

Chapter 12

Micro-Macro-Models for Two-Phase Flow of Dilute Polymeric Solutions: Macroscopic Limit, Analysis, and Numerics

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Abstract We derive a diffuse-interface model for two-phase flow of incompressible fluids with dissolved noninteracting polymers. Describing the polymers as bead chains governed by general elastic spring potentials, including in particular Hookean and finitely extensible, nonlinear elastic (FENE) potentials, it couples a Fokker-Planck type equation describing distribution and orientation of the polymer chains with Cahn–Hilliard and Navier–Stokes type equations describing the balance of mass and momentum. Allowing for different solubility properties which are modelled by Henry type energy functionals, the presented model covers the case of one Newtonian fluid and one non-Newtonian fluid as well as the case of two non-Newtonian fluids. In the case of Hookean spring potentials, we derive a macroscopic diffuse-interface model for two-phase flow of Oldroyd-B-type liquids.

In the case of dumbbell models, we show existence of solutions and present numerical simulations in two space dimensions on oscillating polymeric droplets.

12.1 Introduction

We are concerned with modelling and analysis of two-phase flow of dilute polymeric solutions. For the ease of presentation, we focus initially on dumbbells to describe polymer chains. These dumbbells consist of two beads which are connected by an elastic spring with some spring potential U . We are not only interested in the spatial distribution of the polymers, but also in their configuration, i.e. in their elongation and orientation. Therefore, we have to distinguish between the spatial coordinate $\mathbf{x} \in \Omega$ referring to the barycenter of the dumbbell and the configurational coordinate $\mathbf{q} \in D$ describing its configuration. Consequently, we will use $\nabla_{\mathbf{x}}$, $\operatorname{div}_{\mathbf{x}}$, $\nabla_{\mathbf{q}}$ and $\operatorname{div}_{\mathbf{q}}$ to denote the differential operators with respect to \mathbf{x} and \mathbf{q} , respectively.

In recent years, many authors have contributed to a mathematical theory for multi-scale modeling of dilute polymeric flows (see [3–5, 9, 11, 15, 18–20, 22,

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23, 27, 29, 31] and the references therein). To describe dilute polymeric solutions, different approaches are at hand. Without claiming to be exhaustive, we list the concepts of the stochastic Brownian configuration field approaches coupling stochastic differential equations describing the evolution of the polymer chains with macroscopic equations describing the balance of momentum, deterministic Fokker–Planck approaches, and purely macroscopic approaches like Oldroyd-B type models. For the theoretical background, we refer to [17] and the references therein. Information on the numerical treatment of these approaches can be found e.g. in [13]. Focussing on Fokker–Planck–Navier–Stokes approaches, a generic single phase model reads as

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla_{\mathbf{x}}) \mathbf{u} - \operatorname{div}_{\mathbf{x}} \{2\eta \mathbf{D}\mathbf{u}\} + \nabla_{\mathbf{x}} p = \operatorname{div}_{\mathbf{x}} \left\{ \int_D \psi U'(\tfrac{1}{2} |\mathbf{q}|^2) \mathbf{q} \otimes \mathbf{q} - \int_D \psi \mathbb{1} \right\}, \quad (12.1a)$$

$$\operatorname{div}_{\mathbf{x}} \mathbf{u} = 0 \quad \text{in } \Omega \times (0, T), \quad (12.1b)$$

$$\partial_t \psi + \mathbf{u} \cdot \nabla_{\mathbf{x}} \psi + \operatorname{div}_{\mathbf{q}} \{ \psi \nabla_{\mathbf{x}} \mathbf{u} \cdot \mathbf{q} \} = c_{\mathbf{q}} \operatorname{div}_{\mathbf{q}} \{ \psi \nabla_{\mathbf{q}} \mu_{\psi} \} + c_{\mathbf{x}} \operatorname{div}_{\mathbf{x}} \{ \psi \nabla_{\mathbf{x}} \mu_{\psi} \}, \quad (12.1c)$$

$$\mu_{\psi} = \log \left(\frac{\psi}{M} \right) \quad \text{in } \Omega \times D \times (0, T) \quad (12.1d)$$

with $\eta, c_{\mathbf{q}} > 0$, $c_{\mathbf{x}} \geq 0$ and the symmetrized gradient $\mathbf{D} := \frac{1}{2} (\nabla_{\mathbf{x}} + \nabla_{\mathbf{x}}^T)$. The function $\psi(\mathbf{x}, t) : D \rightarrow \mathbb{R}_0^+$ describes a distribution on the configuration space $D \subset \mathbb{R}^d$ of admissible elongations/orientations of the polymers. In particular, the marginal

$$\omega(\mathbf{x}, t) := \int_D \psi(\mathbf{x}, t, \mathbf{q}) d\mathbf{q}$$

gives the number density of the polymers. The function

$$M(\mathbf{q}) := \left(\int_D \exp \left(-U(\tfrac{1}{2} |\bar{\mathbf{q}}|^2) \right) d\bar{\mathbf{q}} \right)^{-1} \exp \left(-U(\tfrac{1}{2} |\mathbf{q}|^2) \right) \quad (12.2)$$

denotes the Maxwellian associated with the spring potential U . Velocity and pressure field are denoted by (\mathbf{u}, p) . The tensor on the right-hand side of Eq. (12.1a) is the Kramers stress tensor (see [7, 16] and the references therein) which models effects exerted by the polymers on the solvent flow and gives rise to non-Newtonian effects. Equation (12.1c) is the usual evolution equation for the probability density on the configuration space. Note that $\operatorname{div}_{\mathbf{x}} \{ \psi \nabla_{\mathbf{x}} \mu_{\psi} \}$ describes the center-of-mass diffusion of the dumbbells. Although the parameter $c_{\mathbf{x}}$ is magnitudes smaller than one, it seems reasonable to keep the corresponding diffusion term for mathematical

reasons: It guarantees parabolicity of (12.1c). For approaches setting $c_x \equiv 0$, see [22, 23] and the references therein.

In [14], we extend (12.1) to the case of two-phase flows with different mass densities. Allowing for different solubility properties, the resulting model covers the case of one Newtonian fluid and one non-Newtonian fluid as well as the case of two non-Newtonian fluids.

12.2 The Governing Equations

12.2.1 Derivation of the Model: A Novel Approach Based on Onsager's Variational Principle

To derive a micro-macro model describing two-phase flow of dilute polymeric solutions, we apply Onsager's variational principle of minimum energy dissipation (cf. [26]), which turned out to be an efficient workhorse in the derivation of thermodynamically consistent models. There are various examples where it has successfully been applied in fluid dynamics. First, Qian et al. [28] introduced it to model contact line motion for two-phase flow with wall contact. Other applications range from different models for two-phase flow with general mass densities (cf. [21] and [2]) to models for species transport (cf. [2]), electrowetting and other electrokinetic phenomena [8]. Onsager's principle is supposed to provide the most probable evolution of a dissipative process by postulating a linear relation between the rates of displacement from the thermodynamic equilibrium and the applied forces, i.e. the rate of energy (cf. (12.8) below).

In general, there are many examples of models having an underlying energetic structure which may be derived by the Onsager formalism. It is worth mentioning that the micro-macro model obtained in [4] to describe single-phase flows of dilute polymeric solutions, can also be derived by the Onsager method.

Recapitulating the approach of [14], we start with general balance equations and—based on the above observation—apply Onsager's variational principle of minimum energy dissipation to obtain a thermodynamically consistent model for two-phase flow of polymeric solutions. Concerning the balance of mass and momentum, we apply the diffuse-interface method which was used e.g. in [10, 21], and [2] and which allows for a smooth transition between the fluid phases. Following in particular the approach used in [2], we define volume fractions $\phi_i := \frac{\rho_i}{\tilde{\rho}_i}$ ($i = 1, 2$), where $\tilde{\rho}_i$ denotes the mass density of the i th fluid in a pure phase and ρ_i denotes the actual mass density in the two-phase flow. Assuming $\phi_1 + \phi_2 \equiv 1$, the conservation of the phase-field parameter $\phi := \phi_2 - \phi_1$ implies also conservation of the individual mass densities. Defining the momentum as $(\rho \mathbf{u})$, where \mathbf{u} is the solenoidal, volume averaged velocity field, and imposing that the momentum is transported with the

same velocity as the mass—i.e. relative velocities are taken into account—yields

$$\partial_t \phi + \mathbf{u} \cdot \nabla_{\mathbf{x}} \phi + \operatorname{div}_{\mathbf{x}} \mathbf{J}_{\phi} = 0, \tag{12.3}$$

$$\rho(\phi) \partial_t \mathbf{u} + \left(\left(\rho(\phi) \mathbf{u} + \frac{\partial \rho}{\partial \phi} \mathbf{J}_{\phi} \right) \cdot \nabla_{\mathbf{x}} \right) \mathbf{u} = \operatorname{div}_{\mathbf{x}} \mathbf{S} - \nabla_{\mathbf{x}} p + \mathbf{k}, \tag{12.4}$$

with the correction flux \mathbf{J}_{ϕ} , the symmetric stress tensor \mathbf{S} and the force term \mathbf{k} which still are to be determined. For further details, we refer to [2].

In the same spirit we state a balance equation for the configurational density ψ on $\Omega \times D$,

$$\partial_t \psi + \operatorname{div}_{\mathbf{x}} \{ \tilde{\mathbf{v}}_{\mathbf{x}} \psi \} + \operatorname{div}_{\mathbf{q}} \{ \tilde{\mathbf{v}}_{\mathbf{q}} \psi \} = 0. \tag{12.5}$$

The next step is to decompose $\tilde{\mathbf{v}}_{\mathbf{x}} \psi$ into $\mathbf{u} \psi + \mathbf{J}_{\psi, \mathbf{x}}$ and $\tilde{\mathbf{v}}_{\mathbf{q}} \psi$ into $\mathbf{u}_{\mathbf{q}} \psi + \mathbf{J}_{\psi, \mathbf{q}}$ with correction fluxes $\mathbf{J}_{\psi, \mathbf{x}}$ and $\mathbf{J}_{\psi, \mathbf{q}}$, respectively, which are unknowns at this stage of the derivation. Note that there are two velocities to be distinguished—on the physical space the hydrodynamic velocity \mathbf{u} , on the configurational space a drift velocity $\mathbf{u}_{\mathbf{q}}$ which is intended to model the drift caused by the different velocities experienced by the dumbbell at head and tail. It is given by

$$\mathbf{u}_{\mathbf{q}}(\mathbf{x}, \mathbf{q}, t) := \frac{\mathbf{u}(\mathbf{x} + \frac{\varepsilon}{2} \mathbf{q}, t) - \mathbf{u}(\mathbf{x} - \frac{\varepsilon}{2} \mathbf{q}, t)}{\varepsilon} = \nabla_{\mathbf{x}} \left\{ \frac{1}{\varepsilon} \int_{-\frac{\varepsilon}{2}}^{\frac{\varepsilon}{2}} \mathbf{u}(\mathbf{x} + \theta \mathbf{q}, t) d\theta \right\} \cdot \mathbf{q}, \tag{12.6}$$

where the parameter ε reflects the different length scales in Ω and D .

Following the approach in [4], we replace the directional mollifier on the right-hand side of (12.6) by an isotropic one which we denote by $\mathcal{J}_{\varepsilon}$ in the scalar case and \mathbf{J}_{ε} or $\mathfrak{J}_{\varepsilon}$, if applied to vector-valued or matrix-valued quantities. Therefore, the last balance equation reads

$$\partial_t \psi + \mathbf{u} \cdot \nabla_{\mathbf{x}} \psi + \operatorname{div}_{\mathbf{q}} \{ \nabla_{\mathbf{x}} \mathbf{J}_{\varepsilon} \{ \mathbf{u} \} \cdot \mathbf{q} \psi \} = - \operatorname{div}_{\mathbf{x}} \mathbf{J}_{\psi, \mathbf{x}} - \operatorname{div}_{\mathbf{q}} \mathbf{J}_{\psi, \mathbf{q}}. \tag{12.7}$$

Imposing suitable, mass conserving boundary conditions, the unknown quantities are determined using Onsager’s variational principle which is supposed to model the most probable behavior of an irreversible process and postulates the relation

$$\delta_{(\mathbf{J}_{\phi}, \mathbf{J}_{\psi, \mathbf{x}}, \mathbf{J}_{\psi, \mathbf{q}}, \mathbf{S})} \left(\frac{d\mathcal{E}}{dt} + \Phi \right) \stackrel{!}{=} 0 \tag{12.8}$$

between thermodynamical forces (given by the rate of energy in the system) and an appropriate dissipation function Φ which will be defined in (12.9). In (12.8), $\delta_{(\mathbf{J}_{\phi}, \mathbf{J}_{\psi, \mathbf{x}}, \mathbf{J}_{\psi, \mathbf{q}}, \mathbf{S})}$ denotes the first variation with respect to the quantities \mathbf{J}_{ϕ} , $\mathbf{J}_{\psi, \mathbf{x}}$, $\mathbf{J}_{\psi, \mathbf{q}}$, and \mathbf{S} .

The energy of the system is assumed to be the sum of the kinetic energy $\frac{1}{2} \int_{\Omega} |\mathbf{u}|^2$, a Cahn-Hilliard energy $\frac{\delta}{2} \int_{\Omega} |\nabla_{\mathbf{x}} \phi|^2 + \frac{1}{\delta} \int_{\Omega} W(\phi)$, where $W(\phi) = \frac{1}{4} (1 - \phi^2)^2$ is a

standard double-well potential, an entropic component $\int_{\Omega \times D} \psi \left(\log \left(\frac{\psi}{M} \right) - 1 \right)$, and the so called Henry energy $\int_{\Omega} \beta(\phi) \mathcal{J}_{\varepsilon} \left\{ \int_D \psi \, d\mathbf{q} \right\} \, d\mathbf{x}$. By choosing an appropriate function β , the latter energy component will allow to constrain the polymers to one dedicated phase, and therefore allows for one Newtonian phase. Assuming a dissipation functional of the form

$$\Phi(\mathbf{J}_{\phi}, \mathbf{J}_{\psi, \mathbf{x}}, \mathbf{J}_{\psi, \mathbf{q}}, \mathbf{S}) := \int_{\Omega} \frac{|\mathbf{J}_{\phi}|^2}{2m(\phi)} + \int_{\Omega \times D} \frac{|\mathbf{J}_{\psi, \mathbf{x}}|^2}{2c_{\mathbf{x}}\psi} + \int_{\Omega \times D} \frac{|\mathbf{J}_{\psi, \mathbf{q}}|^2}{2c_{\mathbf{q}}\psi} + \int_{\Omega} \frac{|\mathbf{S}|^2}{4\eta(\phi)} \quad (12.9)$$

with $m, c_{\mathbf{x}}, c_{\mathbf{q}}, \eta > 0$ leads to the following set of equations.

$$\begin{aligned} \rho(\phi) \partial_t \mathbf{u} + \left((\rho(\phi) \mathbf{u} - m(\phi) \frac{\partial \rho}{\partial \phi} \nabla_{\mathbf{x}} \mu_{\phi}) \cdot \nabla_{\mathbf{x}} \right) \mathbf{u} - \operatorname{div}_{\mathbf{x}} \{2\eta(\phi) \mathbf{D}\mathbf{u}\} + \nabla_{\mathbf{x}} p \\ = \mu_{\phi} \nabla_{\mathbf{x}} \phi + \int_D \mu_{\psi} \nabla_{\mathbf{x}} \psi + \operatorname{div}_{\mathbf{x}} \left\{ \mathfrak{J}_{\varepsilon} \left\{ \int_D M \nabla_{\mathbf{q}} \frac{\psi}{M} \otimes \mathbf{q} \right\} \right\}, \end{aligned} \quad (12.10a)$$

$$\operatorname{div}_{\mathbf{x}} \mathbf{u} = 0, \quad (12.10b)$$

$$\partial_t \phi + \mathbf{u} \cdot \nabla_{\mathbf{x}} \phi - \operatorname{div}_{\mathbf{x}} \{m(\phi) \nabla_{\mathbf{x}} \mu_{\phi}\} = 0, \quad (12.10c)$$

$$\mu_{\phi} = -\delta \Delta_{\mathbf{x}} \phi + \frac{1}{8} W'(\phi) + \beta'(\phi) \mathcal{J}_{\varepsilon} \left\{ \int_D \psi \right\}, \quad (12.10d)$$

$$\partial_t \psi + \mathbf{u} \cdot \nabla_{\mathbf{x}} \psi + \operatorname{div}_{\mathbf{q}} \{\psi \nabla_{\mathbf{x}} \mathbf{J}_{\varepsilon} \{\mathbf{u}\} \cdot \mathbf{q}\} = \operatorname{div}_{\mathbf{q}} \{c_{\mathbf{q}} \psi \nabla_{\mathbf{q}} \mu_{\psi}\} + \operatorname{div}_{\mathbf{x}} \{c_{\mathbf{x}} \psi \nabla_{\mathbf{x}} \mu_{\psi}\}, \quad (12.10e)$$

$$\mu_{\psi} = \log \left(\frac{\psi}{M} \right) + \mathcal{J}_{\varepsilon} \{\beta(\phi)\}, \quad (12.10f)$$

on $\Omega \times \mathbb{R}^+$ or $\Omega \times D \times \mathbb{R}^+$, respectively, with the boundary conditions

$$\mathbf{u} = 0 \quad \text{on } \partial\Omega \times \mathbb{R}^+, \quad (12.11a)$$

$$\nabla_{\mathbf{x}} \phi \cdot \mathbf{n}_{\mathbf{x}} = 0 \quad \text{on } \partial\Omega \times \mathbb{R}^+, \quad (12.11b)$$

$$\nabla_{\mathbf{x}} \mu_{\phi} \cdot \mathbf{n}_{\mathbf{x}} = 0 \quad \text{on } \partial\Omega \times \mathbb{R}^+, \quad (12.11c)$$

$$\psi \nabla_{\mathbf{x}} \mu_{\psi} \cdot \mathbf{n}_{\mathbf{x}} = 0 \quad \text{on } \partial\Omega \times D \times \mathbb{R}^+, \quad (12.11d)$$

$$\psi (\nabla_{\mathbf{x}} \mathbf{J}_{\varepsilon} \{\mathbf{u}\} \cdot \mathbf{q} - c_{\mathbf{q}} \nabla_{\mathbf{q}} \mu_{\psi}) \cdot \mathbf{n}_{\mathbf{q}} = 0 \quad \text{on } \Omega \times \partial D \times \mathbb{R}^+. \quad (12.11e)$$

Restricting (12.10) to the case of a single-phase flow, i.e. ϕ, ρ , and η constant, allows to recover the set of equations derived in [4]. In practical applications, the constant $c_{\mathbf{x}}$ is magnitudes smaller than $c_{\mathbf{q}}$. Therefore, some authors decided to neglect

diffusion in \mathbf{x} -direction (cf. [3], [22, 23]). As the \mathbf{x} -diffusion guarantees parabolicity of the Fokker–Planck type equation which is convenient for the analytical treatment, we follow the ansatz used e.g. in [4] and keep the $c_x > 0$.

It is straight forward to adapt this modeling approach to polymer models consisting of $K + 1$ beads. In this case, we have to consider K elongation vectors $(\mathbf{q}_i)_{i=1,\dots,K} \in \bigotimes_{i=1}^K D_i =: D \subset \mathbb{R}^{Kd}$. Each of these vectors has its own entropic potential U_i associated with a Maxwellian M_i . The Maxwellian of the complete chain is defined as $M(\mathbf{q}) := \prod_{i=1}^K M_i(\mathbf{q}_i)$ (cf. [5]). Consequently, the momentum and Fokker–Planck equations are changed to become

$$\begin{aligned} \rho(\phi) \partial_t \mathbf{u} + \left(\left(\rho(\phi) \mathbf{u} - m(\phi) \frac{\partial \rho}{\partial \phi} \nabla_x \mu_\phi \right) \cdot \nabla_x \right) \mathbf{u} - \operatorname{div}_x \{ 2\eta(\phi) \mathbf{D}\mathbf{u} \} + \nabla_x p \\ = \mu_\phi \nabla_x \phi + \int_D \mu_\psi \nabla_x \psi + \operatorname{div}_x \left\{ \mathfrak{J}_\varepsilon \left\{ \int_D M \sum_{i=1}^K \nabla_{\mathbf{q}_i} \frac{\psi}{M} \otimes \mathbf{q}_i \right\} \right\}, \end{aligned} \tag{12.12a}$$

$$\begin{aligned} \partial_t \psi + \mathbf{u} \cdot \nabla_x \psi + \sum_{i=1}^K \operatorname{div}_{\mathbf{q}_i} \{ \psi \nabla_x \mathbf{J}_\varepsilon \{ \mathbf{u} \} \cdot \mathbf{q}_i \} \\ = \sum_{i=1}^K \sum_{j=1}^K \operatorname{div}_{\mathbf{q}_i} \{ A_{ij} \psi \nabla_{\mathbf{q}_i} \mu_\psi \} + \operatorname{div}_x \{ c_x \psi \nabla_x \mu_\psi \}, \end{aligned} \tag{12.12b}$$

$$\mu_\psi = \log \left(\frac{\psi}{M} \right) + \mathcal{J}_\varepsilon \{ \beta(\phi) \}, \tag{12.12c}$$

on $\Omega \times \mathbb{R}^+$ or $\Omega \times D \times \mathbb{R}^+$, respectively. The matrix $A = (A_{ij})_{i,j=1}^K$ is the symmetric positive definite Rouse matrix, or connectivity matrix. For further information we refer to [25] and the references therein. Moreover, the boundary conditions need to be adapted to guarantee conservation of particle number.

12.2.2 A Two-Phase Oldroyd-B Model

It is well known that micro-macro models may be used to derive deterministic viscoelastic models by taking the expected value in the Fokker–Planck equation. If the elastic potential is of Hookean type, i.e. $U(s) = s$ and $D = \mathbb{R}^d$, particular versions of the Oldroyd-B model are obtained (see [4] and the references therein). As the elastic potential U and therefore the admissible configurational space D was not specified in the derivation of our model, we may assume that our potential is of Hookean type and formulate a Oldroyd-B type model for two-phase flow by deriving an evolution equation for the additional stress tensor $\mathbf{C} := \int_D M \nabla_{\mathbf{q}} \frac{\psi}{M} \otimes \mathbf{q}$. In [14] the authors derived the following set of equations.

$$\begin{aligned} \rho(\phi) \partial_t \mathbf{u} + \left(\left(\rho(\phi) \mathbf{u} - m(\phi) \frac{\partial \rho}{\partial \phi} \nabla_x \mu_\phi \right) \cdot \nabla_x \right) \mathbf{u} - \operatorname{div}_x \{ 2\eta(\phi) \mathbf{D}\mathbf{u} \} + \nabla_x p \\ = \mu_\phi \nabla_x \phi + \mathcal{J}_\varepsilon \{ \beta(\phi) \} \nabla_x \omega + \operatorname{div}_x \{ \mathfrak{J}_\varepsilon \{ \mathbf{C} - \omega \mathbb{1} \} \}, \end{aligned} \quad (12.13a)$$

$$\operatorname{div}_x \mathbf{u} = 0, \quad (12.13b)$$

$$\partial_t \phi + \mathbf{u} \cdot \nabla_x \phi - \operatorname{div}_x \{ m(\phi) \nabla_x \mu_\phi \} = 0, \quad (12.13c)$$

$$\mu_\phi = -\delta \Delta_x \phi + \frac{1}{\delta} W'(\phi) + \beta'(\phi) \mathcal{J}_\varepsilon \{ \omega \}, \quad (12.13d)$$

$$\begin{aligned} \partial_t \mathbf{C} + (\mathbf{u} \cdot \nabla_x) \mathbf{C} - \nabla_x \mathcal{J}_\varepsilon \{ \mathbf{u} \} \mathbf{C} - \mathbf{C} (\nabla_x \mathcal{J}_\varepsilon \{ \mathbf{u} \})^T \\ = 2c_q \omega \mathbb{1} - 2c_q \mathbf{C} + c_x \Delta_x \mathbf{C} + c_x \operatorname{div}_x \{ \mathbf{C} \otimes \nabla_x \mathcal{J}_\varepsilon \{ \beta(\phi) \} \}, \end{aligned} \quad (12.13e)$$

$$\partial_t \omega + (\mathbf{u} \cdot \nabla_x) \omega - c_x \Delta_x \omega = c_x \operatorname{div}_x \{ \omega \nabla_x \mathcal{J}_\varepsilon \{ \beta(\phi) \} \}, \quad (12.13f)$$

on $\Omega \times \mathbb{R}^+$.

Model (12.13) seems to be the first two-phase model for visco-elastic polymeric flows which takes the density of the polymers in the different fluid phases and their impact on the rheology into account. This way, it may serve to model two-phase flow with Newtonian and visco-elastic phases, too. Conceptually, this approach is different from other methods found in the literature (see e.g. [30]).

To point out this difference, we rewrite (12.13e) in terms of $\mathbf{K} := \mathbf{C} - \omega \mathbb{1}$.

$$\begin{aligned} \partial_t \mathbf{K} + (\mathbf{u} \cdot \nabla_x) \mathbf{K} - \nabla_x \mathcal{J}_\varepsilon \{ \mathbf{u} \} \cdot \mathbf{K} - \mathbf{K} \cdot (\nabla_x \mathcal{J}_\varepsilon \{ \mathbf{u} \})^T - 2\omega \mathbf{D}\mathcal{J}_\varepsilon \{ \mathbf{u} \} \\ = -2c_q \mathbf{K} + c_x \Delta_x \mathbf{K} + c_x \operatorname{div}_x \{ \mathbf{K} \otimes \nabla_x \mathcal{J}_\varepsilon \{ \beta(\phi) \} \}. \end{aligned} \quad (12.14)$$

Denoting the upper convected time derivative, i.e. the first four terms in (12.14), by \mathbf{K}^* (cf. [4]), we obtain

$$\mathbf{K} + \frac{1}{2c_q} \mathbf{K}^* = \frac{\omega}{c_q} \mathbf{D}\mathcal{J}_\varepsilon \{ \mathbf{u} \}, \quad (12.15)$$

as evolution equation for \mathbf{K} after setting $c_x = 0$. I.e. the velocity field \mathbf{u} depends on an additional stress tensor \mathbf{K} in both fluids, but the back coupling of the velocity field depends on the number density of the fluids which may be chosen fluid-dependent. A different approach was used in [30]. Yue et al. used

$$\mathbf{K} + \lambda_H \mathbf{K}^* = 2\mu_P \mathbf{D}\mathbf{u} \quad (12.16)$$

with two constants λ_H and μ_P as an evolution equation for the additional stress tensor. As (12.16) is independent of the phase-field and the species concentration, they had to distinguish between the Newtonian and the non-Newtonian fluid by using $\frac{1}{2}(1 + \phi)\mathbf{K}$ on the right-hand side of (12.13a), i.e. they considered the

additional stress tensor only in the non-Newtonian fluid indicated by $\phi = 1$. In particular, the model in [30] does not allow for gradual changes in the rheology.

12.3 Existence of Solutions

One disadvantage of Hookean elasticity is well known—it permits arbitrarily large polymer elongations. Instead, one may use the FENE (*f*initely *e*xtensible, *n*onlinear *e*lastic) spring potential which reads

$$U(s) := -\frac{Q_{\max}^2}{2} \log \left(1 - \frac{2s}{Q_{\max}^2} \right). \tag{12.17}$$

In this case the critical polymer length of Q_{\max} may not be exceeded, i.e. $D = B(0, Q_{\max})$. Making appropriate assumptions, the existence of weak solutions to (12.10) was established in [14] for the case of equal mass densities and a constant mobility m .

To describe the regularity of these solutions, we introduce the weighted Lebesgue and Sobolev spaces

$$L^2(\Omega \times D; M^{-1}) := \left\{ \theta \in L^1_{\text{loc}}(\Omega \times D) : \int_{\Omega \times D} M^{-1} |\theta|^2 < \infty \right\}, \tag{12.18}$$

$$X := \left\{ \theta \in L^2(\Omega \times D; M^{-1}) : \int_{\Omega \times D} M |\nabla_{\mathbf{x}} \frac{\theta}{M}|^2 + \int_{\Omega \times D} M |\nabla_{\mathbf{q}} \frac{\theta}{M}|^2 < \infty \right\}, \tag{12.19}$$

$$X_+ := \{ \theta \in X : \theta(\mathbf{x}, \mathbf{q}) \geq 0 \text{ for a.e. } (\mathbf{x}, \mathbf{q}) \in \Omega \times D \}. \tag{12.20}$$

Furthermore, we denote the dual space of $H^1_{0,\text{div}}(\Omega) := \{ \mathbf{w} \in H^1_0(\Omega) : \text{div}_{\mathbf{x}} \mathbf{w} = 0 \}$ by $(H^1_{0,\text{div}}(\Omega))'$ and the associated dual pairing by $\langle \cdot, \cdot \rangle$. The following result was deduced in [14] by proving existence of solutions to a time discrete version of (12.10) and passing to the limit. For a detailed list of assumptions, we refer to [14].

Theorem 1 *Let $d \in \{2, 3\}$. Given initial data $(\phi_0, \mathbf{u}_0, \psi_0) \in H^2(\Omega) \times H^1_{0,\text{div}}(\Omega) \times L^2(\Omega \times D; M^{-1})$, there is a quadruple $(\phi, \mu, \mathbf{u}, \psi)$ which solves the equal-density version of system (12.10) combined with the boundary conditions (12.11) in the following weak sense.*

$$\int_{\Omega_T} (\phi_0 - \phi) \partial_t \theta - \int_{\Omega_T} \phi \mathbf{u} \cdot \nabla_{\mathbf{x}} \theta + \int_{\Omega_T} \nabla_{\mathbf{x}} \mu_{\phi} \cdot \nabla_{\mathbf{x}} \theta = 0$$

$$\forall \theta \in C^1([0, T]; H^1(\Omega)) \text{ with } \theta(\cdot, T) \equiv 0, \tag{12.21a}$$

$$\int_{\Omega_T} \mu_\phi \theta = \int_{\Omega_T} \delta \nabla_x \phi \cdot \nabla_x \theta + \int_{\Omega_T} \frac{1}{\delta} W'(\phi) \theta + \int_{\Omega_T} \beta'(\phi) \mathcal{J}_\varepsilon \left\{ \int_D \psi \right\} \theta$$

$$\forall \theta \in L^2(0, T; H^1(\Omega)), \quad (12.21b)$$

$$\int_0^T \langle \partial_t \mathbf{u}, \mathbf{w} \rangle + \int_{\Omega_T} (\mathbf{u} \cdot \nabla_x) \mathbf{u} \cdot \mathbf{w} + \int_{\Omega_T} 2\eta(\phi) \mathbf{D}\mathbf{u} : \mathbf{D}\mathbf{w}$$

$$= \int_{\Omega_T} \operatorname{div}_x \left\{ \tilde{\mathfrak{J}}_\varepsilon \left\{ \int_D \psi U' \mathbf{q} \otimes \mathbf{q} \right\} \right\} \cdot \mathbf{w} + \int_{\Omega_T} \mu_\phi \nabla_x \phi \cdot \mathbf{w}$$

$$+ \int_0^T \int_{\Omega \times D} \mathcal{J}_\varepsilon \{ \beta(\phi) \} \nabla_x \psi \cdot \mathbf{w}$$

$$\forall \mathbf{w} \in L^{4/(4-d)}(0, T; H_{0,\operatorname{div}}^1(\Omega)), \quad (12.21c)$$

$$\int_0^T \int_{\Omega \times D} (\psi_0 - \psi) \partial_t \frac{\theta}{M} + \int_0^T \int_{\Omega \times D} M \frac{\theta}{M} \mathbf{u} \cdot \nabla_x \frac{\psi}{M} - \int_0^T \int_{\Omega \times D} \psi (\nabla_x \mathbf{J}_\varepsilon \{ \mathbf{u} \} \cdot \mathbf{q}) \cdot \nabla_x \frac{\theta}{M}$$

$$+ c_q \int_0^T \int_{\Omega \times D} M \nabla_q \frac{\psi}{M} \cdot \nabla_q \frac{\theta}{M} + c_x \int_0^T \int_{\Omega \times D} M \nabla_x \frac{\psi}{M} \cdot \nabla_x \frac{\theta}{M}$$

$$+ c_x \int_0^T \int_{\Omega \times D} \psi \nabla_x \mathcal{J}_\varepsilon \{ \beta(\phi) \} \cdot \nabla_x \frac{\theta}{M} = 0$$

$$(12.21d)$$

for all θ such that $\frac{\theta}{M} \in C^1([0, T]; C^\infty(\overline{\Omega \times D}))$ and $\theta(\cdot, T) \equiv 0$. Moreover, the solution has the following regularity properties.

$$\mathbf{u} \in L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; H_{0,\operatorname{div}}^1(\Omega)) \cap W^{1,4/d}(0, T; (H_{0,\operatorname{div}}^1(\Omega))'), \quad (12.22a)$$

$$\phi \in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H^2(\Omega)), \quad (12.22b)$$

$$\mu_\phi \in L^2(0, T; H^1(\Omega)), \quad (12.22c)$$

$$\psi \in L^2(0, T; X_+) \cap L^\infty(0, T; L^2(\Omega \times D; M^{-1})), \quad (12.22d)$$

$$\omega := \int_D \psi(\cdot, \mathbf{q}) d\mathbf{q} \in L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega)), \quad (12.22e)$$

with $\omega \geq 0$ a.e. in Ω_T .

The above mentioned result relies on the mollification of certain terms to compensate for the little regularity for the configurational density ψ provided by the first stability result. For single-phase flow, this lack of regularity may also be overcome by using a cut-off operator in the \mathbf{q} -convective term, although revoking the cut-off

when passing to the limit is not an easy task and requires an L^∞ -bound on the marginal $\int_D \psi$ in space and time (cf. [5]). With a view to the numerical treatment of the system, the application of the mollifier also seems to be preferable, as by now the cut-off operator may not be revoked when passing to the limit simultaneously in space and time (cf. [6]).

Similar considerations apply to the convolution in the Henry energy. The strong nonlinear coupling between (12.10c) and (12.10e) requires some regularization. Without mollification, a s -Dirichlet integral might be introduced in the Cahn–Hilliard energy density (cf. [1, 12])—leading, however, to additional severe nonlinearities in the chemical potential.

12.4 Simulations Based on a Convergent Finite Element Scheme

A stable, fully discrete finite element scheme suitable for the numerical treatment of model (12.10) is proposed in [24]. Simulations based on this scheme are used for a qualitative validation of the presented model. Placing an elliptical shaped, non-Newtonian droplet ($\phi = 1$) with axes of length 1.3 and 0.7 and barycenter at $(0, 0)$ in a domain $(\Omega = (-1, 1)^2)$ filled with a Newtonian fluid ($\phi = -1$), we observe its oscillatory behaviour and compute the stresses induced by the additional stress tensor (see Fig. 12.1). As the polymer chains are initially assumed to be in equilibrium, i.e. their distribution on the configurational space $D = B(0, 10)$ is prescribed by the Maxwellian (i.e. $\psi_0(\mathbf{x}, \mathbf{q}) = \max\{0, \phi_0(\mathbf{x})\}3M(\mathbf{q})$), there are no additional stresses at the beginning of the simulation. The remaining physical parameters are listed below, where σ represents the surface tension and weights the Cahn–Hilliard energy.

$$\sigma \left| \delta \right| m \left| \rho(\pm 1) \right| \eta(\pm 1) \left| c_x \right| c_q \left| \beta(-1) \right| \beta(+1) \left| \varepsilon \right|$$

$$10 \left| 0.01 \right| 10^{-4} \left| 2 \right| 0.005 \left| 0.01 \right| 0.1 \left| 5 \right| 1 \left| 0.01 \right|$$

While the triangulation of Ω is adaptive and consists of simplices with diameters between approximately 0.0667 and 0.0083, the approximation of D is adapted to the Maxwellian and consists of simplices with diameters between approximately 3.5355 and 0.3115. Concerning the discretization in time, we decided for a fixed time increment $\tau = 10^{-4}$. For the discrete scheme and discretization related regularization parameters, we refer to [24] (in particular Sect. 4.3.1).

In the course of the simulation, the droplet tries to attain an energetically more preferable circular shape and thereby gives rise to velocity fields. As these velocity fields induce deviations in the configurational distribution of the polymers, additional stresses arise. To visualize those stresses, we computed the eigenvalues and eigenvectors of the stress tensor on every simplex of the triangulation and depicted the eigenvector to the largest positive, real eigenvalue as a yellow line in Fig. 12.1. In comparison to its initial state, the droplet is stretched vertically and therefore the eigenvectors also point mainly in vertical direction.

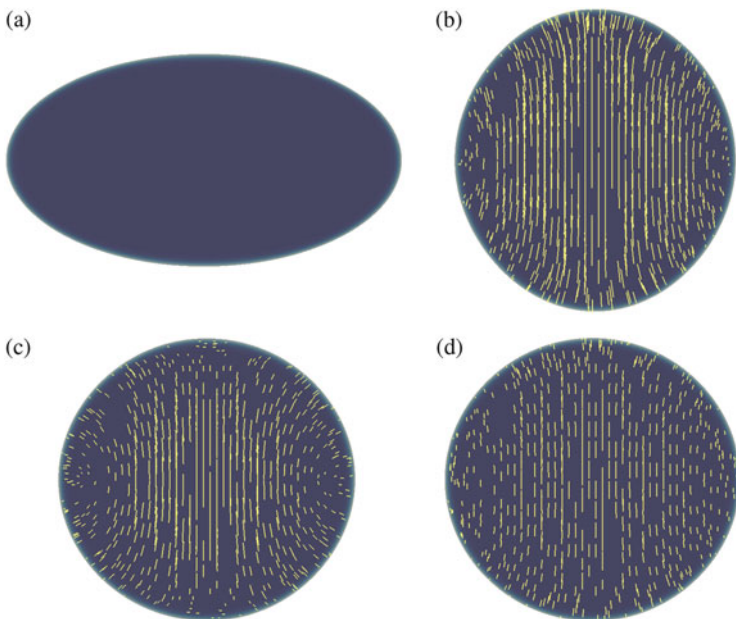


Fig. 12.1 Evolution of a non-Newtonian droplet. (a) $t = 0.0$. (b) $t = 0.2$. (c) $t = 1.0$. (d) $t = 2.0$

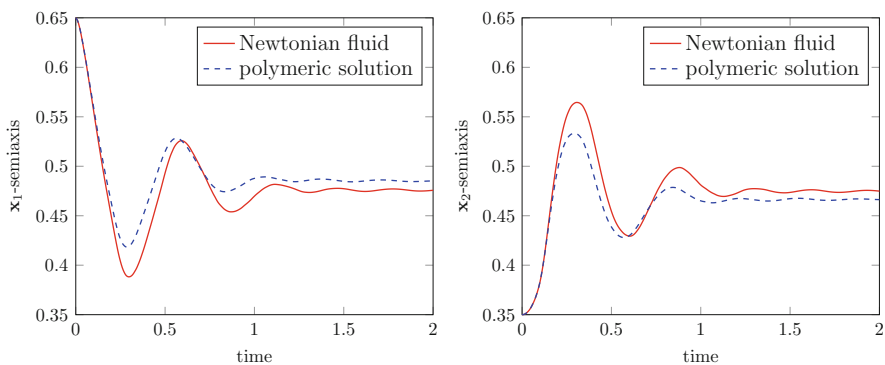


Fig. 12.2 Length of the semi-axes of oscillating droplets

To compare the oscillatory behaviour of a Newtonian and a non-Newtonian droplet, we measured and plotted the length of the x_1 - and x_2 -semi-axes of the droplets (see Fig. 12.2). When comparing the evolution of the axes' length, two phenomena are noticeable. First, the damping of the oscillation is asymmetric for the non-Newtonian droplet. In comparison to the axes of the Newtonian droplet, the maximal elongation of the vertical axis is smaller, while the horizontal axis reaches

almost the same length in the ensuing oscillation as the one of the Newtonian droplet. Secondly, the shape of the non-Newtonian droplet is not completely circular at the end of the simulation, as the stresses induced by the deformation of the polymer chains are not completely released (cf. Fig. 12.1d).

Details on the scheme and the implementation, as well as the proof of stability can be found in [24]. Given fluids with equal mass densities, the convergence of discrete solutions towards solutions of a continuous weak formulation, which is comparable to the one in Theorem 1, is also proven in [24].

References

1. Abels, H.: Existence of weak solutions for a diffuse interface model for viscous incompressible fluids with general densities. *Commun. Math. Phys.* **289**(1), 45–73 (2009)
2. Abels, H., Garcke, H., Grün, G.: Thermodynamically consistent, frame indifferent diffuse interface models for incompressible two-phase flows with different densities. *Math. Models Methods Appl. Sci.* **22**(3), 1150013 (2012)
3. Barrett, J.W., Schwab, C., Süli, E.: Existence of global weak solutions for some polymeric flow models. *Math. Models Methods Appl. Sci.* **15**, 939–983 (2005)
4. Barrett, J.W., Süli, E.: Existence of global weak solutions to some regularized kinetic models for dilute polymers. *Multiscale Model. Simul.* **6**, 506–546 (2007)
5. Barrett, J.W., Süli, E.: Existence and equilibration of global weak solutions to kinetic models for dilute polymers I: Finitely extensible nonlinear bead-spring chains. *Math. Models Methods Appl. Sci.* **21**, 1211–1289 (2011)
6. Barrett, J.W., Süli, E.: Finite element approximation of finitely extensible nonlinear elastic dumbbell models for dilute polymers. *ESAIM: Math. Modell. Numer. Anal.* **46**, 949–978 (2012)
7. Bird, R.B., Curtiss, C.F.: Molecular theory expressions for the stress tensor in flowing polymeric liquids. *J. Polymer Sci.: Polym. Symp.* **73**, 187–199 (1985)
8. Campillo-Funollet, E., Grün, G., Klingbeil, F.: On modeling and simulation of electrokinetic phenomena in two-phase flow with general mass densities. *SIAM J. Appl. Math.* **72**(6), 1899–1925 (2012)
9. Constantin, P.: Nonlinear Fokker–Planck Navier–Stokes systems. *Commun. Math. Sci.* **3**(4), 531–544 (2005)
10. Ding, H., Spelt, P.D.M., Shu, C.: Diffuse interface model for incompressible two-phase flows with large density ratios. *J. Comput. Phys.* **226**, 2078–2095 (2007)
11. E, W., Li, T., Zhang, P.-W.: Well-posedness for the dumbbell model of polymeric fluids. *Commun. Math. Phys.* **248**(2), 409–427 (2004). MR2073140 (2005d:35210)
12. Fontelos, M.A., Grün, G., Jörres, S.: On a phase-field model for electrowetting and other electrokinetic phenomena. *SIAM J. Math. Anal.* **43**(1), 527–563 (2011)
13. Griebel, M., Rüttgers, A.: Multiscale simulations of three-dimensional viscoelastic flows in a square-square contraction. *J. Non-Newtonian Fluid Mech.* **205**, 41–63 (2014)
14. Grün, G., Metzger, S.: On micro-macro-models for two-phase flow with dilute polymeric solutions – modeling and analysis. *Math. Models Methods Appl. Sci.* **26**(05), 823–866 (2016)
15. Jourdain, B., Lelièvre, T., Le Bris, C.: Existence of solution for a micro–macro model of polymeric fluid: the FENE model. *J. Funct. Anal.* **209**(1), 162–193 (2004)
16. Kramers, H.A.: Het gedrag van macromoleculen in een stroomende vloeistof. *Physica* **11**, 1–19 (1944)

17. Le Bris, C., Lelièvre, T.: Multiscale modelling of complex fluids: a mathematical initiation. In: Engquist, B., Lötstedt, P., Runborg, O. (eds.) *Multiscale Modeling and Simulation in Science. Lecture Notes in Computational Science and Engineering*, vol. 66, pp. 49–137. Springer, Berlin (2009)
18. Le Bris, C., Lelièvre, T.: Micro-macro models for viscoelastic fluids: modelling, mathematics and numerics. *Sci. China Math.* **55**(2), 353–384 (2012)
19. Li, T., Zhang, H., Zhang, P.-W.: Local existence for the dumbbell model of polymeric fluids. *Commun. Partial Differ. Equ.* **29**(5–6), 903–923 (2004)
20. Lions, P.L., Masmoudi, N.: Global existence of weak solutions to some micro-macro models. *C. R. Math. Acad. Sci. Paris* **345**(1), 15–20 (2007)
21. Lowengrub, J., Truskinovsky, L.: Quasi-incompressible Cahn–Hilliard fluids and topological transitions. *Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci.* **454**(1978), 2617–2654 (1998)
22. Masmoudi, N.: Well-posedness for the fene dumbbell model of polymeric flows. *Commun. Pure Appl. Math.* **61**(12), 1685–1714 (2008)
23. Masmoudi, N.: Global existence of weak solutions to the FENE dumbbell model of polymeric flows. *Invent. Math.* **191**(2), 427–500 (2013)
24. Metzger, S.: Diffuse interface models for complex flow scenarios: modeling, analysis, and simulation. Ph.D. thesis, Friedrich-Alexander-Universität Erlangen-Nürnberg (2017)
25. Nitta, K.: A graph-theoretical approach to statistics and dynamics of tree-like molecules. *J. Math. Chem.* **25**(2), 133–143 (1999)
26. Onsager, L.: Reciprocal relations in irreversible processes. II. *Phys. Rev.* **38**(12), 2265–2279 (1931)
27. Otto, F., Tzavaras, A.: Continuity of velocity gradients in suspensions of rod-like molecules. *Commun. Math. Phys.* **277**(3), 729–758 (2008) (English)
28. Qian, T., Wang, X.-P., Sheng, P.: A variational approach to the moving contact line hydrodynamics. *J. Fluid Mech.* **564**, 333–360 (2006)
29. Renardy, M.: An existence theorem for model equations resulting from kinetic theories of polymer solutions. *SIAM J. Math. Anal.* **22**(2), 313–327 (1991)
30. Yue, P., Feng, J.J., Liu, C., Shen, J.: A diffuse-interface method for simulating two-phase flows of complex fluids. *J. Fluid Mech* **515**, 293–317 (2004)
31. Zhang, H., Zhang, P.-W.: Local existence for the fene-dumbbell model of polymeric fluids. *Arch. Ration. Mech. Anal.* **181**(2), 373–400 (2006)