Commun. Comput. Phys.
doi: 10.4208/cicp.281009.120210a

Vol. 8, No. 4, pp. 735-757
October 2010

Numerical Simulation of Moving Contact Lines with Surfactant by Immersed Boundary Method

Ming-Chih Lai[1,*], Yu-Hau Tseng[1] and Huaxiong Huang[2]

[1] *Center of Mathematical Modeling and Scientific Computing Department of Applied Mathematics, National Chiao Tung University, 1001, Ta Hsueh Road, Hsinchu 300, Taiwan.*
[2] *Department of Mathematics and Statistics, York University, Toronto, Ontario, M3J 1P3, Canada.*

Received 28 October 2009; Accepted (in revised version) 12 February 2010

Available online 17 May 2010

Abstract. In this paper, we present an immersed boundary method for simulating moving contact lines with surfactant. The governing equations are the incompressible Navier-Stokes equations with the usual mixture of Eulerian fluid variables and Lagrangian interfacial markers. The immersed boundary force has two components: one from the nonhomogeneous surface tension determined by the distribution of surfactant along the fluid interface, and the other from unbalanced Young's force at the moving contact lines. An artificial tangential velocity has been added to the Lagrangian markers to ensure that the markers are uniformly distributed at all times. The corresponding modified surfactant equation is solved in a way such that the total surfactant mass is conserved. Numerical experiments including convergence analysis are carefully conducted. The effect of the surfactant on the motion of hydrophilic and hydrophobic drops are investigated in detail.

AMS subject classifications: 65M06, 76D45

Key words: Immersed boundary method, interfacial flow, Navier-Stokes equations, surfactant, moving contact line, hydrophilic drop, hydrophobic drop, wetting.

1 Introduction

Surfactant are surface active agents that adhere to the fluid interface and reduce the interface tension by lowering the surface energy. Surfactant play an important role in many applications in the food, cosmetics and oil industries. For instance, extraction of ore relies

*Corresponding author. *Email addresses:* mclai@math.nctu.edu.tw (M.-C. Lai), yhtseng@math.nctu.edu.tw (Y.-H. Tseng), hhuang@yorku.ca (H. Huang)

on the subtle effects introduced by the presence of surfactant [3]. 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 at the liquid-gas interface. In microsystems with the 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 [33].

When a fluid-fluid interface is in contact with a solid substrate, surfactant can change the wetting properties by altering the value of the contact angle. This simple fact has found may interesting applications in our daily life and industrial processes. For example, we add detergents (surfactant) in washing machine to clean our clothes more effectively. The detergent helps to remove drops of grease from clothes by increasing the contact angle (measured from inside the drop). An idealization of this problem can be found in a photo shown in [33] or a figure in [3] where it is demonstrated that a drop on clothes can become less ”wetting” (from the drop point of view) by increasing surfactant concentration. By adding surfactant, a drop which sticks to clothes becomes less "sticky" and the water currents can wash away the drop readily. The physical situation corresponding to this idealized system includes a solid-drop (grease)-water system and the surfactant. Mathematically, as discussed more detail in the main text of this paper, this is a moving contact line problem since the solid-drop (grease)-water triple intersection forms a contact line. The main issue we will try to address in this paper is how surfactant, by changing the contact angle, affects the movement of the contact line.

In the past few years, several numerical methods have been developed for interfacial flows with surfactant, such as the level set method [35], volume-of-fluid method [14], front-tracking method [16, 20], and hybrid methods [1]. Recently, we have proposed an immersed boundary method for simulating the motion of two-dimensional fluid interfaces with insoluble surfactant [15]. The mathematical models include the incompressible Navier-Stokes equations and a surfactant concentration equation along the moving interface. A numerical scheme that conserves the total surfactant mass is introduced and drop deformation under shear flow is studied in detail. In the present work, the Navier-Stokes solver is similar to our previous one in [15] with one modification. Instead of moving with the fluid as in [15], the present Lagrangian markers are uniformly distributed along the interface during the time evolution. This is achieved by using an artificial tangential velocity. Despite this modification, our new scheme for the surfactant equation still conserves the total surfactant mass exactly.

Moving contact line problems arise when one fluid is displaced by another immiscible fluid on a solid surface. They appear in the process of wetting, coating and many biological applications [3, 21, 29]. It is well-known that the no-slip boundary condition in the vicinity of the moving contact line leads to a non-integrable stress singularity [5, 12, 29]. In other words, if the no-slip boundary condition is imposed on the solid substrate, an infinite force is required to move the contact line. For the past three decades, many attempts have been made to resolve this physically unrealistic force singularity. It has been