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 in-

terface 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 $\boldsymbol{x}$, are described using a moving curvilinear coordinate system [20]:

$$\boldsymbol{x} = \bar{\boldsymbol{x}}(\underset{\sim}{\chi}, t), \tag{1}$$

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

$$\dot{\boldsymbol{x}} = \left. \frac{\partial \bar{\boldsymbol{x}}}{\partial t} \right|_{\underset{\sim}{\chi}}, \tag{2}$$

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

$$\dot{\boldsymbol{x}} = \boldsymbol{u}. \tag{3}$$

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

$$\dot{\boldsymbol{x}} \cdot \boldsymbol{n} = \boldsymbol{u} \cdot \boldsymbol{n}, \tag{4}$$

where $\boldsymbol{n}$ 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]:

$$\boldsymbol{\tau}_{\mathrm{si}} = \sigma (\boldsymbol{I} - \boldsymbol{nn}) \delta(n), \tag{5}$$

where σ is the (constant) surface tension, $\boldsymbol{I}$ 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 $\boldsymbol{\tau}_{\mathrm{si}}$ is used in the literature (e.g. [24]), by taking the deviatoric part of $\boldsymbol{\tau}_{\mathrm{si}}$ 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]:

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

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

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

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:

$$\frac{\mathrm{D}\phi}{\mathrm{D}t} = \nabla \cdot (M\nabla\mu), \tag{8}$$

where $\mathrm{D}(\ )/\mathrm{D}t$ is the material derivative, M is the constant Cahn–Hilliard mobility and the chemical potential is given by definition as

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

where $\delta()/\delta\phi$ 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]:

$$\phi(x) = \phi_{\mathrm{B}} \tanh\left(\frac{x}{\sqrt{2}\xi}\right), \tag{10}$$

where $\phi_{\mathrm{B}} = \sqrt{\alpha/\beta}$ 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]:

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

To determine the Cahn–Hilliard parameters, we first set $\alpha = \beta$, from which follows $\phi_{\mathrm{B}} = \pm 1$. 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]:

$$\boldsymbol{\tau}_{\mathrm{di}} = \kappa \left(|\nabla\phi|^2 \boldsymbol{I} - \nabla\phi\nabla\phi \right), \tag{12}$$

where an isotropic term was added to $\boldsymbol{\tau}_{\mathrm{di}}$ 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 $\boldsymbol{\tau}_{\mathrm{di}}$ are the yy- and zz-component, which are parallel to the interface and are written as $(\tau_{\mathrm{di}})_{yy} = (\tau_{\mathrm{di}})_{zz} = \kappa(d\phi/dx)^2$. In the limit of ξ goes to zero, these components can be written as:

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