

A continuum model of interfacial surfactant transport for particle methods

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ABSTRACT

Employing the moving particle semi-implicit (MPS) method, this study proposes a numerical framework of Lagrangian particle method to solve the Navier–Stokes equations for multiphase flows coupled with soluble surfactant transport equations. Each particle carries interfacial and bulk surfactant concentrations, as well as momentum. With a diffuse-interface approximation, the discontinuous of the interfacial surfactant across the interface is replaced by a smooth continuous distribution. The interfacial surfactant transport equation is redefined and solved at all particles in a fluid domain. The discrete form of surfactant dynamics is derived in conservative form, and thus, global mass of surfactant is conserved exactly. An artificial normal diffusion is introduced to prevent interfacial mass from leaking from a fuzzy interface. The suitable normal diffusivity depends on the rate of surface contraction and the size of grid. A criterion to determine the size of grid at a given characteristic speed and length scale is discussed.

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1. Introduction

The surface tension on the interface between two fluids dominates the flow fields in small scale such as microfluidic devices [1–3]. Surfactant modifies the surface tension and its surface-gradient induces the Marangoni stress. The presence of surfactant significantly affects the surface tension-dominated flows. The study of modeling for surfactant transport is important in technological applications as well as biological/clinical aspects. Pulmonary surfactant plays a vital role in reducing the surface tension of the liquid lining alveoli and airways, and significantly influences the behavior of the liquid in lung [4–6].

Surfactant can exist on the interface and in the bulk fluid if it is soluble to the fluid. Only interfacial surfactant modifies the surface tension. The typical mathematical model for a soluble surfactant transport is described by two separate transport equations. The interfacial surfactant transport equation describes the mass balance of the interfacial surfactant, which is applied on the interface only. The bulk surfactant transport equation is applied over the bulk fluid. The two equations are coupled through a surfactant mass flux between the interface and the bulk, which depends on the adsorption and desorption kinetics. Both transport equations are solved coupled with flow equations because the interfacial surfactant affects the motion and deformation of the fluid.

Computational modeling of surfactant-contaminated free-surface flows is a highly challenging task. The interfacial surfactant equation must be solved on moving and complex domains where the interfaces may contract/stretch, or breakup/merge. There have been proposed some numerical methods, where the mesh-system and the scheme to track or capture the interface are different. The suitable method depends on the problem to solve. A body-fitted mesh-system is appropriate for steady or small interface-deformation problem with a simple domain shape. Since a grid line (a plane for 3D) of the bulk fluid grid corresponds to an interface line (a plane), it is possible to determine the surface force on the exact interface

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location, and relatively easier to keep a conservation of surfactant mass over the domain. This method has been widely used [7–12], however, there are difficulties to solve the problems with large deformations and topological changes of interface.

There have been proposed numerical methods, which are capable for unsteady problems with a large deformation of interface. Unlike the body-fitted mesh method, they employ a separate mesh system for interface from a bulk fluid mesh. The front-tracking method, where the flow is computed on a fixed grid, while a set of connected marker particles tracks the interface and any interfacial quantities. The front-tracking method for soluble surfactants was studied in Muradoglu and Tryggvason [13]. The immersed boundary method was used to simulate interfacial flows with insoluble surfactants in [14,15].

The volume-of-fluid (VOF) and the level-set methods are the category of interface capturing method, where the interface is not tracked explicitly. They use a transport of fraction, level-set, or phase-field function to capture interfaces. Those methods are capable for the problems that involve large deformations and topological changes of interface. A volume-of-fluid (VOF) method for insoluble surfactants was developed in James and Lowengrub [16]. A level-set method for solving the surfactant equation was presented in Xu et al. [17]. The diffuse-interface approach is applied by Teigen et al. [18]. These studies successfully solved the transport of interfacial surfactant on same grid as the bulk fluid without use of interfacial grids or marker-points.

The smoothed particle hydrodynamics (SPH) and the moving particle semi-implicit (MPS) [19] methods are in the category of particle method. Both methods are a full Lagrangian mesh-less method. Essentially, the computational volume/area is discretized with particles, therefore it is relatively easier to achieve the conservation of mass. Although there are some differences in the derivative models, both methods use a kernel function to govern the interaction among adjacent particles when they are within a cutoff distance. Both methods can handle complex geometries and topological changes in interface. The SPH method has been developed initially for astrophysical problems and recently applied for fluid dynamics with a weak compressibility. The SPH method with a soluble surfactant was proposed by Adami et al. [20].

The MPS method has been developed by Koshizuka and Oka [19] to solve incompressible flows. The major difference from SPH is that the MPS method solves pressure fields implicitly, where the governing equations are transformed based on particle representations, resulting in a Poisson equation for pressure. This method was originally developed for free-surface problems. In MPS, interfaces are also represented by particles. Those interfacial particles cannot be predetermined, which must be identified by a numerical scheme. There are several studies that employed the MPS method to solve flow with a constant surface tension. But, there is no attempt to solve the transport of surfactant.

Employing the MPS method, the present study proposes a scheme to solve surfactant transport equations coupled with flow equations. In this scheme, each particle carries both bulk and interfacial surfactants as well as the momentum. In Section 2, the governing equations for the flow field and the surfactant dynamics are presented. In 2.1, a modified interfacial surfactant transport model is introduced to make all particles capable to carry interfacial surfactant. The numerical procedure is described in Section 3 including a brief introduction of the MPS method. Since the interfacial surfactant must stay in an interface, a discussion is made in 3.2 to simulate this nature. In 4.1, the surfactant dynamics during surface contraction/stretch is presented to examine the proposed model. In 4.2, a drop in a shear flow of a surfactant laden fluid is presented. Conclusions are given in Section 5.

2. Mathematical formulation

2.1. Interfacial surfactant transport model

Considering a material surface element S , we think about the mass balance on S as shown in Fig. 1 [21]. In the continuum interface theory/the diffuse-interface approximation, the discontinuity of the interfacial surfactant across the interface can be replaced by a smooth continuous distribution. The conservation of surfactant mass on S can be transformed into the conservation within a volume V as

$$\frac{d}{dt} \int_S \Gamma dS \simeq \frac{d}{dt} \int_V \Gamma \delta_S dV = \int_V \left\{ \frac{\partial(\delta_S \Gamma)}{\partial t} + \mathbf{u} \cdot \nabla(\delta_S \Gamma) \right\} dV, \quad (1)$$

where δ_S is the Dirac delta function, Γ is the interfacial surfactant concentration, and $\mathbf{u}$ is the velocity. Note that Γ is a surface concentration and the dimension is mass per a unit area. Since the surface element S moves and deforms with flows, the

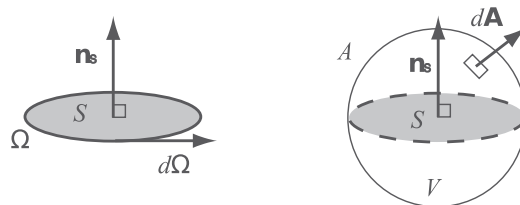


Fig. 1. An illustration of a surface element.

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