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On the use of a diffuse-interface model for the simulation of rigid particles in two-phase Newtonian and viscoelastic fluids

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Abstract

For the simulation of particles in two-phase flows, the diffuse-interface model is frequently employed to describe the fluid-fluid interface. The diffuse-interface model can naturally handle moving contact lines and topological changes, but the thickness of the interface is in general chosen larger than the physical one. We systematically investigated the effect of both the interface thickness and the diffusion of the fluids on the motion of rigid particles in two-phase flows, using a diffuse-interface model for the fluid-fluid interface. A sharp-interface model is considered for the fluid-fluid interface as well, which is expected to behave as the limiting case of the interface thickness going to zero.

The first case that was investigated is a spherical particle in a closed cylindrical container filled with two Newtonian fluids, where the particle is moved toward the fluid-fluid interface by a force. The second case that was investigated is that of the migration of a rigid particle in a two-phase viscoelastic shear flow. The migration of the particle is due a contrast in the viscoelastic properties of the fluids, a phenomenon that was not reported before in the literature. For both cases, the results for the diffuse-interface model converge to the sharp-interface model when the interface thickness is decreased. However, it is shown that both the interface thickness and the diffusion of the fluids play crucial roles in the resulting dynamics of a particle interacting with a diffuse fluid-fluid interface.

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1 Introduction

Particles at interfaces are important in a large number of industrial, biological and natural processes. An example is the so-called Pickering emulsion, where dispersed droplets of one fluid inside a matrix of a second fluid are prevented from coalescence by particles at the fluid-fluid interface [1]. A crucial step in manufacturing Pickering emulsions, is the adsorption of the particles at the fluid-fluid interface. Although the problem of a rigid particle interacting with a fluid-interface has been studied before [2–8], the exact mechanism of particle adsorption and the role of the moving contact line remains unclear.

Modeling offers a valuable tool in the analysis of particles at interfaces, but the large range of length scales that needs to be resolved is challenging. The macroscopic length scale, the particle size and the molecular scale of the fluid-fluid interface should be modeled appropriately. The length over which the transition from one fluid to the other fluid takes place will be referred to as the interface thickness, which is typically of the order of 1 nm for small molecular fluids [9], but can be larger for macromolecular fluids and/or at elevated temperatures [10, 11]. If the interface thickness is small compared to the particle size, a good approximation is to regard the interface as an infinitely thin “membrane”. In this classical fluid mechanics approach, employed by e.g. Young, Laplace and Gauss [12, 13], the effect of the interfacial tension is imposed as a boundary condition. We will refer to this model as the sharp-interface model. The sharp-interface model, combined with a sharp particle boundary, was used in [4–6] to study particles at or close to fluid-fluid interfaces. An alternative approach is to assume a diffuse fluid-fluid interface and a sharp particle boundary [14–17]. A third approach is to model both the fluid-fluid interface and the particle boundary as diffuse [18].

The combination of the diffuse-interface model for the fluid-fluid interface and the sharp-interface model for the particle boundary circumvents the stress singularity of a sharp interface in contact with a solid, which leads to an infinite force needed to submerge a floating object [19]. However, the ratio of the interface thickness to the particle size is often chosen larger than the physical value, due to the intractable difference in length-scales (the ratio can be as small as 10^{-6} for a particle size of 1 mm and interface thickness of 1 nm). In this paper, we present simulations of non-Brownian particles interacting with fluid-fluid interfaces. The particle boundary is assumed to be sharp, and a diffuse-interface model is used for the fluid-

fluid interface. A sharp-interface model is employed for the fluid-fluid interface as well, which is used as a limiting case of the interface thickness going to zero. The influence of the interface thickness and diffusion of the fluids on the motion and adsorption of the particle is systematically investigated. The analysis is carried out for two cases: 1) a particle in a closed cylindrical container containing two Newtonian fluids, and 2) a particle in a two-phase shear flow, where one of the fluids is viscoelastic. In the first case, the particle is moved toward the interface by a force. In the second case, the particle migrates toward the interface due to a contrast in viscoelastic properties of the fluids, a mechanism for particle migration that was not reported before in the literature.

2 Modeling fluid-fluid interfaces

2.1 The sharp-interface model

In the sharp-interface model, the interface is a surface “membrane”, which will be denoted by A . The coordinates of the interface, denoted by $\mathbf{x}$, are described using a moving curvilinear coordinate system [20]:

$$\mathbf{x} = \bar{\mathbf{x}}(\underline{\chi}, t), \quad (1)$$

where $\underline{\chi} = (\chi^1, \chi^2)$ are curvilinear coordinates and $\bar{\mathbf{x}}$ is the time-dependent function that maps the curvilinear coordinates on the spatial coordinates $\mathbf{x}$. The motion of the interface is described through [21]:

$$\dot{\mathbf{x}} = \left. \frac{\partial \bar{\mathbf{x}}}{\partial t} \right|_{\underline{\chi}}, \quad (2)$$

where $\underline{\chi}$ is kept constant. Using a Lagrangian description of the interface motion, the interface will be convected by the fluid velocity $\mathbf{u}$:

$$\dot{\mathbf{x}} = \mathbf{u}. \quad (3)$$

However, in the sharp-interface model only the convection normal to the interface needs to be taken into account [21]:

$$\dot{\mathbf{x}} \cdot \mathbf{n} = \mathbf{u} \cdot \mathbf{n}, \quad (4)$$

where $\mathbf{n}$ is the unit normal vector to the interface. From a computational point of view, updating only the normal component has the advantage that the interface is steady if the motion is purely tangential, e.g. a tank-treading droplet in a shear flow [20]. Furthermore, an arbitrary tangential velocity can be added to the velocity on the interface, while still satisfying Eq. (4). A possible use of this tangential velocity is to move nodes on the interface, such that the elements on the interface are evenly distributed [20, 22]. However, we will use the tangential velocity to keep the horizontal coordinates of the end-points of the interface fixed in the problem of a particle in shear flow, as will be explained in Section 5.4.

The capillary stress tensor in the sharp-interface model can be described by a tension parallel to the interface, which can be written as [23]:

$$\boldsymbol{\tau}_{\text{si}} = \sigma (\mathbf{I} - \mathbf{n}\mathbf{n}) \delta(n), \quad (5)$$

where σ is the (constant) surface tension, $\mathbf{I}$ is the unit tensor and $\delta(n)$ is the delta function (with unit 1/length) with n the coordinate perpendicular to the interface. An alternative expression for $\boldsymbol{\tau}_{\text{si}}$ is used in the literature (e.g. [24]), by taking the deviatoric part of $\boldsymbol{\tau}_{\text{si}}$ as defined in Eq. (5), and absorbing the isotropic part in the pressure, which yields zero stress for spherical drops [25].

2.2 The diffuse-interface model

Cahn and Hilliard [26] hypothesized that the Helmholtz free energy density f of a two-phase fluid is a function of the local composition ϕ and the composition of the immediate surroundings, included through gradients of the composition [27]:

$$f(\phi, \nabla\phi) = f_0(\phi) + \frac{\kappa}{2} |\nabla\phi|^2, \quad (6)$$

where $f_0(\phi)$ is a double-well function and κ is the gradient energy parameter. In this paper, the double-well function is described by

$$f_0(\phi) = -\frac{1}{2}\alpha\phi^2 + \frac{1}{4}\beta\phi^4 \quad (7)$$

where α and β are constants that can be used to control the shape of the double-well function. The free energy of such a system can be lowered by a diffusive flux of ϕ toward areas of lower chemical potential μ . This leads to the Cahn-Hilliard equation, which describes the evolution of ϕ and is given by [12]:

$$\frac{D\phi}{Dt} = \nabla \cdot (M \nabla \mu), \quad (8)$$

where $D(\cdot)/Dt$ is the material derivative, M is the constant Cahn-Hilliard mobility and the chemical potential is given by definition as

$$\mu = \frac{\delta f}{\delta \phi} = -\alpha\phi + \beta\phi^3 - \kappa \nabla^2 \phi, \quad (9)$$

where $\delta(\cdot)/\delta\phi$ denotes the variational derivative to ϕ . For a planar interface in equilibrium, Eqs. (8) and (9) can be solved analytically, which yields the solution [26]:

$$\phi(x) = \phi_B \tanh\left(\frac{x}{\sqrt{2}\xi}\right), \quad (10)$$

where $\phi_B = \sqrt{\alpha/\beta}$ is the bulk value of the composition and $\xi = \sqrt{\kappa/\alpha}$ is the interface thickness. The planar interface in equilibrium is endowed with an interfacial energy [13]:

$$\sigma^* = \int_{-\infty}^{\infty} \kappa \left(\frac{d\phi}{dx} \right)^2 dx = \frac{2\sqrt{2}}{3} \frac{\kappa \phi_B^2}{\xi}. \quad (11)$$

To determine the Cahn-Hilliard parameters, we first set $\alpha = \beta$, from which follows $\phi_B = \pm 1$. Then, for desired values of ξ and σ^* , the values of κ and α are chosen such that Eqs. (10) and (11) are satisfied. In this paper, we will set the Cahn-Hilliard interfacial energy σ^* equal to σ , but is important to note that the interfacial energy in the diffuse-interface model is in general not constant because flow can move the composition profile away from the equilibrium profile as given in Eq. (10).

Due to the $\nabla\phi$ terms in the free energy, there will be a contribution to the stress tensor of the form [28]:

$$\boldsymbol{\tau}_{\text{di}} = \kappa (|\nabla\phi|^2 \mathbf{I} - \nabla\phi \nabla\phi), \quad (12)$$

where an isotropic term was added to $\boldsymbol{\tau}_{\text{di}}$ to ensure the capillary stress is parallel to the interface [29, 30]. When ξ approaches zero, the diffuse-interface model converges to the sharp-interface

model [31]. This can be shown for a planar interface ($\phi = \phi(x)$) in 3D space: the non-zero components of $\boldsymbol{\tau}_{\text{di}}$ are the yy - and zz -component, which are parallel to the interface and are written as $(\tau_{\text{di}})_{yy} = (\tau_{\text{di}})_{zz} = \kappa(d\phi/dx)^2$. In the limit of ξ goes to zero, these components can be written as:

$$\kappa \left(\frac{d\phi}{dx} \right)^2 = \frac{1}{2} \frac{\kappa \phi_{\text{B}}^2}{\xi^2} \text{sech}^4 \left(\frac{x}{\sqrt{2}\xi} \right) = \frac{2\sqrt{2}}{3} \frac{\kappa \phi_{\text{B}}^2}{\xi} \delta(x) = \sigma^* \delta(x). \quad (13)$$

In the second equal sign in Eq. (13) the following relation was used [32]:

$$\lim_{\xi \rightarrow 0} \left[\frac{3}{4\sqrt{2}\xi} \text{sech}^4 \left(\frac{x}{\sqrt{2}\xi} \right) \right] = \delta(x). \quad (14)$$

Thus, in the limit of ξ goes to zero, the surface tension is concentrated in an infinitely thin surface and is directed parallel to this surface. It is interesting to note the equivalence of $\boldsymbol{\tau}_{\text{si}}$ as defined in Eq. (5) and $\boldsymbol{\tau}_{\text{di}}$ as defined in in Eq. (12), which become equal as ξ goes to zero, but it should be emphasized that this is only valid for a planar interface in equilibrium. For curved interfaces, there is an error in the interfacial tension of the order of the interface thickness squared times the curvature [33]. Furthermore, flow can compress or dilute the tanh profile of ϕ , which can locally change the interfacial tension [28, 33].

We conclude this section by remarking that there are many variants of the diffuse-interface model available in the literature. Especially the case of varying densities and phase-dependent mobility has received considerable attention [34–37]. For simplicity in the analysis presented in this work, we assume equal densities of the fluids and a constant mobility.

3 Governing equations

It is assumed that inertia can be neglected, which is in general the case for highly viscous polymeric fluids. We furthermore assume that the fluids are incompressible and density-matched. This yields the balance of momentum and mass written as:

$$\begin{aligned} -\nabla \cdot \boldsymbol{\sigma} &= \mathbf{0}, \\ \nabla \cdot \mathbf{u} &= 0, \end{aligned} \quad (15)$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor. When using the sharp-interface model, the Cauchy stress tensor can be written as

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\eta\mathbf{D} + \boldsymbol{\tau}_p + \boldsymbol{\tau}_{\text{si}}, \quad (16)$$

where p is the pressure, η is a Newtonian viscosity, $\mathbf{D} = (\nabla\mathbf{u} + (\nabla\mathbf{u})^T)/2$ is the rate of deformation tensor, $\boldsymbol{\tau}_p$ is the viscoelastic (polymer) stress tensor and $\boldsymbol{\tau}_{\text{si}}$ is the sharp-interface stress as given in Eq. (5). In the viscoelastic fluid, the Newtonian fluid assumes the role of a solvent. When using the diffuse-interface model, the Cauchy stress tensor is written as

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\eta\mathbf{D} + \boldsymbol{\tau}_p + \boldsymbol{\tau}_{\text{di}}, \quad (17)$$

where $\boldsymbol{\tau}_{\text{di}}$ is the diffuse-interface stress as given in Eq. (12).

In the sharp-interface model, the two fluids form two distinct domains and $\boldsymbol{\sigma}$ can be defined for each fluid separately. This makes it straightforward to assign different material parameters to each fluid. In the diffuse-interface model, different material parameters for each fluid can be obtained by making the material parameters a function of ϕ , e.g. by using a linear mixing rule. For example, the viscosity is given by

$$\eta(\phi) = \eta_1 \frac{\phi + 1}{2} + \eta_2 \frac{1 - \phi}{2}. \quad (18)$$

where η_1 is the viscosity for the fluid where $\phi = 1$ and η_2 is the viscosity for the fluid where $\phi = -1$. Note, that in the diffuse-interface model, the value for ϕ can attain unphysical values of $\phi > 1$ or $\phi < -1$, as explained in [38]. To avoid unphysical values for the viscosity, in those cases we manually set ϕ to 1 or -1 , respectively, for defining the viscosity $\eta(\phi)$.

3.1 Viscoelastic stress

The viscoelastic stress is described using the Giesekus constitutive equation, which is written in the conformation tensor form:

$$\boldsymbol{\tau}_p = G(\mathbf{c} - \mathbf{I}), \quad (19)$$

where G is the modulus and $\mathbf{c}$ is the conformation tensor. The evolution of $\mathbf{c}$ is described by

$$\lambda \overset{\nabla}{\mathbf{c}} + \mathbf{c} - \mathbf{I} + \alpha(\mathbf{c} - \mathbf{I})^2 = \mathbf{0}, \quad (20)$$

where λ is the relaxation time and α is the Giesekus mobility, which controls the shear thinning behavior of the fluid. Furthermore, $\overset{\nabla}{(\cdot)}$ denotes the upper-convected derivative, which is defined by

$$\overset{\nabla}{(\cdot)} = \frac{D(\cdot)}{Dt} - (\nabla \mathbf{u})^T \cdot (\cdot) - (\cdot) \cdot \nabla \mathbf{u}. \quad (21)$$

The polymer viscosity η_p is related to the modulus and relaxation time through $\lambda = \eta_p/G$.

Again, making one or both of the fluids viscoelastic in the sharp-interface model is straightforward, since the fluids form two distinct domains. To make one of the two fluids viscoelastic in the diffuse-interface model, we can define a modulus that is dependent on ϕ , where we again use a linear mixing rule:

$$G(\phi) = G_1 \frac{\phi + 1}{2} + G_2 \frac{1 - \phi}{2}, \quad (22)$$

where G_1 is the modulus for the fluid where $\phi = 1$ and G_2 is the modulus for the fluid where $\phi = -1$. This approach can be interpreted as a linear change of the polymer density with ϕ across the interface [28].

3.2 Motion of the particle

For the fluid-fluid interface, both a sharp-interface and a diffuse-interface model are employed in this paper. In both approaches, the interface between the particle and the fluids is modeled as a sharp interface. Furthermore, it is assumed that the inertia of the particle can be neglected, which yields a balance of forces and torques on the particle:

$$\int_{\partial P} \boldsymbol{\sigma} \cdot \mathbf{n}_p dS = \mathbf{F}, \quad (23)$$

$$\int_{\partial P} (\mathbf{x} - \mathbf{X}) \times (\boldsymbol{\sigma} \cdot \mathbf{n}_p) dS = \mathbf{0}, \quad (24)$$

where $\mathbf{n}_p$ is the outwardly directed unit normal vector on the particle boundary ∂P , $\mathbf{X}$ denotes the location of the center point of the particle and $\mathbf{F}$ is an external force acting on the particle. Furthermore, $\boldsymbol{\sigma}$ is evaluated on the “fluid side” of the boundary ∂P . Lastly, a kinematic

equation yields the relation between the particle position and velocity:

$$\frac{d\mathbf{X}}{dt} = \mathbf{U}. \quad (25)$$

Due to the particle being circular or spherical, the rotation angle of the particle is not needed.

4 Boundary and initial conditions

In this section, the cases treated in this paper, and their boundary and initial conditions, are defined. It is assumed that if the fluid-fluid interface comes into contact with a solid boundary, the contact angle is 90° : the solid boundaries are wetted equally by the fluids.

4.1 Case 1

Case 1 is an axisymmetric problem of a spherical particle in a closed, cylindrical container containing two Newtonian fluids with matched viscosities. The particle is moved toward the fluid-fluid interface by a force $\mathbf{F}$, which is directed along the axis of the cylinder (see Fig 1). The axial coordinate is given by z and the radial coordinate by r , using the convention $[z, r]$. The particle location is denoted by $\mathbf{X} = [Z, 0]$, the force acting on the particle by $\mathbf{F} = [F, 0]$ and the particle translational velocity by $\mathbf{U} = [U, 0]$.

4.1.1 Sharp-interface model for case 1

When using the sharp-interface model for case 1, the boundary conditions for the velocity are given by:

$$\mathbf{u} = \mathbf{0} \quad \text{on } \Gamma_1 \text{ and } \Gamma_3 \quad (26)$$

$$u_z = U \quad \text{on } \partial P. \quad (27)$$

Furthermore, the radial velocity is set to zero on the symmetry line, the particle boundary and on the side of the cylinder:

$$u_r = 0 \quad \text{on } r = 0, \partial P \text{ and } \Gamma_2. \quad (28)$$

Fig. 1: Case 1 is a spherical particle in a closed cylinder.

The fluid-fluid interface A makes contact with the side of the cylinder. The combination of a no-slip condition with the sharp-interface model would fix the contact point on the wall, yielding large deformations of the interface and unphysical results. To circumvent this problem, perfect slip is assumed on the side of the cylinder:

$$\sigma_{zr} = 0 \quad \text{on } \Gamma_2. \quad (29)$$

The boundary conditions on A are given by the continuity of the velocity and traction (taking the pressure jump due to the curvature of the interface into account):

$$\mathbf{u}|_1 = \mathbf{u}|_2, \quad (30)$$

$$(\boldsymbol{\sigma} \cdot \mathbf{n})|_1 - (\boldsymbol{\sigma} \cdot \mathbf{n})|_2 = \sigma \mathbf{n} \nabla \cdot \mathbf{n}, \quad (31)$$

where the notation $|_i$ means the term is evaluated on the side of the interface of fluid i . Initial conditions are needed for the particle location and interface position, which are given by

$$\mathbf{X}(t = 0) = \mathbf{X}_0, \quad (32)$$

$$\mathbf{x}(t = 0) = \mathbf{x}_0. \quad (33)$$

4.1.2 Diffuse-interface model for case 1

For the diffuse-interface model, the boundary conditions for the velocity are similar to Eqs. (26–29). Note, that the perfect-slip condition on Γ_2 is not strictly needed since the diffuse interface can move through diffusion, but for comparison to the sharp-interface model we impose it here as well. Boundary conditions are needed for ϕ and μ . Assuming a 90° contact angle of the fluid-fluid interface with the rigid boundaries and zero diffusive flux of ϕ across the boundaries yields:

$$\frac{\partial \phi}{\partial n} = 0 \quad \text{and} \quad \frac{\partial \mu}{\partial n} = 0 \quad \text{on } \Gamma_1, \Gamma_2, \Gamma_3 \text{ and } \partial P, \quad (34)$$

where $\partial()/\partial n$ is the directional derivative normal to the boundary.

Initial conditions are needed for the particle position and the ϕ -field. For the initial particle position we use Eq. (32). The initial ϕ -field is given by the planar equilibrium composition given in Eq. (10), where we make sure that the location of the interface (defined by $\phi_0 = 0$) coincides with the location of the sharp interface $\mathbf{x}_0$.

4.2 Case 2

The second problem is a circular particle in a two-phase shear flow (with the average shear rate given by $\dot{\gamma} = 2U_w/H$), where the bottom fluid is viscoelastic, whereas the top fluid is Newtonian (see Fig. 2). Periodicity is assumed in x -direction. Initially, the particle is located in the viscoelastic fluid, and its vertical migration is investigated. The particle location is denoted by $\mathbf{X} = [X, Y]$ and its translational velocity by $\mathbf{U} = [U_x, U_y]$. For case 2, no external force is placed on the particle: $\mathbf{F} = \mathbf{0}$.

Fig. 2: Case 2 is a circular particle in a two-phase shear flow.

4.2.1 Sharp-interface model for case 2

When using the sharp-interface model for case 2, the boundary conditions due to no-slip on the particle boundary and rigid walls and periodicity of the velocity and traction are given by:

$$\mathbf{u} = [-U_w, 0] \quad \text{on } \Gamma_1, \quad (35)$$

$$\mathbf{u} = [U_w, 0] \quad \text{on } \Gamma_3, \quad (36)$$

$$\mathbf{u} = \mathbf{U} + \boldsymbol{\omega} \times (\mathbf{x} - \mathbf{X}) \quad \text{on } \partial P, \quad (37)$$

$$(\mathbf{u})_{\Gamma_2} = (\mathbf{u})_{\Gamma_4}, \quad (38)$$

$$(\mathbf{t})_{\Gamma_2} = -(\mathbf{t})_{\Gamma_4}, \quad (39)$$

where $\mathbf{t} = \boldsymbol{\sigma} \cdot \mathbf{m}$ is the traction vector on the outer boundary of the domain, where $\mathbf{m}$ is the outwardly directed unit normal vector on the outer boundary.

The boundary conditions on A are given by the continuity of the velocity and traction

(taking the pressure jump due to the curvature of the interface into account).

$$\mathbf{u}|_1 = \mathbf{u}|_2, \quad (40)$$

$$(\boldsymbol{\sigma} \cdot \mathbf{n})|_1 - (\boldsymbol{\sigma} \cdot \mathbf{n})|_2 = \sigma \mathbf{n} \nabla \cdot \mathbf{n}. \quad (41)$$

The interface is not in contact with a solid boundary, and will remain so due to the assumption of a sharp interface. Furthermore, periodicity yields the following boundary conditions for the conformation tensor:

$$(\mathbf{c})_{\Gamma_2} = (\mathbf{c})_{\Gamma_4}. \quad (42)$$

The initial conditions for the particle location and interface position are again denoted by

$$\begin{aligned} \mathbf{X}(t=0) &= \mathbf{X}_0, \\ \mathbf{x}(t=0) &= \mathbf{x}_0. \end{aligned} \quad (43)$$

In addition, an initial conformation tensor needs to be defined, denoted by

$$\mathbf{c}(t=0) = \mathbf{c}_0, \quad (44)$$

which is set to $\mathbf{c}_0 = \mathbf{I}$, which effectively means that the initial viscoelastic stress is zero.

4.2.2 Diffuse-interface model for case 2

For the diffuse-interface model, the boundary conditions for the velocity, traction and conformation tensor are similar to the ones given for the sharp-interface model. The boundary conditions for ϕ and μ follow again from the assumption of a 90° contact angle of the fluid-fluid interface with the solid boundaries and zero flux of ϕ across the boundaries (Eq. (34)). Furthermore, periodicity in x -direction yields:

$$(\phi)_{\Gamma_2} = (\phi)_{\Gamma_4}, \quad (45)$$

$$(\mu)_{\Gamma_2} = (\mu)_{\Gamma_4}. \quad (46)$$

The initial ϕ -field is given by the planar equilibrium composition given in Eq. (10), where we make sure that the location of the interface (defined by $\phi_0 = 0$) coincides with the location of the sharp interface $\mathbf{x}_0$.

5 Numerical method

In this section, we will first present the weak forms of the system of equations for both the sharp-interface model and the diffuse-interface model. Note, that the weak forms are different for the two cases simulated in this paper, with the main difference being how the velocity of the particle is taken into account. We will give the weak forms for case 2, for which the unknown particle velocity is denoted by $\mathbf{U}$ and the unknown angular velocity by $\boldsymbol{\omega}$. For case 1, the weak forms are similar, but the unknown particle velocity is a scalar U and there is no angular velocity. In both the diffuse-interface and sharp-interface model, the motion of the particle is included as a constraint, using the combined equation of motion approach. In this approach, the particle translational and angular velocities are solved as additional unknowns, such that Eqs. (23) and (24) are satisfied [39]. This yields a Lagrange multiplier on the particle boundary denoted by $\boldsymbol{\lambda}$. In the second part of this section, we will explain the time-integration employed for these systems. It should be noted that the diffuse-interface equations are solved implicitly for $\mathbf{u}$, p , ϕ and μ in one system, greatly enhancing stability [40]. For the sharp-interface model, implementing an implicit scheme is not trivial, and thus a semi-implicit approach is taken.

5.1 Weak form sharp-interface model

For the sharp-interface model, the weak form of the balance of momentum and mass is written as: find $\mathbf{u}$, p , $\mathbf{U}$, $\boldsymbol{\omega}$ and $\boldsymbol{\lambda}$ such that

$$(\mathbf{D}_v, 2\eta\mathbf{D} + \boldsymbol{\tau}_p) - (\nabla \cdot \mathbf{v}, p) + \langle \mathbf{v} - (\mathbf{V} + \boldsymbol{\chi} \times (\mathbf{x} - \mathbf{X}), \boldsymbol{\lambda}) \rangle_{\partial P} + \int_A (\nabla \mathbf{v})^T : \sigma(\mathbf{I} - \mathbf{n}\mathbf{n}) dS = 0, \quad (47)$$

$$(q, \nabla \cdot \mathbf{u}) = 0, \quad (48)$$

$$\langle \boldsymbol{\mu}, \mathbf{u} - (\mathbf{U} + \boldsymbol{\omega} \times (\mathbf{x} - \mathbf{X})) \rangle_{\partial P} = 0, \quad (49)$$

for all admissible test functions $\mathbf{v}$, q , $\mathbf{V}$, $\boldsymbol{\chi}$, and $\boldsymbol{\mu}$. Furthermore, $\mathbf{D}_v = (\nabla \mathbf{v} + (\nabla \mathbf{v})^T)/2$, $(\cdot, \cdot)$ is a proper inner product on Ω and $\langle \cdot, \cdot \rangle_{\partial P}$ is an inner product on ∂P , which will be defined later in this section. The last term on the left hand side of Eq. (47) is derived as follows:

$$\begin{aligned}
- \int_{\Omega} \mathbf{v} \cdot \nabla \cdot (\sigma(\mathbf{I} - \mathbf{n}\mathbf{n})\delta(n)) dV = \\
\int_{\Omega} (\nabla \mathbf{v})^T : \sigma(\mathbf{I} - \mathbf{n}\mathbf{n})\delta(n) dV - \int_{\Omega} \nabla \cdot (\mathbf{v} \cdot \sigma(\mathbf{I} - \mathbf{n}\mathbf{n})\delta(n)) dV = \\
\int_A (\nabla \mathbf{v})^T : \sigma(\mathbf{I} - \mathbf{n}\mathbf{n}) dS - \int_A \mathbf{n}^* \cdot \mathbf{v} \cdot \sigma(\mathbf{I} - \mathbf{n}\mathbf{n}) dS = \\
\int_A (\nabla \mathbf{v})^T : \sigma(\mathbf{I} - \mathbf{n}\mathbf{n}) dS - \int_C \mathbf{v} \cdot \sigma \mathbf{b} dl, \quad (50)
\end{aligned}$$

where C is the curve that delineates the surface A (in case A is not closed). Furthermore, $\mathbf{b}$ is the binormal on C : the unit vector that is tangential to A and normal to C , pointing away from A . The term involving a volume integral of $\nabla \cdot (\mathbf{v} \cdot \sigma(\mathbf{I} - \mathbf{n}\mathbf{n})\delta(n))$ is converted to a surface integral, where $\mathbf{n}^*$ is the normal to the “box” that encloses A . As shown in Fig. 3, as the thickness of the box goes to zero, the term $\mathbf{n}^* \cdot (\mathbf{I} - \mathbf{n}\mathbf{n})$ is zero for the top and bottom of the box, whereas $\mathbf{n}^* \cdot (\mathbf{I} - \mathbf{n}\mathbf{n})$ yields the binormal $\mathbf{b}$ on the sides of the box. Note, that we assume that the term involving $\sigma \mathbf{b}$ integrated over C is equal to zero, which follows from the assumption of a 90° contact angle of the fluid-fluid interface with the rigid walls.

Fig. 3: As the thickness of the box is decreased in (a), the term $\mathbf{n}^* \cdot (\mathbf{I} - \mathbf{n}\mathbf{n})$ will become zero on the top and bottom of A , and $\mathbf{n}^*$ will become equal to the binormal $\mathbf{b}$, as is shown in (b).

5.2 Weak form diffuse-interface model

The diffuse-interface equations are solved implicitly for $\mathbf{u}$, p , ϕ , μ , $\mathbf{U}$, and $\boldsymbol{\omega}$ in one system, greatly enhancing stability [40]. The weak form is given by: find $\mathbf{u}$, p , ϕ , μ , $\mathbf{U}$, $\boldsymbol{\omega}$ and $\boldsymbol{\lambda}$ such that

$$(\mathbf{D}_v, \boldsymbol{\tau}_s + \boldsymbol{\tau}_p + \boldsymbol{\tau}_c) - (\nabla \cdot \mathbf{v}, p) + \langle \mathbf{v} - (\mathbf{V} + \boldsymbol{\chi} \times (\mathbf{x} - \mathbf{X})), \boldsymbol{\lambda} \rangle_{\partial P} = 0, \quad (51)$$

$$(q, \nabla \cdot \mathbf{u}) = 0, \quad (52)$$

$$\langle \boldsymbol{\mu}, \mathbf{u} - (\mathbf{U} + \boldsymbol{\omega} \times (\mathbf{x} - \mathbf{X})) \rangle_{\partial P} = 0, \quad (53)$$

$$(r, \frac{D\phi}{Dt}) + M(\nabla r, \nabla \mu) = 0, \quad (54)$$

$$(s, -\beta\phi^3 + \alpha\phi) - \kappa(\nabla s, \nabla \phi) + (s, \mu) = 0, \quad (55)$$

for all admissible test functions $\mathbf{v} = (v_x, v_y)$, q , r , s , $\mathbf{V}$, $\boldsymbol{\chi}$, $\boldsymbol{\mu}$.

5.3 Discretization in space

The equations are solved using the finite element method on boundary-fitted meshes that are moved in time. Triangular $P_2P_1P_1$ elements are used for $\mathbf{u}$, p and $\mathbf{c}$, whereas P_2P_2 elements are used for ϕ and μ . For the diffuse-interface model, the meshes are only aligned with the particle boundary. For the sharp-interface model, the meshes are aligned with both the particle boundary and the fluid-fluid interface and both p and $\mathbf{c}$ are allowed to be discontinuous across the interface. Although we only employ 2D meshes in this paper, this approach can be fairly easily extended to full 3D problems with multiple interfaces (see e.g. [41]). For both models, we employ adaptive meshing to ensure that the mesh close to the particle and fluid-fluid interface is refined, whereas it is coarser in the rest of the domain. Since the fluids are described on a grid that moves with the particle, but not necessarily with the fluid, the arbitrary Lagrange Euler framework is employed. When identifying the computational mesh with the moving grid, the material derivative is rewritten to [42]:

$$\frac{D(\cdot)}{Dt} = \frac{\partial(\cdot)}{\partial t} \Big|_{\mathbf{x}_m} + (\mathbf{u} - \mathbf{u}_m) \cdot \nabla (\cdot), \quad (56)$$

where the mesh coordinates $\mathbf{x}_m$ remain constant in the partial derivative and $\mathbf{u}_m$ is the mesh velocity. The implementation is done by generating meshes for the separate fluid domains using Gmsh [43]. These meshes are conform on the interface A and aligned to the particle boundary. The inner product on the particle boundary is defined using a collocation method:

$$\langle \boldsymbol{\mu}, \mathbf{u} - (\mathbf{U} + \boldsymbol{\omega} \times (\mathbf{x} - \mathbf{X})) \rangle_{\partial P} = \sum_{k=1}^{n_{\text{coll}}} \boldsymbol{\mu}_k \cdot [\mathbf{u}(\mathbf{x}_k) - (\mathbf{U} + \boldsymbol{\omega} \times (\mathbf{x} - \mathbf{X}))], \quad (57)$$

where n_{coll} is the number of collocation points, which are identified with the nodes on the particle boundary, and $\boldsymbol{\mu}_k$ and $\mathbf{x}_k$ are the Lagrange multiplier and nodal coordinate of the k -th collocation point, respectively. Continuity of the velocity and traction on A is imposed by connecting the meshes node-by-node with an additional constraint equation, using a collocation method similar to Eq. (57). In this way, the pressure and conformation tensor are allowed to be discontinuous across the interface.

5.4 Time integration sharp-interface model

Time integration is started by generating a mesh (with nodal coordinates $(\mathbf{x}_m)_0$) based on the initial particle position $\mathbf{X}_0$ and interface position $\mathbf{x}_0$. On this mesh, the weak form of the balance equations, Eqs. (47) to (49), is solved to obtain the initial velocities $\mathbf{u}_0$, $\mathbf{U}_0$ and $\boldsymbol{\omega}_0$ (note that initially $\boldsymbol{\tau}_p = \mathbf{0}$). The new interface position is then obtained using a first-order extrapolation, $\hat{\mathbf{x}}_1 = \mathbf{x}_0$, whereas the new particle position follows from an explicit Euler scheme:

$$\mathbf{X}_1 = \mathbf{X}_0 + \Delta t \mathbf{U}_0. \quad (58)$$

For subsequent steps, a second-order prediction is used for the interface position $\hat{\mathbf{x}}_{n+1} = 2\mathbf{x}_n - \mathbf{x}_{n-1}$ and a second-order Adams-Bashforth scheme is used for the particle position:

$$\mathbf{X}_{n+1} = \mathbf{X}_n + \Delta t \left(\frac{3}{2} \mathbf{U}_n - \frac{1}{2} \mathbf{U}_{n-1} \right). \quad (59)$$

Using the displacement of the particle, denoted by $\Delta \mathbf{X}_{n+1} = \mathbf{X}_{n+1} - \mathbf{X}_n$, and the displacement of the interface, denoted by $\Delta \mathbf{x}_{n+1} = \hat{\mathbf{x}}_{n+1} - \mathbf{x}_n$, the mesh is updated by solving a Poisson problem for the mesh displacement $(\Delta \mathbf{x}_m)_{n+1}$, where $\Delta \mathbf{X}_{n+1}$ and $\Delta \mathbf{x}_{n+1}$ are used as boundary conditions on the particle boundary and interface, respectively. Note, that in the problem of

a particle in a shear flow, the x -position of the particle will be kept fixed, which minimized mesh distortion [44]. However the proper mesh velocity needs to be taken into account in the material derivative, as will be explained later in this section. The displacement of the remaining boundaries is set to zero and in the Poisson problem a diffusion coefficient is used that is proportional to the inverse of the element size, which ensures that larger elements deform more than smaller elements [42]. The new mesh is found from $(\mathbf{x}_m)_{n+1} = (\mathbf{x}_m)_n + (\Delta \mathbf{x}_m)_{n+1}$. An example of the mesh movement for the problem of a particle in a cylinder is shown in Fig. 4. The mesh velocity, which is needed in the evolution equation of the conformation tensor

Fig. 4: The mesh at t_n (a) is moved according to the displacement of the particle and interface to obtain the mesh at t_{n+1} (b). If mesh distortion is too large, a remeshing is performed, where the interface and bulk mesh are refined in regions where the particle is close to the interface and/or where the curvature of the interface is large (c). The red line depicts the fluid-fluid interface.

(Eq. (20)), is found using a first-order backward differencing scheme for the first step:

$$(\mathbf{u}_m)_1 = \frac{(\mathbf{x}_m)_1 - (\mathbf{x}_m)_0}{\Delta t}, \quad (60)$$

whereas a second-order backward differencing scheme is used for subsequent steps:

$$(\mathbf{u}_m)_{n+1} = \frac{\frac{3}{2}(\mathbf{x}_m)_{n+1} - 2(\mathbf{x}_m)_n + \frac{1}{2}(\mathbf{x}_m)_{n-1}}{\Delta t}. \quad (61)$$

For the problem of a particle in a shear flow, the mesh is fixed in x -direction with respect to the particle motion. This means that there is an additional contribution to the mesh velocity in x -direction, which is equal to the particle velocity in x -direction. This velocity is obtained by

backward differencing of the particle location X similar to Eq. (60) for first-order, or Eq. (61) for second-order time integration.

Once the mesh becomes too distorted, a remeshing is performed based on the particle position $\mathbf{X}_{n+1}$ and interface position $\hat{\mathbf{x}}_{n+1}$, as shown in Fig. 4. Mesh refinement is performed in regions where the particle is close to the interface and/or where the curvature of the interface is large, by splitting elements on the interface, as is shown in Fig. 5. Note, that the previous interface coordinates, $\mathbf{x}_n$ and $\mathbf{x}_{n-1}$, needed for the time integration, are found by splitting the same elements at the previous times. The conformation tensor and mesh coordinates at the previous time steps, which are needed for the time integration, are projected onto the new mesh using a similar procedure as was presented in [45], and the time integration can continue.

On the mesh with nodal coordinates $(\mathbf{x}_m)_{n+1}$, the balance equations are solved to find $\mathbf{u}_{n+1}$, p_{n+1} , $\mathbf{U}_{n+1}$ and $\boldsymbol{\omega}_{n+1}$, where in the problem of a particle in shear, a prediction of the conformation tensor, denoted by $\hat{\mathbf{c}}^{n+1}$ is used to estimate the polymer stress according to D’Avino and Hulsen [46]. This semi-implicit approach to include the polymer stress in the momentum balance was shown to improve stability and allows for the simulation of viscoelastic fluids with little or no solvent contribution. After solving for the new velocities and pressures, the actual conformation tensor $\mathbf{c}^{n+1}$ is found using a second-order backward differencing scheme for equation Eq. (20), using SUPG [47] and the log conformation representation [48] for stability.

Lastly in a time step, a corrector step is performed to find the actual interface coordinates $\mathbf{x}_{n+1}$. For case 1, the interface is updated in a Lagrangian manner according to Eq. (3), where the velocity is simply taken in the nodes on the interface. Using a first-order backward differencing scheme for Eq. (3) yields for the first time step

$$\mathbf{x}_1 = \mathbf{x}_0 + \Delta t \mathbf{u}_1. \quad (62)$$

For subsequent steps, a second-order backward differencing scheme is used:

$$\mathbf{x}_{n+1} = \frac{2}{3} \left(2\mathbf{x}_n - \frac{1}{2}\mathbf{x}_{n-1} + \Delta t \mathbf{u}_{n+1} \right). \quad (63)$$

For case 2, a particle in a shear flow, using the Lagrangian approach would be problematic: the interface will move in x -direction with respect to the particle. The situation improves by

Fig. 5: The interface is refined by splitting elements based on the curvature of the interface and the distance between the interface and the particle. The different colors represent the different fluid domains.

updating only the normal component of the interface according to Eq. (4), but the same problem occurs as the interface deforms and the normal to the interface obtains a horizontal component. However, as was mentioned in Section 2.1, any tangential motion can be added to the interface, a property that can be used to keep the interface in “frame”. Introducing a tangential velocity $\mathbf{u}_t$, Eq. (4) can be written as [20]:

$$\dot{\mathbf{x}} + \mathbf{u} \cdot \nabla_s \mathbf{x} = \mathbf{u} + \mathbf{u}_t, \quad (64)$$

where ∇_s is the surface gradient operator. As is shown in Fig. 6, the tangential velocity can be chosen such that the (periodic) end points of A only move vertically. However, when solving Eq. (64) in a semi-implicit manner, where $\mathbf{u}_t$ needs to be specified, this velocity is not known yet. We use an approach where two “intermediate solutions” are combined such that the end-points of the interface only move in vertical direction. The approach is illustrated using the following simplified problem: we want to find the solution x to the following equation

$$\mathcal{L}(x) = f_1 + cf_2, \quad (65)$$

where $\mathcal{L}$ is a linear operator, f_1 and f_2 are known terms and c is a constant of unknown magnitude. This system can be solved in two steps:

$$\mathcal{L}(x_1) = f_1, \quad (66)$$

$$\mathcal{L}(x_2) = f_2, \quad (67)$$

where x_1 and x_2 are two “intermediate solutions”. Due to the linearity of the operator $\mathcal{L}$, the solution $x = x_1 + cx_2$, where the magnitude of c is arbitrary, also satisfies Eq. (65). The value of c can be chosen such that the solution x fulfills a certain condition.

This approach is implemented by solving Eq. (64) for the unknowns $\mathbf{x}_{n+1}$ in a semi-implicit manner using SUPG stabilization [47], similarly to [20]. The periodicity of the end points of A is enforced using a constraint, and the resulting system matrix is identified with the linear operator $\mathcal{L}$. As explained before, the solution is obtained in two steps. In the first step, a prediction for the tangential velocity is used (based on the predicted location of the interface), which is denoted by $\hat{\mathbf{u}}_t$, and which is chosen such that the x -displacement of the end points is approximately zero. For stability, it is essential that $\hat{\mathbf{u}}_t$ is included in the SUPG terms. The prediction $\hat{\mathbf{u}}_t$ (plus the additional terms needed for the time-integration of Eq. (64)) is identified with f_1 in Eq. (65). Solving the resulting system yields the first solution $(\mathbf{x}_1)_{n+1}$. The end points will now have an x -displacement that is approximately zero, but not exactly. This will be corrected in the second step, where the right hand side is replaced by the unit tangent vector to A , which is denoted by $\mathbf{k}$. The unit tangent vector $\mathbf{k}$ is identified with f_2 in Eq. (67). Solving the second system yields the solution $(\mathbf{x}_2)_{n+1}$. The final solution, which satisfies Eq. (65), is now given by $\mathbf{x}_{n+1} = (\mathbf{x}_1)_{n+1} + c(\mathbf{x}_2)_{n+1}$, where c is chosen such that the end points only move in vertical direction. The actual tangential velocity in Eq. (64) is thus given by $\mathbf{u}_t = \hat{\mathbf{u}}_t + c\mathbf{k}$.

5.5 Time integration diffuse-interface model

During the time-integration of the diffuse-interface model, we solve for $\mathbf{u}$, p , ϕ , μ , $\mathbf{U}$ and $\boldsymbol{\omega}$ in one system. It was shown that this implicit approach greatly enhances stability [40]. Although our previous work on particles in Cahn-Hilliard fluids was not done using this implicit approach, there is a large amount of overlap, so here only the notable differences are explained. For details, the reader is referred to [45, 49].

Fig. 6: By adding a tangential velocity $\mathbf{u}_t$ to the velocity on the interface, the end points of A can be fixed in horizontal direction. In (a) the interface can be seen as it moves “out of frame”, whereas in (b) the interface was moved back by $\mathbf{u}_t$.

Initially, a mesh is created based on the initial particle location $\mathbf{X}_0$. The mesh is refined near the interface (defined by $\phi = 0$). To find the initial particle velocity $\mathbf{U}_0$, the system given by Eqs. (51) to (55) is solved by substituting the known ϕ_0 -field, and solving for $\mathbf{u}_0$, p_0 , μ_0 , $\mathbf{U}_0$ and $\boldsymbol{\omega}_0$. The new particle position is found using an explicit first-order Euler scheme for the first time step, or a second-order Adams-Bashfort scheme for subsequent time steps (Eqs. (58) and (59)). The new particle position is then used to update the mesh by solving a Poisson problem using the displacement of the particle as a boundary condition, similar to the sharp-interface model. The mesh-velocity is found using a first-order backward-differencing scheme for the first time step or a second-order backward-differencing scheme for subsequent time steps (Eqs. (62) and (63)). If mesh deformation becomes too large, or if the interface moves out of the refined area, remeshing is performed. We use similar criteria for remeshing as presented in [45]. To solve the system given by Eqs. (51–55), the phase-dependent viscosity and modulus are needed. We determine these in the following way:

$$\hat{\eta}_{n+1} = \eta(\hat{\phi}_{n+1}) \quad (68)$$

$$\hat{G}_{n+1} = G(\hat{\phi}_{n+1}) \quad (69)$$

where $\hat{\eta}_{n+1}$ and $\hat{G}_{n+1}$ are predictions for the viscosity and polymer modulus respectively, and $\hat{\phi}$ is a first-order extrapolation for the first time step ($\hat{\phi}_1 = \phi_0$) or a second-order extrapolation for subsequent time steps ($\hat{\phi}_{n+1} = 2\phi_n - \phi_{n-1}$). Similar to the sharp-interface problem, a prediction for the conformation tensor is used to determine the polymer stress [46]. Solving the system yields the new solutions $\mathbf{u}_{n+1}$, p_{n+1} , ϕ_{n+1} , μ_{n+1} , $\mathbf{U}_{n+1}$ and $\boldsymbol{\omega}_{n+1}$ which are then used to solve for the real $\mathbf{c}_{n+1}$ using a backward differencing scheme for equation Eq. (20), and using SUPG

[47] and the log conformation representation [48] for stability.

6 Results

When simulating particles that are larger than the micrometer scale, using the actual physical interface thickness, which is of the order of nanometers, leads to an intractable problem. In this case, the diffuse-interface model can be applied with an interface thickness that is larger than the real interface thickness and often scaling is applied to correct for this [50]. The interface thickness in dimensionless form is called the Cahn number and is defined as

$$\text{Cn} = \frac{\xi}{a}. \quad (70)$$

Furthermore, the effect of diffusion of the fluids can be described by the dimensionless parameter S , which can be interpreted as a diffusion length over a macroscopic length and is defined as [51]:

$$S = \frac{\sqrt{\eta M}}{a}. \quad (71)$$

Due to the use of a Cahn number that is larger than the physical value, the interface can be diluted or compressed due to flow. This effect can be countered by setting S to a value that is much larger than the physical value, to ensure that the interface maintains its tanh profile. A rule of thumb, is that the mobility should be large enough to maintain this profile, but not too large as to overly damp the flow [33]. The results presented here will be used to investigate the role that Cn and S play in describing a particle that approaches a fluid-fluid interface. The sharp-interface model is expected to behave as the limiting case of Cn going to zero. Note, that diffusion of the fluids does not play a role for the sharp-interface model.

6.1 Case 1

The problem of a spherical particle in a closed, cylindrical container filled with viscosity-matched Newtonian fluids, is completely described by the geometry of the domain and a dimensionless force $F^* = F/F_{\max} = F/(\sigma a \pi)$, where $F_{\max}$ denotes the maximum force on the particle that the interface can support, as was shown in [45]. The subsequent results will be presented in

dimensionless form: time is normalized by $\eta a^2/F$ and lengths are normalized by the particle radius a , unless mentioned otherwise. For all simulations, the dimensions of the cylinder are set to $L_1 = 10$, $L_2 = 20$ and $R = 4$. For the diffuse-interface model, simulations are performed on locally refined meshes, with an element size near the interface of ξ . This yields around ten second-order points on the interface, which has been given as a criterion for mesh-convergence [28]. For the sharp-interface model, the initial element size on the interface is set to $R/40$, but refinement is performed in regions where the particle is close to the interface and/or where the curvature of the interface is large. For both the diffuse-interface and the sharp-interface simulations, the element size near the particle is chosen as $2\pi a/64$: there are 64 elements on the circumference of the particle. Due to the use of a fully implicit scheme, a relatively large time step of $\Delta t = 0.1$ could be used for the diffuse-interface simulations. The semi-implicit time integration for the sharp interface, allowed for a time step of $\Delta t = 0.01$.

Simulations were performed for $F^* = 2$, using both the sharp-interface model and the diffuse-interface model with Cahn numbers ranging from 0.01 to 0.08, and $S = 0.1, 0.01$ and 0.001. Snapshots of the composition ϕ for $S = 0.01$ in are shown in Fig. 7. It can be observed that for the sharp-interface model, the particle remains on top of the interface during the entire simulation. This type of interface deformation was called the film-drainage mode by Geller et al. [52]. Also note that a film of non-uniform thickness is developed with a symmetric dimple on the bottom of the particle, as was observed experimentally by Hartland [2, 3]. However, for $Cn > 0$, the particle makes contact with the interface, and subsequently moves into the lower fluid. This phenomenon is delayed for lower values of Cn . As the particle goes through the interface, some of the upper fluid remains attached to the particle. For $Cn = 0.08$, these droplets quickly disappear since they are below a critical volume [38]. The droplets remain on the particle for $Cn \leq 0.04$, but appear to be larger for smaller values of Cn .

The resulting particle velocity U as a function of time is presented Fig. 8. Note, that the particle velocity is scaled by the velocity of an isolated sphere in an unbounded flow, which follows from Stokes' law: $U_s = F/(6\pi a\eta)$. It can be seen that due to the interfacial tension, the particle velocity shows a strong decrease. For the sharp-interface model, the velocity keeps decreasing and remains small until the end of the simulation at $t = 1000$. The particle velocity for the diffuse-interface depends strongly on Cn and S . For $S = 0.1$, the velocity is similar to

Fig. 7: Snapshots of the composition field for $F^* = 2$ and $S = 0.01$. The number below each figure denotes the Cahn number for that simulation.

the sharp-interface solution until around $t = 100$. Depending on the Cahn number, the particle velocity then increases as the particle goes through the interface. For $S = 0.01$, the velocity until $t = 100$ deviates slightly from the sharp-interface solutions, especially for larger values of Cn. Again, depending on the Cahn number, the particle velocity suddenly increases as the particle goes through the interface. For $Cn = 0.01$, the adsorption of the particle is delayed until $t = 800$. For $S = 0.001$, none of the particles penetrate the interface but the particle velocity during the initial stage of the simulation deviates from the sharp interface solution, especially for the larger Cahn numbers. However, when inspecting the particle velocity for $S = 0.001$ on a log-scale, as presented in Fig. 8d, it appears that the particle velocity goes to a small, but

non-zero value. Moreover, for $Cn = 0.08$, an increase of the particle velocity is observed toward the end of the simulation, which indicates that the particle is in the process of moving through the interface. It is interesting to note that for $S = 0.001$, the simulation qualitatively agrees

Fig. 8: The particle velocity as a function of time for $F^* = 2$ using $S = 0.1$ (a), $S = 0.01$ (b), $S = 0.001$ (c) and $S = 0.001$ on a log-scale (d).

with the sharp-interface simulation, where no particle adsorption is observed during the entire simulation time. The final composition field for $S = 0.001$ is shown in Fig. 9.

To further investigate the influence of Cn and S on the particle velocity, simulations were performed for $F^* = 4$, again using the sharp-interface model and the diffuse-interface model with Cn varying between 0.01 and 0.08, and $S = 0.1, 0.01$ and 0.001. The resulting composition field is shown for $S = 0.001$ in Fig. 10. For the sharp-interface model, the particle goes through the interface, dragging a thread of the upper fluid along with it. This type of interface deformation

Fig. 9: The composition field at $t = 1000$ for $F^* = 2$ and $S = 0.001$. The number below each figure denotes the Cahn number for that simulation.

was called the tailing mode by Geller et al. [52]. The thread becomes unstable and is pinched off close to the original position of the interface. At this point, the sharp interface model can only continue when applying “mesh surgery” to account for topological changes, which is outside the scope of this paper. The breakup of the thread can be described by the diffuse-interface model. Depending on the Cahn number, multiple satellite drops are formed, which appear to become smaller toward the particle.

Results of the particle velocity for $F^* = 4$ are presented in Fig. 11, where the sharp-interface model shows a decrease in velocity, followed by an increase, which is associated with the pinch-off of the fluid thread. Furthermore, similar observation as for $F^* = 2$ can be made: at $S = 0.1$, the velocity matches well during the initial part of the simulation, but starts to deviate as the particle goes through the interface, which happens earlier for larger values of Cn . For $S = 0.01$, the simulations using the sharp-interface model and diffuse-interface model coincide remarkably well for $Cn \leq 0.02$. For $S = 0.001$, deviations are observed in the particle velocity, which appears to be much lower for larger Cn . The results indicate that for low values of S the process of the particle penetrating the interface is delayed with increasing Cn , for which we offer the following explanation: in front of the particle, the interface is compressed due to the flow, effectively lowering the interface thickness. For low values of S , diffusion cannot restore the interface to its equilibrium tanh profile, leading to an effective increase in $|\nabla\phi|$ across the interface and thus an increase in the Cahn-Hilliard interfacial tension σ^* (see Eq. (11)). This increase in interfacial

Fig. 10: Snapshots of the composition field for $F^* = 4$ and $S = 0.001$. The number below each figure denotes the Cahn number for that simulation.

tension causes an increase in Laplace pressure, slowing the particle down. This effect becomes stronger for higher values of Cn. Jacqmin [33] already reported this effect, and suggested that the Cahn-Hilliard diffusion should be set large enough such that the equilibrium tanh shape of the interface can be maintained. However, as was shown in this section, a large value of S results in the particle moving through the interface much faster. This might not always describe the true physics well, especially when the actual interface thickness is much smaller than the numerical one. Another approach is suggested by Yue et al. [28], where the κ parameter in Eq. (11) is adapted to “match” the surface tension σ , but an implementation in the implicit scheme used here is not trivial. Finally, it should be emphasized that the problem becomes

less significant for smaller values of Cn . When S is chosen with care, the particle velocity for the diffuse-interface mode and sharp-interface model agree well. For the problem investigated in this section, $S = 0.01$ appears to be an appropriate choice, with the diffuse-interface model converging to the sharp-interface model around $Cn = 0.02$ up until the pinch-off of the fluid thread, as is shown in Fig. 11b.

Fig. 11: The particle velocity as a function of time for $F^* = 4$ for $S = 0.1$ (a), $S = 0.01$ (b) and $S = 0.001$ (c).

6.2 Case 2

The second problem under investigation is a two-phase shear flow, where one of the fluids is viscoelastic and contains a rigid particle. The movement of the particle toward the interface is (as opposed to case 1) not the result of an external force, but is due to gradients in normal

stresses. This migration of particles is well known for flow geometries where the shear rate is not constant, e.g. a wide-gap Couette device [53]. In the current work, the gradients in normal stresses are due to differences in viscoelastic properties of the two fluids, a phenomenon that is important in e.g. the processing of filled polymer blends. Although the migration of particles in polymer blends has been reported in the literature [54], the contrast in viscoelastic properties has not been investigated before as a possible mechanism for particle migration. Here, we focus on the description of the fluid-fluid interface, and the full analysis of particle migration in two-phase viscoelastic flows is topic of future research.

The Newtonian viscosity in Eq. (17) is different for fluid 1 and fluid 2, and is denoted by η_1 and η_2 , respectively. Note, that in fluid 2, the Newtonian fluid acts as a solvent. The average shear rate is defined as $\dot{\gamma} = 2U_w/H$. In addition to Cn and S, there are a number of dimensionless parameters that govern this problem. These are the Weissenberg number, which is defined as $Wi = \lambda\dot{\gamma}$, the Giesekus mobility α , the ratio between the viscosity of the Newtonian fluid and the zero-shear viscosity of the viscoelastic fluid, defined by $\delta = \eta_1/(\eta_p + \eta_2)$ and the ratio between the solvent viscosity and zero-shear viscosity of the viscoelastic fluid, defined by $\beta = \eta_2/(\eta_p + \eta_2)$. Furthermore, the effect of the interfacial tension is described by the capillary number, defined as $Ca = (\dot{\gamma}(\eta_p + \eta_2))/(\sigma/a)$. For this problem, time is normalized by the inverse of the shear rate $\dot{\gamma}^{-1}$ and lengths are normalized by the particle radius a , unless mentioned otherwise. The size of the domain is set to $W = 4$ and $H = 40$. Furthermore, the strain rate is slowly increased from zero to its actual value between $t\dot{\gamma} = 0$ and $t\dot{\gamma} = 25$, to avoid large oscillations of the interface at the initial stage of the simulation.

For the simulations using the diffuse-interface model, the equations are solved on meshes with an element size of ξ near the interface. For the sharp-interface simulations, the element size on the interface is initially set to $W/40$, but refinement is performed as the simulation progresses. For both the diffuse-interface and the sharp-interface simulations, the element size near the particle is chosen as $2\pi a/64$: there are 64 elements on the circumference of the particle. For the diffuse-interface simulations, a time step of $\Delta t = 0.08$ is used, whereas the time step for the sharp interface simulations are set to $\Delta t = 0.01$, due to stability considerations.

Simulations were performed for both the sharp-interface model and diffuse-interface model, for several values of Cn and S. The remaining parameters are $Wi = 2$, $\alpha = 0.2$, $\delta = 1$, $\beta = 0.1$

and $Ca = 5$ for all results presented in this section. Depending on the values of Cn and S , we identified three possible scenarios: 1) the particle makes contact with the interface and subsequently migrates into the upper fluid (Fig. 12), 2) the particle does not make contact with the interface, but migrates into the upper fluid surrounded by a film of the bottom fluid (Fig. 13) and 3) the particle moves toward the upper fluid but is halted before reaching the interface (Fig. 14). The results indicate that both Cn and S are crucial in describing the migration of a particle in a two-phase viscoelastic flow. It can furthermore be observed that for $Cn = 0.04$ and $S = 0.001$, the interface directly above the particle is compressed due to the flow, and there is too little diffusion to restore it to its equilibrium profile. As explained in Section 6.1, this results in a higher local surface tension, which is enough to halt the migration of the particle. The results for the sharp-interface model are similar to the results for $Cn = 0.02$ and $S = 0.01$ as shown in Fig. 13. Around $t\dot{\gamma} = 200$ the interface is swept underneath the particle, and crosses the periodic boundary. At this stage, the simulation can only continue when “mesh-surgery” is applied, which is outside the scope of this paper.

Fig. 12: Snapshots of the composition field for a migrating particle. $Cn = 0.04$ and $S = 0.1$.

In Fig. 15, the vertical component of the particle velocity is plotted as a function of strain, for the initial part of the simulation. It can be seen that U_y attains a positive value immediately: the particle is migrating toward the upper fluid. Oscillations can be observed, which are due to the particle disturbing the interface and the periodicity of the problem. These oscillations are damped by the surface tension. For $S = 0.1$, the migration velocities overlap relatively well and convergence of the diffuse-interface model to the sharp-interface model is observed as Cn is decreased. When decreasing S to 0.01 and 0.001, the average migration velocities remain roughly the same, although the solutions clearly deviate more than for $S = 0.1$.

Fig. 13: Snapshots of the composition field for a migrating particle. $Cn = 0.02$ and $S = 0.01$.

Fig. 14: Snapshots of the composition field for a migrating particle. $Cn = 0.04$ and $S = 0.001$.

The vertical component of the particle velocity is plotted up to $t\dot{\gamma} = 200$ in Fig. 16 for several values of Cn and S . For $S = 0.1$, clear deviations of the particle velocity can be observed around a strain of 100 for $Cn = 0.08$ and around a strain of 180 for $Cn = 0.04$. For $S = 0.1$ and $Cn \geq 0.04$, the fluid-fluid interface comes into contact with the particle boundary, leading to a rapid increase of the velocity, as the interfacial tension pulls the particle up. The particle then continues moving upward, while “spinning” off the interface, as shown in Fig. 12. For $Cn \leq 0.02$, the results are qualitatively different: a sharp increase in velocity is observed as the interface is swept underneath the particle, as is shown in Fig. 13. The particle moves into the upper fluid, but is encapsulated by the lower fluid. For larger values of Cn , the migration velocity is underestimated, or migration is even halted, which is again attributed to a local increase in surface tension. This effect is strongest present for $S = 0.001$, where there is too little diffusion present to restore the interface to its equilibrium value.

It is well-known that a circular particle in a Newtonian shear flow rotates with an angular

velocity that is half the shear rate [55]. However, both experiments and simulations show that viscoelasticity can significantly reduce the angular velocity of the particle [56, 57]. This decrease in angular velocity plays a large role in e.g. the interaction between particles in viscoelastic fluids [58]. To investigate the role of the fluid-fluid interface on the rotation of the particle, we present the angular velocity in the xy -plane (denoted by ω and defined positive in clockwise direction) in Fig. 17. It should be noted that due to shear thinning of the Giesekus fluid, the shear rate is not the same for both fluids. For the fluid parameters used in this section, the sharp-interface model without a particle yields shear rates of 0.66 and 1.34 times the average shear rate, for the Newtonian fluid and Giesekus fluid, respectively. It can be observed that the angular velocity rapidly grows to a value of 0.215 as the shear rate is gradually increased during the initial stage of the simulation. As the particle approaches the interface, the angular velocity slowly decreases, but remains remarkably similar for all values of S and Cn , up to a strain of $t\dot{\gamma} = 100$. For $t\dot{\gamma} > 100$, the influence of Cn and S increases, and the angular velocity depends largely on the behavior of the particle (e.g. contact with the interface or halted migration).

7 Discussion and conclusion

We have presented simulations of a particle in a closed cylinder filled with two Newtonian fluids, and a particle in a shear flow, where one of the fluids was viscoelastic. Two models were used for the fluid-fluid interface: a sharp-interface model and a diffuse-interface model. In the diffuse-interface model, two additional dimensionless groups appear: the Cahn number Cn , which is a measure for the interface thickness, and a dimensionless diffusion parameter S . The influence of these groups on the movement of the particle was investigated, and the results were compared to the results of the sharp-interface model.

As Cn was decreased, the diffuse-interface model converges to the sharp-interface model. Large values of S yields particle velocities that match well with the sharp-interface model, as long as the particle is far from the interface. This is attributed to the interface maintaining its equilibrium tanh profile, and thus the equilibrium value of the surface tension. However, for large values of S and Cn , the results can be qualitatively different with particle adsorption occurring rapidly, or the particle making contact with the interface, whereas for smaller values of Cn and the sharp-interface model, the particle is encapsulated by the fluid. Decreasing the

Fig. 15: The particle migration velocity as a function of strain for $S = 0.1$ (a), $S = 0.01$ (b) and $S = 0.001$ (c).

value of S has the result that the interface does not maintain its equilibrium profile, which locally changes the surface tension. This results in the particle adsorption being slowed down or halted altogether. The two interface deformation modes as mentioned by Geller et al. [52], the film-drainage mode and the tailing mode, are observed in the sharp-interface model. Furthermore, the typical dimple shape of the fluid film in the film-drainage mode, as reported by Hartland [2, 3], is observed in the simulations with the sharp-interface model. For small values of Cn and S , these phenomena are also observed in the diffuse-interface model, but the particle makes contact with the interface for larger Cn and S . It was shown that also in the case of viscoelastic fluids, the diffuse-interface results converge to the sharp-interface results.

When comparing these results to experiments, the value of the real Cahn number can be

Fig. 16: The particle migration velocity as a function of strain for $S = 0.1$ (a), $S = 0.01$ (b) and $S = 0.001$ (c).

as small as 10^{-6} for particles of the order of millimeters. The results for the specific problems presented here, show that a film of fluid is formed around the particle, and the particle making direct contact with the interface is not likely. The diffuse-interface model is able to capture these results, although care should be taken in the choice of S . Furthermore, using a small value for Cn appears to improve the results, i.e. the model converges to the sharp-interface model. When using diffuse-interface models with Cn larger than its actual value, it is therefore advised to always study the convergence of the problem with Cn . The use of a sharp-interface model can be very useful in that respect.

The combination of rigid particles modeled by a sharp-interface model with a diffuse-interface model for fluid-fluid interfaces is a powerful technique that can be used to gain more

Fig. 17: The particle angular velocity as a function of strain for $S = 0.1$ (a), $S = 0.01$ (b) and $S = 0.001$ (c).

physical insight into problems where particles on interfaces play a role, such a Pickering emulsions and self-assembly of particles at interfaces. However, the choice of the diffuse-interface parameters is not always obvious, and might influence the results, both quantitatively and qualitatively. We believe that the analysis presented in this paper helps in the interpretation of the results, especially with respect to the role of diffusion and the thickness of the interface.

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