A conservative scheme for solving coupled surface-bulk convection–diffusion equations with an application to interfacial flows with soluble surfactant

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ABSTRACT

Many physical problems arising in biological or material sciences involve solving partial differential equations in deformable interfaces or complex domains. For instance, the surfactant (an amphiphilic molecular) which usually favors the presence in the fluid interface may couple with the surfactant soluble in one of bulk domains through adsorption and desorption processes. Thus, it is important to accurately solve coupled surface-bulk convection–diffusion equations especially when the interface is moving. In this paper, we first rewrite the original bulk concentration equation in an irregular domain (soluble region) into a regular computational domain via the usage of the indicator function so that the concentration flux across the interface due to adsorption and desorption processes can be termed as a singular source in the modified equation. Based on the immersed boundary formulation, we then develop a new conservative scheme for solving this coupled surface-bulk concentration equations which the total surfactant mass is conserved in discrete sense. A series of numerical tests has been conducted to validate the present scheme. As an application, we extend our previous work [M.-C. Lai, Y.-H. Tseng, H. Huang, An immersed boundary method for interfacial flows with insoluble surfactant, J. Comput. Phys. 227 (2008) 7279–7293] to the soluble case. The effects of solubility of surfactant on drop deformations in a quiescent and shear flow are investigated in detail.

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1. Introduction

Many problems in biological, physical and material sciences involve solving partial differential equations in complex domains or deformable interfaces. In particular, the underlying material quantities in the bulk domain may couple with the one in the interface through adsorption and desorption processes. Meanwhile, the concentration of surface quantities might change the physical behavior of the interface through the modifications of interfacial forces. For instance, surfactant molecules typically consisting of a hydrophilic head and a hydrophobic tail may adsorb and desorb between bulk fluids and the interface so that the interfacial tension can be reduced. Meanwhile, this non-uniform distribution of surfactant molecules produce extra force (Marangoni force) along the tangential direction to affect the dynamics. In practice, the surfactant may be soluble only to some portion of bulk domain enclosed by the interface where the interface and the soluble region are evolving simultaneously. In order to simulate this problem, we have to introduce two surfactant concentrations in the

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system; namely, the surface concentration along the interface, and the volume concentration in the bulk region. Thus, one need to solve a coupled system of surface-bulk convection–diffusion equations [18,32,25].

Another example comes from cell biology applications where proteins inside the cell can diffuse and bind to the membrane whereas membrane-bound proteins can dissociate and diffuse to the inner cytoplasm [19]. To simulate this problem, one need to solve a coupled system of surface-volume reaction–diffusion equations. Many other examples in physical and biological systems that have the similar adsorption or desorption mechanisms in the dynamics can be found in Ref. [25].

It is known that solving a coupled system of surface-bulk equations in complex domains or deformable interfaces numerically is quite challenging especially when the interface (or the interior boundary of domains) is moving. Even in the case of only surface material (without bulk coupling), developing numerical methods for convection–diffusion equations on an evolving interface is still of major interest in scientific computing community. These methods include surface element method [5,6,9,10], level set method [2,7,29,24,17], and phase field method [23,25,11], just to name a few. Front tracking method is typically more accurate for one-dimensional interface (a curve in 2D space), but it can be more complicated to implement for two-dimensional surface especially the implementation involves surface mesh distortion or even topological changes. In [14], we have successfully developed a mass conservative scheme for convection–diffusion equation on moving interface and applied to simulate the interfacial flows with insoluble surfactant [14–16]. A recent work of Khatri and Tornberg [13] used segment projection method to represent the interface and solve the surfactant equation. More up-to-dated numerical methods for solving Navier–Stokes flows with insoluble surfactant can be found in [13] as well.

In this paper, we shall extend our previous work to soluble surfactant case. However, as a very first step, we need to develop a numerical scheme for solving coupled surface-bulk convection–diffusion equations. There are at least three major numerical issues from our point of view. (1) How to handle the adsorption and desorption between the interface and the bulk accurately? (2) How to maintain the total surfactant mass conserved during the evolution? (3) Since the surfactant might be soluble to only one of buck fluid, how to avoid the surfactant being present in other bulk regions via either convection or diffusion mechanism? Here, we formulate the coupled surface-bulk convection–diffusion equations in the immersed boundary framework so that the adsorption and desorption processes can be termed as a singular source in the bulk equation. Moreover, by using the indicator function, we can embed the bulk equation into the whole computational domain so that regular Eulerian finite difference scheme can be applied without handling the complicated moving irregular domain. We develop a new conservative scheme for solving the coupled bulk-surface concentration equations which the total surfactant mass can be conserved exactly in discrete sense. By introducing the indicator function and solving the bulk equation in the regular computational domain, one can avoid evaluating the surfactant flux across the interface due to adsorption and desorption processes.

The present formulation is similar to other front tracking approaches such as in [32,18] but differs from their numerical computations. For instance, in order to let the surfactant be depleted from only one bulk phase, some one-sided discretized delta functions were used in [32] which results the numerical integration of the discrete function does not yield the exact value of unity. The authors have tried different forms of one-sided delta function and the mass error is within 1%. Here, we use the traditional discrete delta function for the spreading and interpolating operators in the immersed boundary method so that the surfactant mass leaking error is much smaller compared with [32]. There are other numerical methods in literature for interfacial flows with soluble surfactant dynamics such as in [1,4,26,31].

The rest of the paper is organized as follows. In Section 2, we present a coupled surface-bulk concentration model and discuss their conservation property. By employing the indicator function, we then embed the bulk equation into a regular Cartesian computational domain. Based on our immersed boundary formulation, we develop a conservative scheme for solving the coupled surface-bulk equations in Section 3. As an application, we apply the present scheme to solve Navier–Stokes flow with soluble surfactant in Section 4. In Section 5, a detailed numerical tests have been conducted to validate our present scheme and study the effect of soluble surfactant on drop deformations in a quiescent and shear flow.

2. A coupled surface-bulk concentration model

As in [25], we consider the same coupled bulk-surface material (or surfactant) concentration model in which the adsorption and desorption can be occurred on the moving deformable interface. Consider a domain Ω in R^2 and there is an interface Σ, which is a simple closed curve immersed in Ω. The interior of the interface is Ω_0, and the exterior is Ω_1 so that $\Omega = \Omega_0 \cup \Omega_1$, see the illustration of these domains in Fig. 1. The interface is represented by a Lagrangian form $\boldsymbol{X}(\alpha, t), 0 \leqslant \alpha \leqslant L_b$, where α is the Lagrangian material coordinate attached to the interface which is not necessarily to be the arc-length parameter. The unit tangent vector of the interface can be written as $\boldsymbol{\tau} = \frac{\partial \boldsymbol{X}}{\partial \alpha} / |\frac{\partial \boldsymbol{X}}{\partial \alpha}|$; thus, the unit outward normal vector $\boldsymbol{n}$ pointing into Ω_1 can be defined accordingly. In addition, the interface Σ is moving with a given velocity field $\boldsymbol{u} = (u, v)$ in Ω; that is,

$$\frac{\partial \boldsymbol{X}(\alpha, t)}{\partial t} = \boldsymbol{U}(\alpha, t) = \int_{\Omega} \boldsymbol{u}(\boldsymbol{x}, t) \delta(\boldsymbol{x} - \boldsymbol{X}(\alpha, t)) \, d\boldsymbol{x}, \tag{1}$$

where $\delta(\boldsymbol{x}) = \delta(x)\delta(y)$ is the two-dimensional Dirac delta function. We use the above usual delta function formulation in the immersed boundary method [20] to represent the interpolation of the velocity field into the interface. Here we assume