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An immersed boundary method for interfacial flows with insoluble surfactant

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Abstract

In this paper, an immersed boundary method is proposed for the simulation of two-dimensional fluid interfaces with insoluble surfactant. The governing equations are written in a usual immersed boundary formulation where a mixture of Eulerian flow and Lagrangian interfacial variables are used and the linkage between these two set of variables is provided by the Dirac delta function. The immersed boundary force comes from the surface tension which is affected by the distribution of surfactant along the interface. By tracking the interface in a Lagrangian manner, a simplified surfactant transport equation is derived. The numerical method involves solving the Navier–Stokes equations on a staggered grid by a semi-implicit pressure increment projection method where the immersed interfacial forces are calculated at the beginning of each time step. Once the velocity value and interfacial configurations are obtained, surfactant concentration is updated using the transport equation. In this paper, a new symmetric discretization for the surfactant concentration equation is proposed that ensures the surfactant mass conservation numerically. The effect of surfactant on drop deformation in a shear flow is investigated in detail.

Keywords: Immersed boundary method; Interfacial flow; Navier–Stokes equations; Surfactant

1. Introduction

In this paper, we propose an immersed boundary method for the simulation of two-dimensional fluid interfaces with insoluble surfactant. Surfactant are surface active agents that adhere to the fluid interface and affect the interface surface tension. Surfactant play an important role in many applications in the industries of food, cosmetics, oil, etc. For instance, the daily extraction of ore rely on the subtle effects introduced by the presence of surfactant [5]. In a liquid–liquid system, surfactant allow small droplets to be formed and used as an emulsion. Surfactant also play an important role in water purification and other applications where micro-sized bubbles are generated by lowering the surface tension of the liquid–gas interface. In microsystems with the

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presence of interfaces, it is extremely important to consider the effect of surfactant since in such cases the capillary effect dominates the inertia of the fluids [20].

The immersed boundary (IB) method proposed by Peskin [14], has been applied successfully to blood–valve interaction and other biological problems. The IB formulation employs a mixture of Eulerian and Lagrangian variables, where the immersed boundary is represented by a set of discrete Lagrangian markers embedding in the Eulerian fluid domain. Those markers can be treated as force generators to the fluid while being carried by the fluid motion. The interaction between the Lagrangian force generators (markers) and the fluid motion, described by variables defined on the fixed Eulerian grid, is linked by a properly chosen discretized delta function. Most IB applications in the literature belong to the fluid–structure problems, and they can be found in a recent review of Peskin [15]. However, there is comparatively less work on the application of the IB method to viscous, incompressible multi-phase flow problems. Perhaps the most successful one is the front-tracking method proposed by Tryggvason et al. [21,22] which uses an approach similar to the immersed boundary method.

In the case of interfacial flows with surfactant, Ceniceros [4] used a hybrid level set and front tracking approach to study the effects of surfactant on the formation of capillary waves. Lee and Pozrikids [12] used Peskin's immersed boundary idea to study the effects of surfactant on the deformation of drops and bubbles in Navier–Stokes flows. The surfactant convection–diffusion equation in these papers is based on the formulation proposed by Wong et al. [23], and the conservation of total mass of surfactant on the interface has not been rigorously investigated numerically.

James and Lowengrub [9] have proposed a surfactant-conserving volume-of-fluid method for interfacial flows with insoluble surfactant. Instead of solving the surfactant concentration equation based on Stone's derivation [19] directly, the authors relate the surfactant concentration to the ratio of the surfactant mass and surface area so that they are tracked independently. The method has been applied to study the axis-symmetric drop deformation in extensional flows. Recently, Xu et al. [25] develop a level-set method for interfacial Stokes flows with surfactant. Their method couples surfactant transport, solved in an Eulerian domain [26] with Stokes flow field, solved by the immersed interface method [11] with jump conditions across the interface. However, the method does not conserve the mass automatically and numerical scaling is used to enforce the conservation of surfactant on the interface numerically. Recently, Muradoglu and Tryggvason [13] have proposed a front-tracking method for computation of interfacial flows with soluble surfactant. They consider the axis-symmetric motion and deformation of a viscous drop moving in a circular tube.

In this paper, we propose an immersed boundary method to simulate the interfacial problems with insoluble surfactant. By tracking the interface in a Lagrangian manner, the surfactant concentration equation becomes much simpler than the one in [23]. Our numerical method involves solving the Navier–Stokes equations on a staggered grid by a semi-implicit pressure increment projection method where the immersed interfacial forces are calculated at the beginning of each time step. A new symmetric discretization for the surfactant concentration equation is proposed so that the total mass of surfactant is conserved numerically. The effect of surfactant on drop deformation in a shear flow is then investigated in detail.

The rest of the paper is organized as follows. In Section 2, we present the governing equations which includes the immersed boundary formulation and the surfactant concentration equation in Lagrangian coordinates on the interface. The numerical method is described in Section 3 which includes an algorithm of solving the Navier–Stokes equations and a conservative scheme for the surfactant equation. The effect of surfactant on drop deformation in a shear flow is investigated numerically in Section 4. Some concluding remarks and brief discussion on future directions are given in Section 5.

2. The governing equations

Consider an incompressible two-phase flow problem consisting of fluids 1 and 2 in a fixed two-dimensional square domain $\Omega = [a, b] \times [c, d] = \Omega_1 \cup \Omega_2$ where an interface Σ separates Ω_1 from Ω_2. Here, we assume the interface is a simple closed curve immersed in the fluid domain, and is contaminated by the surfactant so that the distribution of the surfactant changes the surface tension accordingly. In each fluid region, the Navier–Stokes equations are satisfied as