Computational Fluid Dynamics Simulation of the Behavior of Droplet Rising in Water Column with the Effect of Surfactant

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Abstract

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Dispersants decrease the oil-water interfacial tension causing oil droplets to breakup into smaller ones and to be dispersed in the water column. This paper presents the analysis of the behavior of an oil droplet in water containing dispersant. We implemented additional equations to account for the oil-water interfacial tension due to the presence of surfactant and those equations were incorporated into FLUENT by using a UDF (User Defined Function). It was observed that the surfactant concentration was higher at the bottom of and the streams of oil emerging from the droplet due to shear. The presence of surfactant affected the deformation process of oil droplets of different diameters: When surfactant is well-mixed in bulk, the oil droplet tended to peel off a big chunk of oil with tip-streaming. However, tip streaming was only at the rear cap for oil droplet premixed with surfactant. The presence of surfactant decreased the rising speed of oil droplets compared to the terminal velocity of clean oil droplet. The results may be valuable to help us to apply surfactant to oil spill in a more efficient way.

Goal of the Study

- Develop a robust numerical model to account for the effect of surfactant
- Understand how surfactant affect the breakup of oil droplet
- The difference in role of premixed surfactant and surfactant in bulk.

Introduction

Dispersant is mixture of solvents, surfactants, and other additives that applied to oil slicks to reduce the oil-water interfacial tension. Surfactant is the main effective component of dispersant to reduce the surface tension of oil droplets to allow the large oil droplets be dispersed into smaller droplets in the open water field.

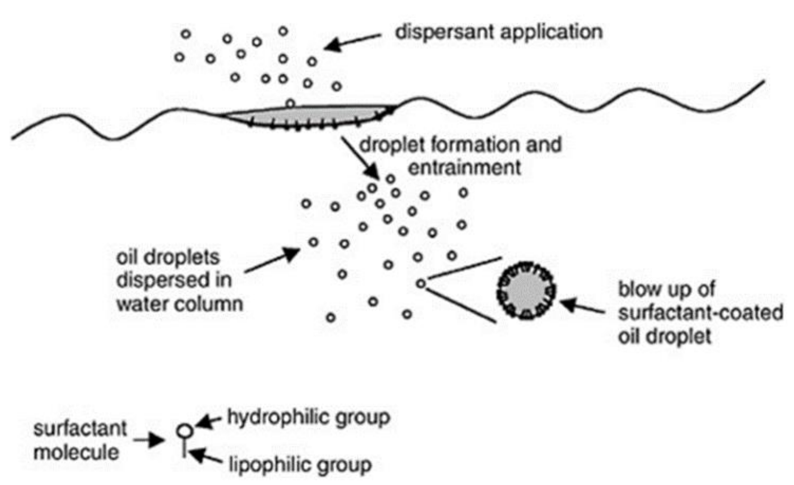

Figure 1: How surfactant works on oil droplet (http://www.nap.edu/read/11283/chapter/5#53)

Methods

Governing equations

The convection-diffusion equations on the interface:

$$\frac{\partial \Gamma}{\partial t} + \nabla_s \cdot (\Gamma \vec{u}_s) = D_s \nabla_s^2 \Gamma + S_\Gamma \qquad (1)$$

where S_Γ represents the source term due to the net adsorption of surfactant at the interface:

$$S_\Gamma = \kappa_a C_s (\Gamma_\infty - \Gamma) - \kappa_d \Gamma \qquad (2)$$

κ_a and κ_d indicate the rate constant of adsorption and desorption, respectively.

The interfacial tension and surfactant concentration:

We assume a linear relationship between interfacial tension (σ) and surfactant concentration(Γ):

$$\sigma = \begin{cases} \sigma_0 - 0.016 * \dfrac{\Gamma}{\Gamma_\infty}, \Gamma < \Gamma_\infty \\ 0.004, \Gamma \geq \Gamma_\infty \end{cases} \qquad (3)$$

In FLUENT, the interface is identified by volume fraction of oil to be 0.5 (e.g., cells with volume fraction is 0.5 is treated as interface).

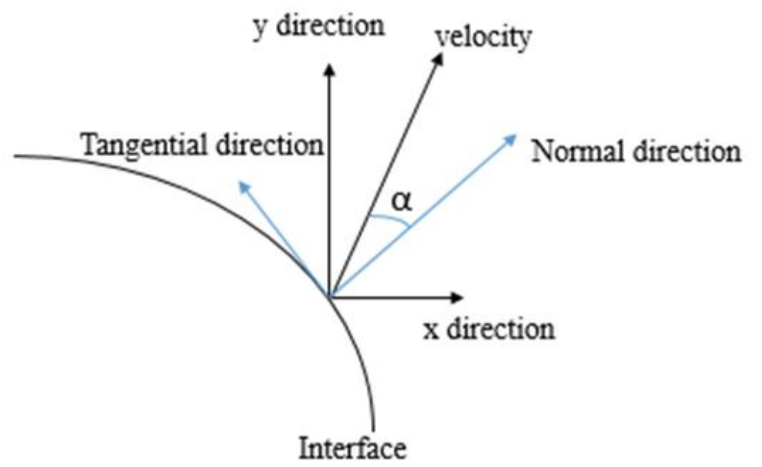

Figure 2: The coordinates in the computational domain.

The velocity along the oil droplet surface (u_s):

$$\vec{u}_s = \cos\alpha * \vec{u} \qquad (4)$$

$$\cos\alpha = \frac{n_x}{\sqrt{n_x^2 + n_y^2}} \qquad (5)$$

Equation (1)-(5) are implemented as User Defined Functions (UDF) in FLUENT to evaluate the influence of surfactant 2D axisymmetric boundary condition is applied.

The solution methods in Fluent:
- Momentum: Second order
- Volume fraction: Geo-Reconstruct
- Surfactant concentration: Second order
- Pressure: PRESTO

Table 2: The information implemented in the present simulation	
Initial bulk concentration (C_0)	0.0021 mol/L
Diffusion coefficient along the interface (D_s)	$1.0*10^{-8}$ m^2/s
Maximum surface excess concentration (Γ_∞)	$4.0*10^{-6}$ mol/m^2
Initial interfacial tension under clean environment (σ_0)	0.02 N/m

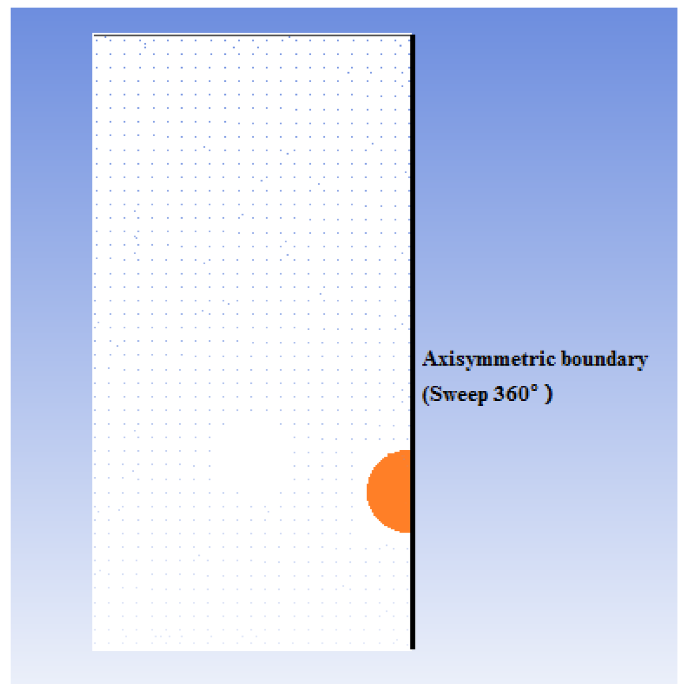

Figure 3: The mesh and axisymmetric boundary conditions used in the present simulation (The plane sweep 360 ° along the axis)

Results

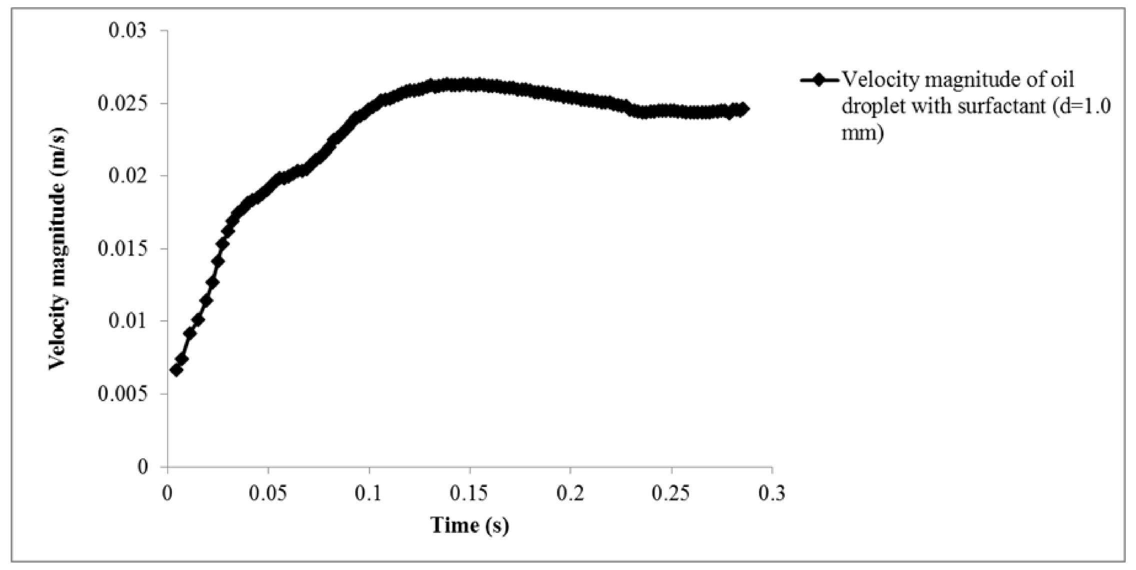

Figure 4: The terminal velocity of premixed oil droplet (d=1.0 mm). When the oil droplet is clean, the terminal velocity is approximately 3.3 cm/s, while that is of 2.5 cm/s when premixed with surfactant, which introduces a 24% decrease compared to the clean situation.

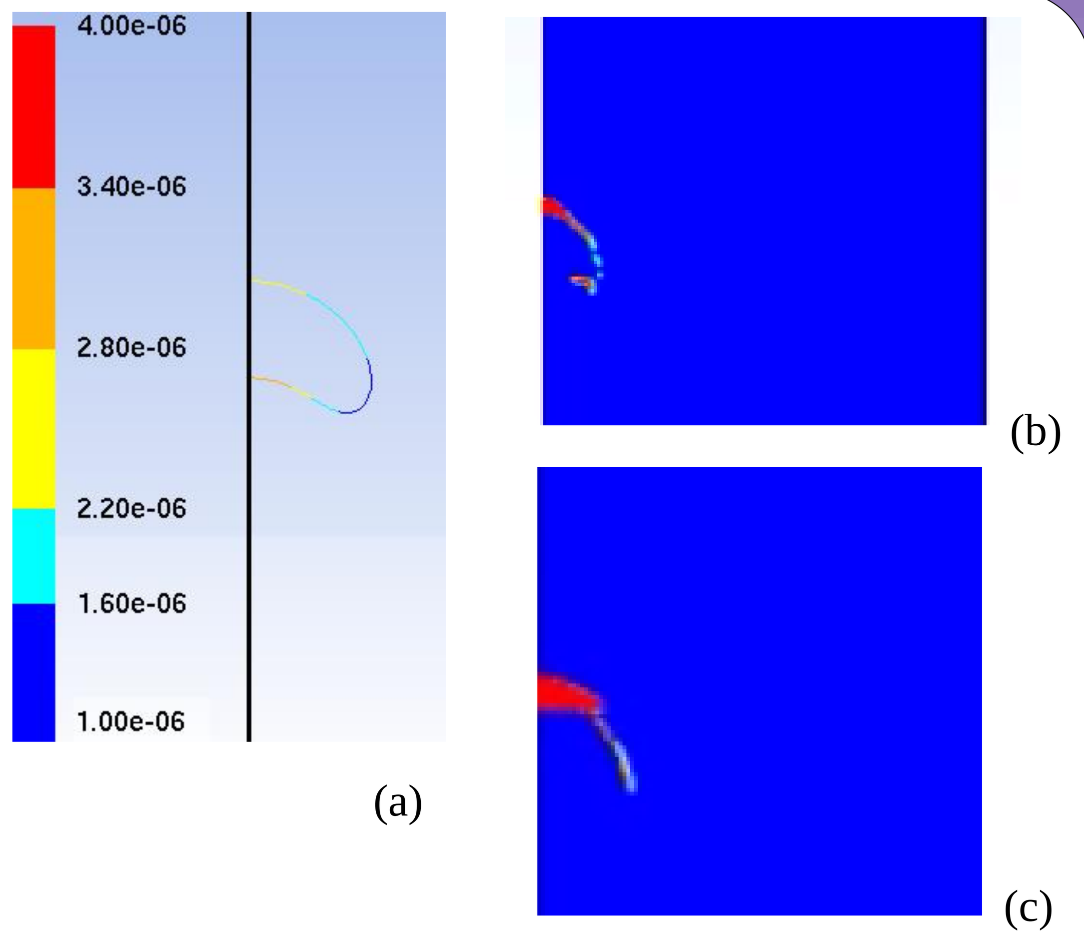

Figure 5: The oil droplet (d=4 mm) (a) surface surfactant concentration at t=0.1 s (b) with surfactant in bulk at =0.25 s (c) with surfactant premixed at t=0.25 s after the initial release. The surfactant is accumulated at the rear cap of the oil droplet due to the shear velocity as it rises. It can be noticed that when surfactant is well-mixed in bulk, the oil droplet tends to peel off a big chunk of oil with tip-streaming. However, it only shows tip streaming at the rear cap for the situation with oil droplet premixed with surfactant.

Conclusions

- We developed a numerical method to account for the effect of surfactant on the oil droplet
- The terminal velocity of oil droplet premixed with surfactant is reduced compared to clean situation.
- The surfactant is accumulated at the rear cap of the oil droplet due to the shear velocity.
- When surfactant is well-mixed in bulk, the oil droplet tend to peel off a big chunk of oil with tip-streaming. However, it only shows tip streaming at the rear cap for the situation with oil droplet premixed with surfactant.

References

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