newly derived numerical schemes for two-dimensional test problems. For the full model (2.7) or (2.15) we apply the splitting scheme (3.13)-(3.16). Here we use the Chorin projection method, see Remark 3.4, and the optimal dissipation 2 approximation for $f(\phi^{n+1}, \phi^n)$, see Remark 3.1.

The simplified model (2.8) is simulated using the second order scheme (3.3) with the optimal dissipation 2 approximation for $f(\phi^{n+1}, \phi^n)$. Note that for our numerical schemes we can use larger Δt than that applied in *Zhou et al.* [30]. For example for our second order scheme for the simplified model we can set $\Delta t = 0.25$ instead of $\Delta t = 0.025$ as in *Zhou et al.* [30]. This is related to the fact that our energy dissipative schemes are more stable.

We start with the experimental error analysis of our numerical scheme (3.3) for the simplified model. For the reference solution z_{ref}, $z \in \{\phi, q\}$ the finest resolution $\Delta t = 2^{-4}\cdot 10^{-3}$ is used. The experimental order of convergence (EOC) in time is given as

$$EOC(z) = \log_2(e(z)/e(z')),$$

where $e(z) = \|z - z_{ref}\|_{L_1(\Omega)}$ and $e(z')$ are the L_1-errors of two numerical solutions computed with the consecutive time steps Δt and $\Delta t' = \Delta t/2$. Table 4.1 presents the corresponding errors and clearly indicates that scheme (3.3) is second order accurate.

In the **first numerical experiment** we solve numerically system (2.7) applying periodic boundary conditions. The computational domain $\Omega = [0,1] \times [0,1]$ is divided into 128×128 grid cells. We follow the parameter set from *Gomez and Hughes* [13]. The initial data of the volume fraction $\phi(t = 0)$ is taken to be a constant $\phi_0 = 0.4$ with a random perturbation distributed in $\omega = [-0.05, 0.05]$. The initial velocities and bulk stress are set to zero. In order to ensure positive definiteness of shear stress tensor we choose $\boldsymbol{\sigma}(t = 0) = B_2(\phi(t = 0))(\sqrt{2} - 1)\mathbb{1}$. Further, we set the temperature to $T = 0.9\bar{3}$ and the interface width $\sqrt{C_0} = \frac{1}{\sqrt{600}}$. For the Flory-Huggins potential the molecular weights are set to $n_p = n_s = 1$ and $\chi_0 = 2.8$. The bulk modulus is set to $A_1(\phi) = M_b^0\left[1 + \tanh\left(\frac{\cot(\pi\phi^*) - \cot(\pi\phi)}{\epsilon}\right)\right] + M_b^1$, where $M_b^0 = 0.5$ and $M_b^1 = 1$, ϕ^* is set to be equal to the initial average polymer volume fraction ϕ_0 and $\epsilon = 0.01$. Furthermore, we set the mobility coefficient $M = 10$ and the relaxation coefficients to $\tau_b^0 = 10, \tau_s^0 = 5$ and $m_s^0 = 0.2$.

This experiment demonstrates phase separation by aggregation of the polymer molecules towards droplets. Figure 4.1 illustrates time evolution of the volume fraction ϕ. The total energy is (strictly) monotonically decreasing over time, which is related to the surface minimization of the

Table 4.1: Experimental order of convergence (EOC) in time for scheme (3.3) using the smooth initial data $\phi_0 = 0.5 + 0.5\sin(2\pi x)\sin(2\pi y)$; other parameters are the same as in the first numerical experiment.

$\Delta t/\Delta t'$	L_1-error ϕ	$EOC(\phi)$	L_1-error q	$EOC(q)$
$8/4 \cdot 10^{-3}$	3.765		1.812	
$4/2 \cdot 10^{-3}$	1.069	1.817	0.4613	1.974
$2/1 \cdot 10^{-3}$	0.2824	1.920	0.1172	1.977
$1/2^{-1} \cdot 10^{-3}$	$7.124 \cdot 10^{-2}$	1.987	$2.907 \cdot 10^{-2}$	2.012
$2^{-1}/2^{-2} \cdot 10^{-3}$	$1.779 \cdot 10^{-2}$	2.002	$7.212 \cdot 10^{-3}$	2.011
$2^{-2}/2^{-3} \cdot 10^{-3}$	$4.803 \cdot 10^{-3}$	1.889	$1.854 \cdot 10^{-3}$	1.960
$2^{-3}/2^{-4} \cdot 10^{-3}$	$1.462 \cdot 10^{-3}$	1.716	$4.401 \cdot 10^{-4}$	2.075

droplets and to droplets merging, see Figure 4.2.

The **second experiment** has been proposed in [30]. Here we solve numerically both, the complete system (2.7) as well as the simplified model (2.8). The computational domain $\Omega = [0, 128] \times [0, 128]$ is divided to 128×128 grid cells, initial volume fraction consists of $\phi_0 = 0.4$ and a small random perturbation distributed in $\omega = [-0.001, 0.001]$. The interface thickness width $\sqrt{C_0} = 1$, which is already very small having the size of one grid cell, and the temperature $T = 1.1$. The initial value of the shear stress is set to zero as in [30]. All other parameters are used as in the first experiment.

Figure 4.3 shows simulation of the complete system (2.7), where the whole viscoelastic phase separation process is exhibited. In the earlier stage the polymer-rich phase forms thin networklike structures. The solvent-rich droplets grow and coagulate. The area of the polymer-rich phase keeps decreasing. This is the well-known volume-shrinking process in polymer phase separation. In the later stage polymer-rich networklike structures are broken and the polymer-rich phase changes from being continuous to being discontinuous. This process is called phase inversion, cf. [30].

Figure 4.4 illustrate the dynamics of the simplified model (2.8). We can clearly see that also this model captures most important physical mechanism of the viscoelastic phase separation. From time $t = 600$ thin networklike structures formed by the matrix-polymer-rich phase can be clearly recognized.

The presented experiments confirm the reliability of our newly developed methods that preserve thermodynamic consistency of the underlying physical model and dissipate free energy on the discrete level, see Figures 4.2 and 4.5. Consequently, they can be applied to model numerically complex polymeric mixtures and provide a detailed view in the dynamics of a phase separation process of a semi-dilute polymer-solvent mixture after a temperature quench, including both key characteristics volume-shrinking and phase inversion.

Conclusions

In this paper we have derived and analysed new linear, energy dissipative numerical schemes for viscoelastic phase separation. The mathematical model is obtained through the variational principle as a minimizer of the free energy. Consequently, the model consisting of the Cahn-Hilliard equation describing the dynamics of interface between polymer and Newtonian solvent and the Oldroyd-B for the viscoelastic flow, can be understood as the gradient flow corresponding to the total free energy.

The linearity of the numerical schemes increases the efficiency of numerical simulations since there is no nonlinear iterative process required. The energy dissipative property is fundamental for phase-separation problems and reflects their thermodynamic consistency on the discrete level. This property has been demonstrated experimentally and proven theoretically up to the numerical
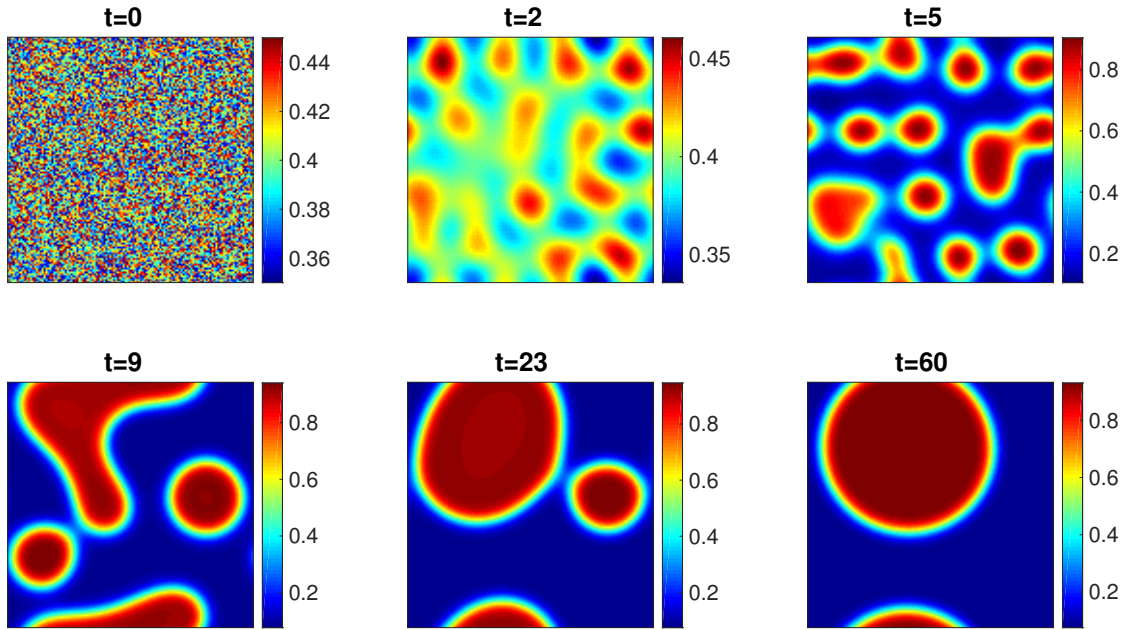
Figure 4.1: Time evolution of the polymer-solvent phase separation after a temperature quench with $T = 0.9\bar{3}$, $\phi_0 = 0.4$ and $\omega = [-0.05, 0.05]$. The computational domain is $\Omega = [0,1] \times [0,1]$ and the interface width $\sqrt{C_0} = \frac{1}{\sqrt{600}}$. The time step is $\Delta t = 10^{-4}$.

dissipation of the potential ND_{phobic}, which is small.

For the simplified model (2.8) the proposed numerical scheme is second order. Numerical experiments confirm that the simplified model can describe the most important physical properties of the viscoelastic phase separation. The full system can be approximated by the fully coupled scheme, Subsection 3.2 and the splitting scheme, Subsection 3.3. Both schemes schemes yield analogous numerical solutions, but we opted here for the splitting scheme, since it is more efficient computationally.

In future our aim is to develop hybrid schemes for multiscale models of viscoelastic phase separation processes. Thus, our aim will be to combine the proposed linear, energy dissipative schemes for macroscopic models coupled with the combined Lattice-Boltzmann and Molecular-Dynamics simulations of mesoscopic models for the viscoelastic phase separation. We refer a reader to [27] and the references therein for more details on the latter scheme. We believe that by such hybrid multiscale simulation the underlying physics will become more clear and can provide deeper insight and perhaps also the development of more refined and accurate macroscopic models.

Acknowledgements

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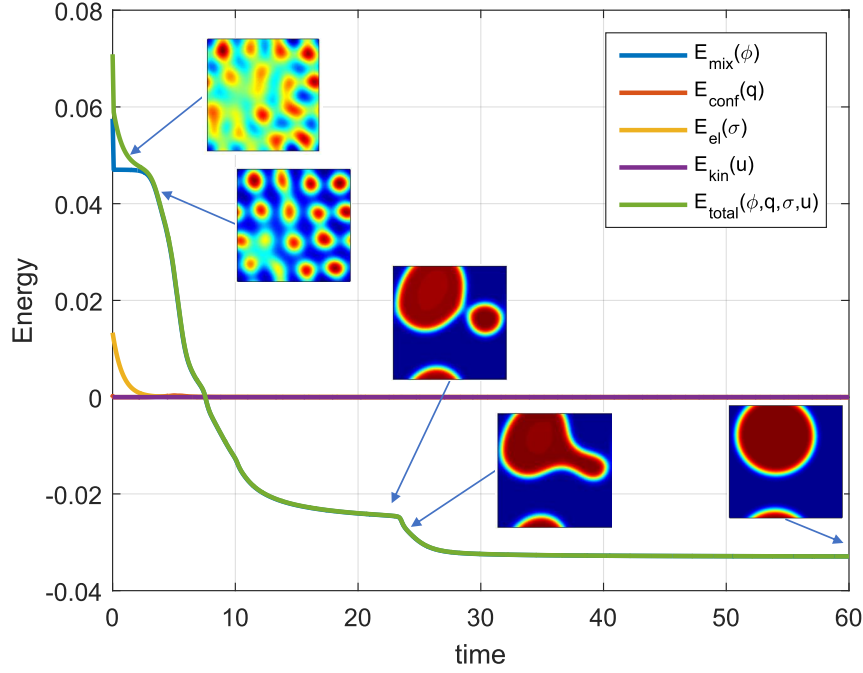
Figure 4.2: Energy evolution of the first numerical experiment corresponding to Figure 4.1 with intermediate states of the phase separation.

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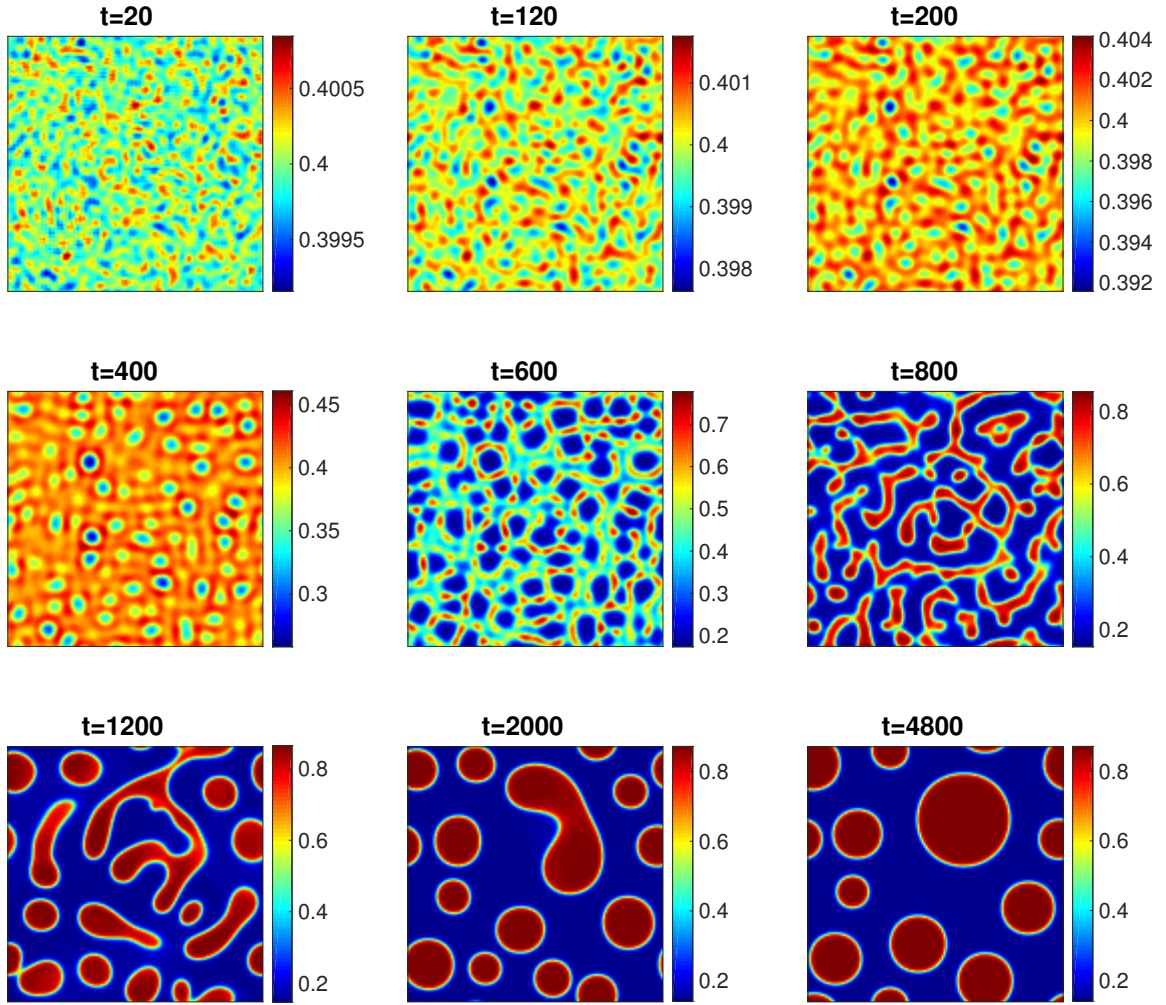
Figure 4.3: Time evolution of the polymer-solvent phase separation after a temperature quench with $T = 1.1, \phi_0 = 0.4$ and $\omega = [-0.001, 0.001]$. The computational domain is $\Omega = [0, 128] \times [0, 128]$ and the interface width $\sqrt{C_0} = 1$. The time step is $\Delta t = 0.025$.

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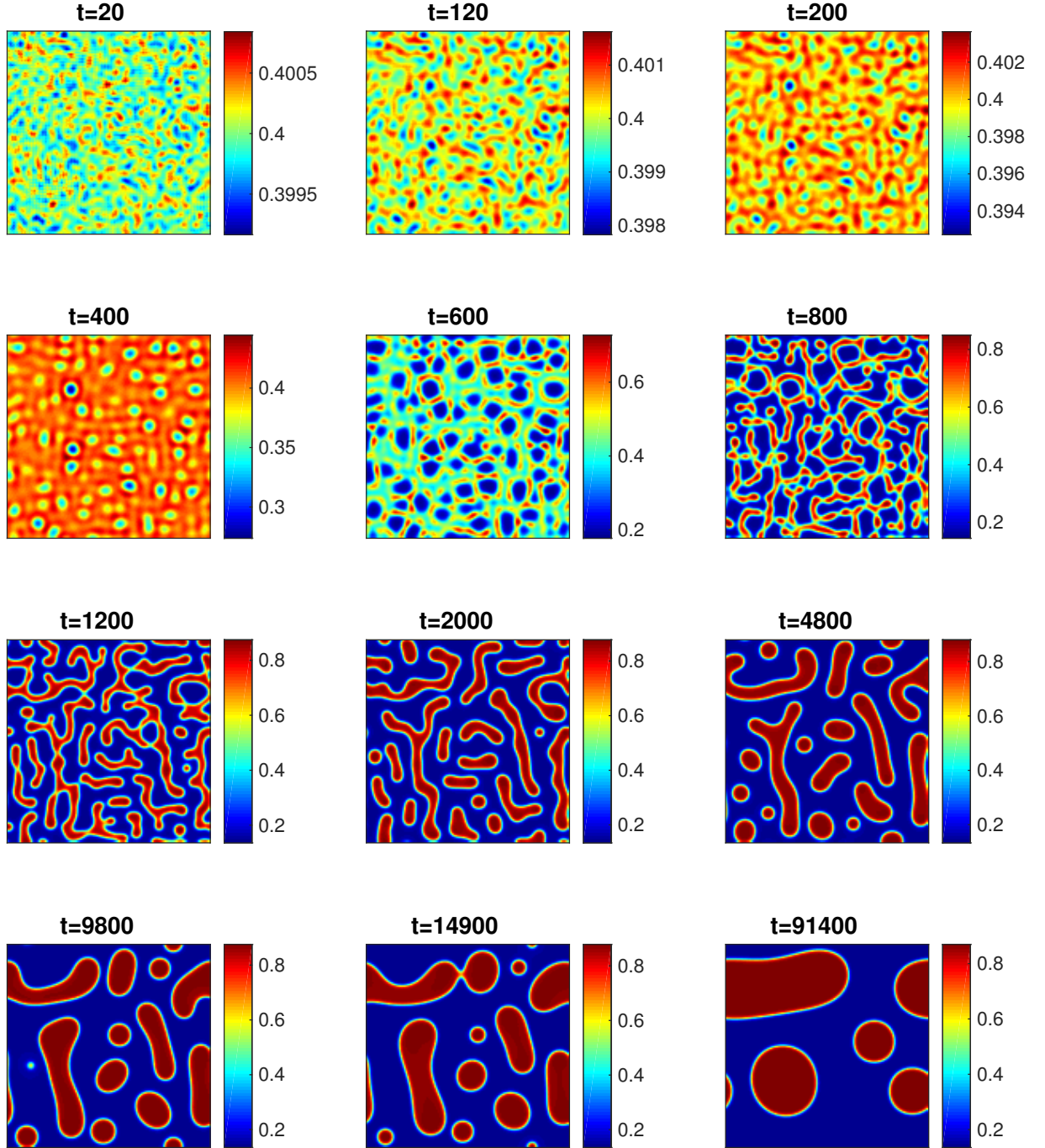
Figure 4.4: Time evolution of the polymer-solvent phase separation after a temperature quench, simulated by the simplified model utilizing the same parameter set used in the experiment from Figure 4.3, except for the time step $\Delta t = 0.25$, since our second order scheme is used.
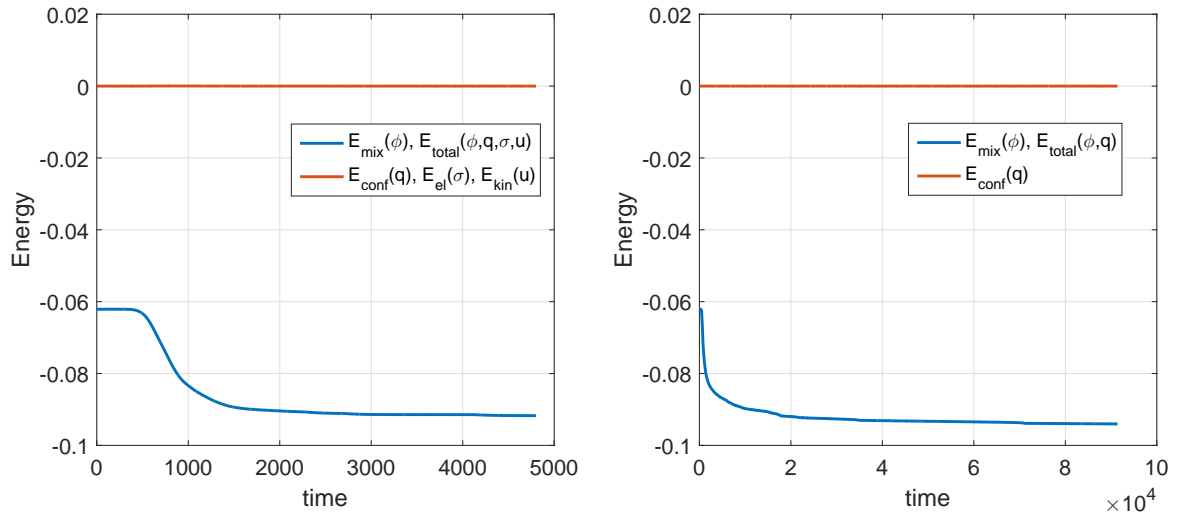
Figure 4.5: Energy evolution of the second numerical experiment corresponding to Figure 4.3 (left) and Figure 4.4 (right).