Journal of Computational Physics 256 (2014) 768–790

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

An embedded boundary method for soluble surfactants with interface tracking for two-phase flows

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ARTICLE INFO

Article history:
Received 14 April 2013
Received in revised form 22 August 2013
Accepted 7 September 2013
Available online 18 September 2013

Keywords:
Soluble surfactants
Embedded boundary method
Interface tracking
Two-phase flows
Strang splitting
Marangoni forces

ABSTRACT

Surfactants, surface reacting agents, lower the surface tension of the interface between fluids in multiphase flow. This capability of surfactants makes them ideal for many applications, including wetting, foaming, and dispersing. Due to their molecular composition, surfactants are adsorbed from the bulk fluid to the interface between the fluids, leading to different concentrations on the interface and in the fluid.

In a previous paper [21], we introduced a new second order method using uniform grids to simulate insoluble surfactants in multiphase flow. This method used Strang splitting allowing for a fully second order treatment in time. Here, we use the same numerical methods to explicitly represent the singular interface, treat the interfacial surfactant concentration, and couple with the Navier–Stokes equations. Now, we introduce a second order method for the surfactants in the bulk that continues to allow the use of regular grids for the full problem. Difficulties arise since the boundary condition for the bulk concentration, which handles the flux of surfactant between the interface and bulk fluid, is applied at the interface which cuts arbitrarily through the regular grid. We extend the embedded boundary method, introduced in [22], to handle this challenge.

Through our results, we present the effect of the solubility of the surfactants. We show results of drop dynamics due to resulting Marangoni stresses and of drop deformations in shear flow in the presence of soluble surfactants. There is a large nondimensional parameter space over which we try to understand the drop dynamics.

1. Introduction

Surfactants, surface reacting agents, are known to decrease the surface tension at interfaces between fluids. Surfactant molecules are composed of hydrophobic tails and hydrophilic heads. Due to this molecular composition, surfactants are adsorbed as a monomolecular layer to the interface between fluids. Soluble surfactants are present both in the surrounding fluid and on the interface, unlike insoluble surfactants which exist only on the interface. The concentration on the interface is different from that in the bulk fluid due to the affinity the molecules have to the interface. Adsorption and desorption of the surfactant molecules to and from the interface plays a role in the dynamics of the flow. A common example of a surfactant which lowers the surface tension of interfaces is detergent [32].

Having control of the surface tension is important in many applications. Surfactants give us the ability to have this control. A recent example includes the use of dispersants by BP in the 2010 Deepwater Horizon oil spill. Dispersants,

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0021-9991/$ – see front matter
http://dx.doi.org/10.1016/j.jcp.2013.09.019

consisting of surfactants, were used to try to dilute and disperse the oil in the spill, by making the oil more soluble in the water. There is not a full understanding of the effects of dispersant use in oil spills [8]. Studies, such as the one presented here, can help to bring more understanding to such situations.

Surfactants are often used in many practical applications. For example, surfactants can help with wetting, foaming, and dispersing, and can be used as an emulsifier. This allows them to be used in microfluidic applications, pharmaceuticals, suspensions, cosmetics, and in many more products [25,34,4]. One example is the use of surfactants to help hydrophobic surfaces adsorb the ink in inkjet printing [17].

Surfactants are also important in biology. Currently, biosurfactants, surfactants of microbial origin, are being studied to be used in the above applications, as chemical surfactants may have a negative environmental impact [5]. Cells of the alveoli in the lung are known to secrete surfactants to lower the surface tension forces in the lung fluid [47]. Another biological application of surfactants is in the treatment of decompression illness. Decompression illness is when gas bubbles enter the bloodstream, often caused by surgery or when the pressure around the body has changed drastically [9,52].

Since surfactants play a major role in many applications and are also present in nature, having an understanding of their behavior is important. In this paper, we present a mathematical model and numerical method to simulate multiphase flow in the presence of soluble surfactants.

An insoluble surfactant is present only at the interface between the two fluids, and is not soluble in the bulk phase. The evolution of insoluble surfactants can be described by a partial differential equation defined on the time dependent interface, which is a challenge to simulate accurately. The strengths of the surface tension forces depend on the interfacial surfactant concentration as modeled e.g. by the Langmuir equation of state. Soluble surfactants are soluble in one or both bulk phases, and hence there will be adsorption of surfactants to the interface and desorption from the interface. Often, it is assumed in models that surfactants are insoluble. By conducting numerical simulations with both insoluble and soluble surfactants, we hope to bring some understanding of when solubility is important. The flux of surfactants between the interface and the bulk can be modeled with a source term in the differential equation for the interfacial surfactant concentration and with a flux boundary condition at the interface for the volume surfactant concentration. Since the flux depends on both the bulk concentration and the interfacial concentration, the boundary condition effectively becomes a mixed Neumann–Dirichlet boundary condition. Hence, treating soluble surfactants yields the additional challenge of solving the advection-diffusion equation on one side of the interface while imposing boundary conditions at the location of the moving and deforming interface.

In recent years, a considerable effort has been made to develop numerical methods able to simulate multiphase flows with insoluble surfactants. These methods are based on different numerical techniques to represent the interfaces, including front tracking and boundary integral methods, level set methods, and finite volume methods. Front tracking and boundary integral methods include Lagrangian points to track the interface and the interfacial surfactant concentration is solved for at these irregularly spaced points [30,14,23]. Also, front tracking methods to represent the interface have been combined with finite volume methods to handle the surfactants [50,24,6,16]. Level set methods track the interface as the zero level set of a function one dimension higher than the interface dimension. The surfactants are also solved for in a band around the interface in this higher dimension [1,49,48]. Volume of fluid (VOF) methods measure the volume of the two immiscible fluids in numerical cells to track the interface. A VOF method is also used then to solve for the surfactant concentration along the interface [18,33,13]. In a previous paper [21], we present a numerical method to model insoluble surfactants using the Segment Projection Method (SPM) [43] to represent the interface. This will be explained further below, as we discuss the extension to soluble surfactants.

The works listed above all model insoluble surfactants. Work has recently begun on developing numerical methods for soluble surfactants. Stebe et al. have presented theory with some experiments and simulations for soluble surfactants in [15,19,39]. They do not solve for the bulk surfactants, but rather assume that the adsorption and desorption of surfactants from the bulk is diffusion dominated and the bulk surfactant concentration is a constant. The front tracking method has been used to represent the interface coupled with a finite difference solver for the surfactants in methods developed by Muradoglu, Tryggvason et al. [29,40] and Zhang, Eckmann, and Ayyaswamy [52]. Also, a few other methods, including the VOF method, smoothed particle hydrodynamics, and phase field-modeling have been used to simulate soluble surfactants [3,2,28,41,51]. Booty and Siegel, in [7], address the issues that arise when there is a large bulk Peclet number.

In the Segment Projection Method (SPM) [43], an interface between two phases of a fluid in two dimensions is modeled by dividing the interface into overlapping segments. Each segment is described as a single valued function of a specific coordinate plane, resulting in a graph representation of the interface. A partial differential equation is used to advect the interface with the fluid flow. This equation is discretized using standard numerical methods on a uniform grid of the same dimension as the interface. The interfacial surfactant concentration is defined on these segments and the partial differential equation for the concentration is solved on the same uniform grids using similar standard numerical methods. This is very useful, as we introduce an implicit in time treatment of the diffusion of surfactants on the interface. By using the SPM, we benefit from both an explicit representation of the interface, as in Lagrangian point representations, and from the use of regular grids as in level set representations, without increasing the dimensionality of the problem.

When the surfactants are soluble in the bulk fluid, we couple the SPM for the interface and interfacial surfactant concentration with a separate advection-diffusion equation for the bulk surfactant concentration, as discussed above. We discretize the bulk surfactant concentration equation on a uniform two-dimensional grid. The mixed Neumann–Dirichlet boundary condition that arises from the exchange with the interfacial surfactants is to be applied at the interface that cuts arbitrarily