Effects of an Insoluble Surfactant on the Deformation of a Falling Drop Towards a Solid Surface

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***Abstract*:** A numerical method is implemented to investigate the influence of an insoluble surfactant on the deformation of a falling drop normal to a solid surface. In the constructed model, the liquid drop falls due to the gravity. The front-tracking method is used to solve free boundary motion of the two-phase Navier-Stokes equations and the surfactant evolution. Results show that the surfactant affects to slow the falling drop; more significant for a relatively small drop than a big one. When the drop has attained the solid surface, the contained-surfactant drop deforms easier than the free-surfactant drop.

***Keywords*:** Insoluble surfactant, falling drop, the front-tracking method**.**

1. Introduction

Surfactants (or surface-active agents) are typically molecules that accumulate at fluid interface and affect to decrease the interfacial tension. The decreasing of the interfacial tension can occur if surfactant concentration is not uniform at the interface, which is called the Marangoni effect. This effect can influence the dynamics of multiphase flow systems [7], including for a falling drop case. The goal of this work is to provide a numerical investigation about the influence of the surfactant to the deformation of falling drop. Its applications can be seen in many fields, ranging from biomedical to enhanced oil recovery.

The deformation of a falling drop has been investigated by many researchers. Pozrikidis [9] investigated numerically the deformation of a viscous drop moving under the action of gravity normal to a plane solid wall. She found that the deformation of the drop depends on the surface tension, the initial position, the initial shape, the viscosity ratio, and the inverse Bond number. While, Middleman [6] reviewed several problems about the slowly approach of a viscous drop to a solid surface, including the terminal velocity of drop in the Stokes flow regime, and the thickness of the separating fluid between a deformable drop and the lower solid surface.

Related to the presence of the surfactant on an interface, there were some early works that studied the influence of the surfactant to the deformation and breakup of drops; mostly for a drop in a shear flow case. Lai et al. [2] proposed the immersed boundary method to examine the effect of surfactant to the deformation of a drop in a steady shear flow. They neglected the gravity and assumed that both fluids have equal viscosity and density. Lee and Pozrikidis [4] also studied this issue for two-dimensional drop with arbitrary viscosity in a simple shear flow. They applied an algorithm which combines Peskin's immersed-interface method with the diffuse-interface approximation. They found the possibility of interface immobilization due to Marangoni tractions. Teigen et al. [8] simulated a drop in shear flow in the presence of a soluble surfactant . They couple the diffuse interface approach with the solution of the Navier–Stokes equations. James and Lowengrub [11] constructed a surfactant-conserving volume-of-fluid method to study the effects of insoluble surfactants on interfacial flows for a drop in an extensional flow. Xu et al. [10] presented a level-set method for computations of interfacial flows with insoluble surfactants then applied it to examine the effects of insoluble surfactants on single drop, drop–drop interactions, and interactions of many drops in Stokes flow under a steady applied shear. Ganesan and Tobiska [1] proposed an interface-resolving moving mesh finite-element scheme for the simulation of 3D-axisymmetric rising bubble with soluble surfactants. One of the results is the presence of surfactant retarding the rising bubble. Wellington et al. [12] studied the three-dimensional deformation of a bubble under shear flow in the presence of an insoluble surfactant. They used a finite-volume discretization with an adaptive mesh refinement/immersed boundary methodology.

In this paper, we examine effects of the surfactant on the deformation of a falling drop towards the solid surface with variety sizes. The drop and the bulk fluid have different viscosity and density. Here we include the gravity force, and the surface force causing by the surfactant. The surfactant is insoluble and is assumed to affect the drop on the interface only.

The paper is organized as follows. In Section 2, we model the problem and state the formulation. In Section 3 we present the numerical simulations. The grid convergence and mass conservation of the drop and the surfactant concentration at the interface are also showed to validate the simulations. Conclusions are written in Sec. 4.

2. The Mathematical Model

We consider two immiscible fluids in a fixed two-dimensional square domain Ω=[a, b] × [c, d]. Fluid 1 is a drop which is surrounded by fluid 2. Both fluids are separated by an interface Σ, which is contaminated by a surfactant (Figure 1). We assume that the surfactant is insoluble and distributed at the interface by convection. Furthermore, the surfactant concentration is assumed to be sufficiently small, hence it affects only to the interfacial tension, without any more complex dynamical or rheological effects.

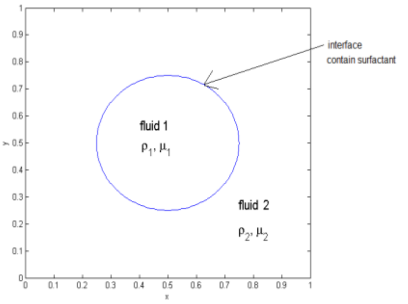


Figure 1. The drop immersed in another fluid.

The motion of the drop and the bulk fluid can be formulated by the two-phase incompressible Navier-Stokes equations [6, 13]:

$$\rho_i \frac{\partial \boldsymbol{u}_i}{\partial t} + \rho_i \nabla.\, \boldsymbol{u}_i \boldsymbol{u}_i = -\nabla p_i + \rho_i \boldsymbol{g} + \nabla.\, \mu_i (\nabla \boldsymbol{u}_i + \nabla^T \boldsymbol{u}_i) + \boldsymbol{f}, \quad (1)$$

$$\nabla \boldsymbol{u}_i = 0, \quad i = 1, 2 \quad (2)$$

where ρ is the density of the fluids, p is the pressure, $\boldsymbol{u}$ is the fluids velocity, $\boldsymbol{g}$ is the gravity, and μ is the viscosity. The notation $\boldsymbol{f}$ is the body force acting on the fluids due to the interfacial force $\boldsymbol{F}$:

$$\boldsymbol{F}(s,t) = \frac{\partial}{\partial s}\left(\sigma(s,t)\boldsymbol{\tau}(s,t)\right), \quad (3)$$

where σ is the surface tension, and $\boldsymbol{\tau}$ is a unit tangent to the interface. The relation between $\boldsymbol{f}$ and $\boldsymbol{F}$ is stated by:

$$\boldsymbol{f}(\boldsymbol{x},t) = \int_0^{Lb} \boldsymbol{F}(\boldsymbol{X}(s),t)\,\delta(\boldsymbol{x} - \boldsymbol{X}(s))\,ds, \quad (4)$$

where $\boldsymbol{X}(s), 0 \le s \le L_b$ is a parameter for the interface Σ, and δ is the two-dimensional dirac delta function. Note that the surface tension force $\boldsymbol{f}$ is different from zero only on the interface, vanishing everywhere else [12].

The interface moves with the fluid flows, which can described by:

$$\frac{\partial \boldsymbol{X}(s,t)}{\partial t} = \boldsymbol{u}(\boldsymbol{X}(s,t)), \quad (5)$$

The relation between surface tension (σ) and surfactant concentration (Γ) can be stated by the simplified nonlinear Langmuir equation [5]:

$$\sigma(\Gamma) = \sigma_c(1 + \ln(1 - \xi\Gamma)), \quad (6)$$

where σ_c is the surface tension related to zero surfactant concentration, and ξ is the sensitivity of surface tension to change because of the surfactant. On the other hand, the dynamic of the surfactant on the interface satisfies:

$$\frac{\partial \Gamma}{\partial t} + (\nabla_s.\, \boldsymbol{u})\Gamma = 0, \quad (7)$$

where ∇_s is the surface divergence.

3. Numerical Results

In this section, we show some numerical results about the effect of the surfactant to the deformation of a falling drop. The numerical solution is obtained by using the front tracking method, which is completely discussed in [14]. We use a computational domain Ω=[0,1] × [0,1], where a circular drop with radius r is initially located at (0.5, 0.3). This point was chosen as an illustration only. The initial surfactant concentration distributes uniformly, $\Gamma(s,0)=1$. The initial fluid velocity is set to be zero everywhere.

3.1 Validation of Numerical Algorithm

An important property reflecting the accuracy of our simulations is the conservation of mass, for the drop and the surfactant concentration. To verify this property, in the Tabel 1 we present the change of the drop area up to time T=0.125, for some refinement grids. The similar treatment also conducted to the surfactant concentration. Here we use A_{ref} and Γ_{ref} are initially the area of drop (πr^2) and the total surfactant concentration ($2\pi r$), respectively. The interface mesh is chosen $\Delta s = \frac{2\pi}{180}$, and the time step size is $\Delta t = 1.25\ 10^{-3}$.

Table 1. The Change of the Drop Area and the Surfactant Concentration

r	Size mesh	$\lvert\Gamma - \Gamma_{ref}\rvert$	Error (%)	$\lvert A - A_{ref}\rvert$	Error (%)
0.25	1/32	0.466	7.424	$2.49\ 10^{-4}$	0.025
0.25	1/64	0.169	2.690	$2\ 10^{-6}$	0
0.1	1/32	0.641	10.202	$4.99\ 10^{-5}$	0.001
0.1	1/64	0.300	4.778	$2.72\ 10^{-5}$	0.086

From the Table 1, we can see that the conservation of mass for the drop is satisfied, whereas the error for the sum of surfactant concentration substantially decreases, as the mesh is refined. Now, we consider the error for the small size mesh $\Delta x = \Delta y = \frac{1}{64}$. The changes of the sum of surfactant concentration for both radius r are less than 4.8%; the numerical error is quite acceptable. These results suggest that our constructed numerical schemes are quite accurate. The simulations of the liquid drop deformation are shown in Section 3.2.

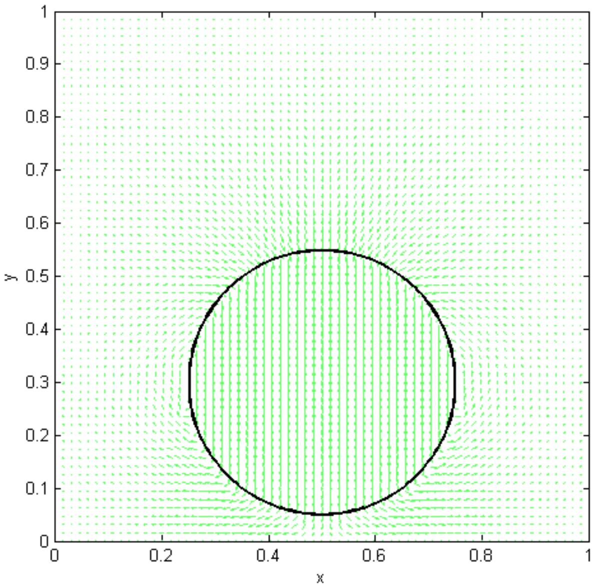
3.2 Simulations

In this section, we present several numerical experiments to investigate the influence of surfactant to deformation of a falling drop. For the following simulation, we choose the mesh width which have small errors, that is $\Delta x = \Delta y = \frac{1}{64}$.

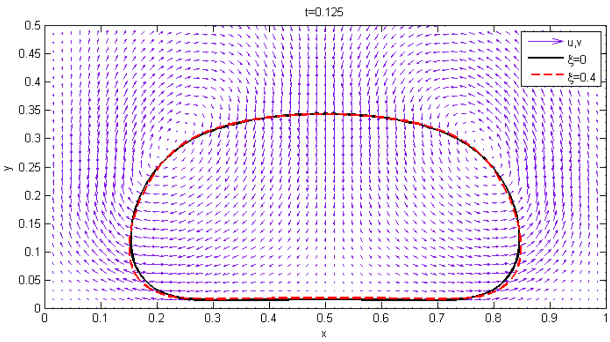
3.2.1 A Big Drop Case

The comparisons of the drop deformation in the absence ($\xi = 0$) and presence ($\xi = 0.4$) of the surfactant, are ilustrated in Figure 2. In this simulation we take the radius of drop r=0.25, with phisycally parameter μ_1=0.01, μ_2=0.1, ρ_1=1, ρ_2=2, g=100. Since the density of the drop is higher than the bulk fluid, then the drop moves down to the solid surface. From the Figure 2(b), it can be seen that the difference of the drops deformation between absence and presence of the surfactant at T=0.125 hardly differs. In order to zoom-in the difference, the heights of the lowest point on the both drops to the solid surface are also compared, which is shown in Figure 3. From this figure, it can be seen that the surfactant slightly delays the time for the drop to attain the solid surface.

However, increasing T to become T=0.25, when the drops has attained the solid surface, both drops behave differently; the surfactant-covered drop deforms easier than the clean drop (see Figure 4). This result can be explained as follows: Figure 5 shows the distribution of surfactant concentration at T=0 (dashed-dotted line), and at T=0.25 (solid line) together with the corresponding surface tension (dotted line). It can be observed that at T=0.25, the surfactant concentration located around 0° and 180° is higher than other locations. This is because the surfactant has been convected in the direction of the fluids velocity (see Figure 4). As the result, the surface tension of the surfactant-covered drop around 0° and 180° significantly decreases, causing the part of the surfactant-covered drop on that spots deforms easier than the clean drop.



(a)



(b)

Figure 2. The deformation of falling drops with radius r=0.25 at time T, (a). T=0, (b). T=0.125.

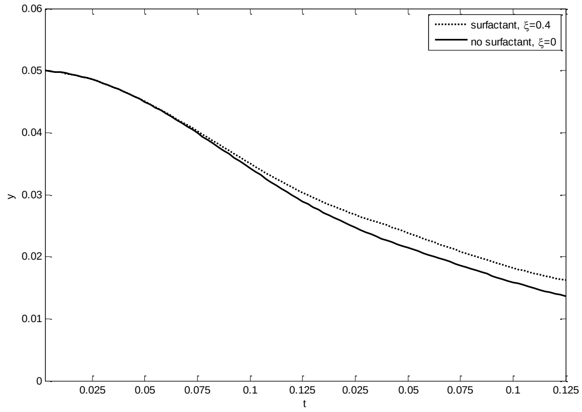


Figure 3. The height of the lowest point of the drop to the solid surface; clean (solid line) and surfactant-covered (dotted line).

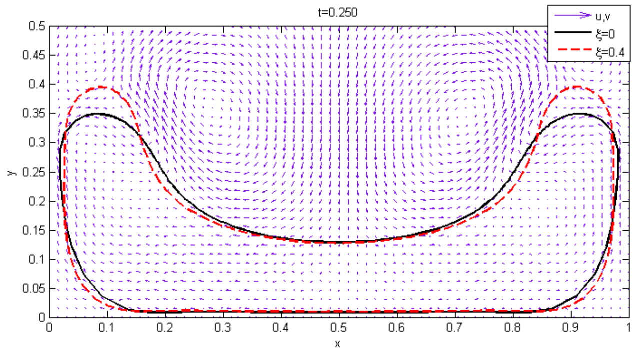


Figure 4. The deformation of drop after attain the solid surface, for absence (solid line) and presence of the surfactant (dashed line).

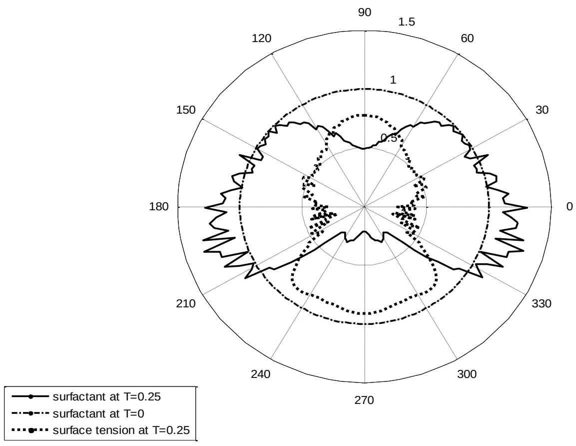


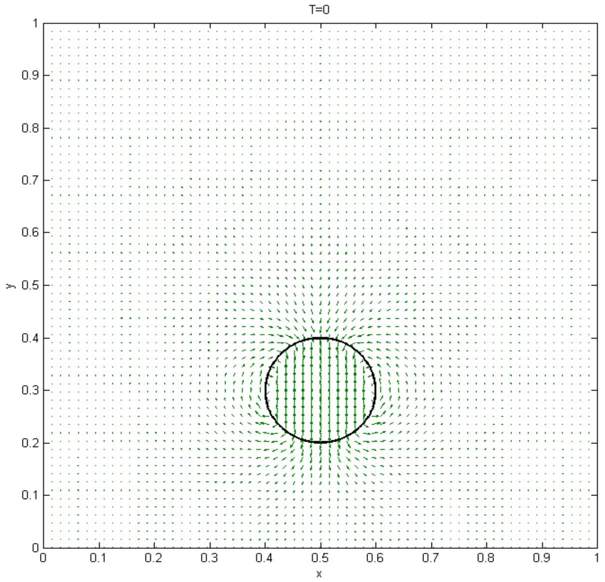
Figure 5. The distribution of surfactant at T=0 and T=0.250, the surface tension at T=0.250.

3.2.2 A Small Drop Case

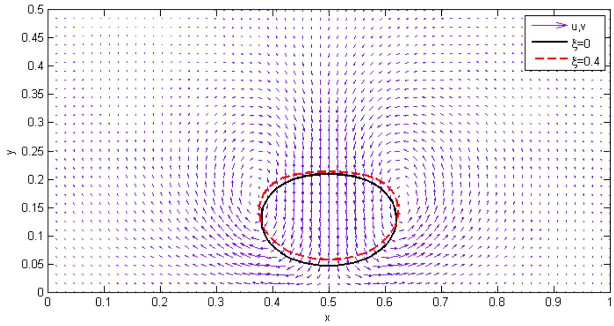
Since the surfactant affects only on the interfacial tension, then in this section we investigate the influence of surfactant for a small drop. Here we take the radius of drop r=0.1, and keep the other parameters as same as in the big drop case.

Similar with the big drop, the surfactant retards the fall of small liquid drop (Figure 6(b)). Furthermore, in Figure 7 we present the position difference for every corresponding point

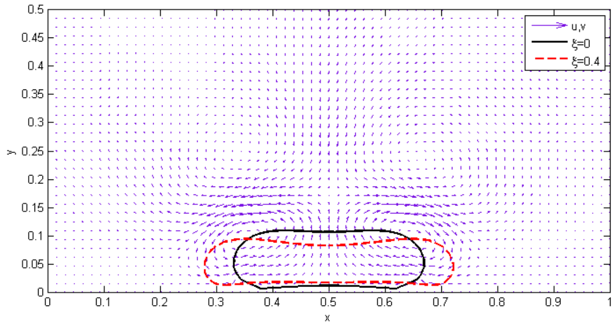
between the clean drop and the covered-surfactant drop at T=0.125; for the small drop (·) and the big drop (*). From that figure, we should have remark that the surfactant effect on the retardation of the drop is clearer for the small drop than the big drop.
In the case the drops have attained the solid surface, the surfactant-covered small drop also deforms easier than the clean-surfactant drop (Figure 6(c)). Similar to the big drop case, this result occurs because the surfactant concentration located around 0° and 180° is higher than other locations.



(a)



(b)



(c)

Figure 6. The deformation of falling drop with radius r=0.1 at time T, (a). T=0, (b).T=0.125, (c). T=0.25.

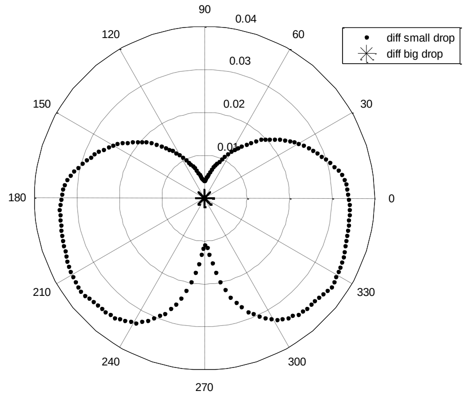


Figure 7. The position difference between clean drop and covered-surfactant drop at T=0.125; for the small drop (·) and the big drop (*).

4. Conclusions

In this paper we developed a model for two-phase incompressible flows with insoluble surfactant that admits mass conservative law. The presence of the surfactant at the interface had effect to slow the falling drop. The surfactant affected more significant for the retardation of a relatively small liquid drop than the big one. When the drop has attained the solid surface, the surfactant-covered drop deforms easier than the clean-surfactant drop.

5. Acknowledgements

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