Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2017-0090

Vol. **23**, No. 3, pp. 640-664
March 2018

An Immersed Boundary Method for Simulating Interfacial Flows with Insoluble Surfactant in Three Dimensions

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Received 12 April 2017; Accepted (in revised version) 29 June 2017

Abstract. In this paper, an immersed boundary (IB) method for simulating the interfacial flows with insoluble surfactant in three dimensions is developed. We consider a doubly periodic interface separating two fluids where the surfactant exists only along the evolving interface. An equi-arclength parametrization is introduced in order to track the moving interface and maintain good Lagrangian meshes, so stable computations can be performed without remeshing. This surface mesh-control technique is done by adding two artificial tangential velocity components into the Lagrangian marker velocity so that the Lagrangian markers can be equi-arclength distributed during the time evolution. As a result, the surfactant equation on the interface must be modified based on the new parametrization. A conservative scheme for solving the modified surfactant equation has been developed and proved to satisfy the total surfactant mass exactly in discrete level. A series of numerical experiments consisting of the validation of Lagrangian mesh control technique, the convergence study, the study of self-healing dynamics, and the simulations of two-layer fluids under Couette flow have been conducted to test our present numerical scheme.

AMS subject classifications: 35Q35, 65M06, 76D45
Key words: Insoluble surfactant, a conservative scheme, mesh control, interfacial flow, Navier-Stokes flow, immersed boundary method.

1 Introduction

Surfactant is a typical compound of amphiphilic molecules with hydrophilic heads and hydrophobic tails. It adheres to the fluid interface and changes the surface tension accordingly. So, in the presence of surfactant, the dynamics of interfacial flows can be

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dramatically altered in complex ways due to the variable surface tension. For instance, a recent work of Pan et al. [37] demonstrates that by simply adding a small amount of surfactant, one can manipulate the impact outcome of droplet collision from coalescence to bouncing. Surfactant also plays a crucial role in numerous industrial applications including oil recovery, ore extraction, emulsification, pharmaceutical, and food industry [24], etc. Nowadays, we are benefited from scientific success with applications to its practical use; however, the understanding of surfactant effects is far from being complete.

For the past two decades, the interfacial flows with insoluble and soluble surfactant have been extensively studied by numerical computations. Those numerical methods are strongly relevant to how the interface is represented and how the surfactant convection-diffusion equation is solved along the evolving interface. For the soluble surfactant case, another coupling bulk convection-diffusion equation needs to be solved in one of bulk regions. In early computational models of surfactant problems, the boundary integral formulations in Stokes flow were extensively employed [12,28,30,31,40,46], refer to [35] for a review. In order to take the inertia effect into account, various numerical methods were proposed to incorporate with Navier-Stokes equations. These methods are based upon volume-of-fluid (VOF) [4, 11, 21], front-tracking method [9, 32, 33], immersed boundary method [7, 25–27], level-set [47, 48], and arbitrary Lagrangian-Eulerian (ALE) finite element method [3, 15–17, 19, 36]. Apart from the methods listed above, other numerical studies include diffuse-interface method [43], segmented projection method [22, 23], lattice Boltzmann method [13], moving particle semi-implicit method [14], and smoothed particle hydrodynamics (SPH) method [1] etc. Some hybrid approaches combining two different methods were proposed as well [6, 29, 49, 51]. In this paper, we extend the third author's previous 2D [25, 26] and axisymmetric [27] works and propose a three-dimensional immersed boundary (IB) method for simulating the evolution of a deforming interface with insoluble surfactant.

As known, solving the surfactant convection-diffusion equation on an evolving interface has already been a numerical challenge, especially in three-dimensional space. From the authors point of view, there are two major numerical issues to be considered carefully. (1) How to maintain the interfacial mesh quality to avoid Lagrangian markers clustering and surface mesh distortion without re-meshing? (2) How to guarantee that the total surfactant mass is conserved along the evolving interface without re-scaling? In this paper, we aim to propose a numerical scheme that can handle both issues systematically for an evolving free interface. Our numerical approach is outlined as follows. We first assume a doubly periodic interface separating two fluids where the surfactant exists only along the evolving interface. An equi-arclength parametrization is introduced in order to track the moving interface and maintain good Lagrangian meshes, so stable computations can be performed without re-meshing. This surface mesh-control technique is done by adding two artificial tangential velocity components into the Lagrangian marker velocity so that the Lagrangian markers can be equi-arclength distributed during the time evolution. As a result, the surfactant equation on the interface must be modified based on the new parametrization. A conservative scheme for solving the modified surfactant equation