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# Effects of surfactant on terminal velocity of a Taylor bubble in a vertical pipe

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### ABSTRACT

Effects of soluble surfactant on the terminal velocity of a Taylor bubble rising through a vertical pipe are investigated using an interface tracking method. A level set method is utilized to track the interface. Transport of surfactant in the bulk liquid and at the interface is taken into account. The amount of adsorption and desorption is evaluated using the Frumkin and Levich model. The normal component of surface tension force is computed using a ghost fluid method, whereas the tangential component, i.e., the Marangoni force, is evaluated by making use of the continuum surface force model. Simulations of small air bubbles contaminated with soluble surfactant are carried out for validation. The Marangoni effects on the bubbles, i.e., the surface immobilization and the increase in drag coefficient, are well predicted. Then Taylor bubbles rising through vertical pipes filled with contaminated water at a low Morton number are simulated for various Eötvös numbers, various bulk surfactant concentrations and two different surfactants, i.e., 1-pentanol and Triton X-100. As a result, the following conclusions are obtained: (1) the reduction of surface tension near the bubble nose is the cause of the increase in terminal velocity, (2) the surfactant does not affect the terminal velocities of high Eötvös number bubbles since the bubbles at high Eötvös numbers are independent of surface tension, (3) the terminal velocity of a low Morton number Taylor bubble can be evaluated by making use of available correlations for clean Taylor bubbles, provided that the degree of contamination near the bubble nose is known and the Marangoni effect in the nose region is negligible, and (4) the Hatta number, which is the ratio of the adsorption velocity to the bubble velocity, is a primary factor governing the degree of contamination in the bubble nose region.

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Multinhase Flow

# 1. Introduction

Slug flow is one of the typical two-phase flow patterns encountered in various industrial applications. The flow is characterized by the presence of large bullet-shaped bubbles, which are called Taylor bubbles.

If a Taylor bubble in a vertical pipe filled with a stagnant liquid is free from a surface-active agent (surfactant), the force balance between the inertial, viscous, surface tension and buoyant forces determines the bubble motion. These forces give three independent dimensionless groups governing the bubble motion, e.g., the Froude number,  $Fr = V_T / \sqrt{\Delta \rho g D / \rho_L}$ , the Eötvös number,  $Eo_D = \Delta \rho g D^2 / \sigma_0$ , and the Morton number,  $M = \mu_L^4 \Delta \rho g / \rho_L^2 \sigma_0^3$ , where  $V_T$ is the bubble terminal velocity,  $\Delta \rho$  the density difference between the two phases, g the magnitude of the acceleration of gravity, D the pipe diameter,  $\rho$  the density,  $\sigma_0$  the surface tension of the clean surface,  $\mu$  the viscosity, and the subscript *L* denotes the continuous liquid phase. A number of studies on the Froude number of the clean Taylor bubble have been carried out and several correlations of Fr applicable to a wide range of M and  $Eo_D$  have been proposed, e.g., Wallis (1969), Viana et al. (2003) and Hayashi et al. (2010). On the other hand, our knowledge on the motion of a Taylor bubble contaminated with surfactant is still insufficient and no Froude number models have been proposed for contaminated Taylor bubbles.

Almatroushi and Borhan (2004) measured terminal velocities of Taylor bubbles in glycerol-water solutions contaminated with sodium dodecyl sulfate at low Reynolds numbers and for  $12 \leq \Delta \rho g D^2 / \sigma_c \leq 26$ , where  $\sigma_c$  is the surface tension at the critical micelle concentration. They pointed out that the presence of surfactant increases  $V_T$  of the Taylor bubbles, and speculated that the cause of the increase in  $V_T$  is the reduction in surface tension due to the surfactant adsorption and the surface immobilization due to the Marangoni effect is weak since large shape deformation dilutes the surfactant concentration at the surface. To the contrary, it is well known that the terminal velocities of Taylor bubbles at high Eo<sub>D</sub> numbers and low *M* numbers are independent of the presence of surfactant. Detailed investigation of these surfactant effects may reveal a key physics in developing the Froude number model for contaminated Taylor bubbles.

Interface tracking methods are useful tools for investigating the motion of a contaminated bubble, since they may be able to

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consider all the surfactant dynamics, i.e., the advection and diffusion of surfactant in the bulk liquid and at the bubble surface and the adsorption-desorption kinetics.

Several interface tracking methods for simulating motions of bubbles contaminated with soluble surfactant have been proposed. Cuenot et al. (1997) carried out simulations of spherical bubbles using a boundary-fitted coordinate (BFC) method. The adsorption and desorption were taken into account by using the Frumkin and Levich model (Frumkin and Levich, 1947; Levich, 1962). Liao and McLaughlin (2000) investigated the motions of small bubbles contaminated with decanoic acid by using a BFC method. Takagi et al. (2003) carried out experiments on nitrogen bubbles in water contaminated with three different surfactants, i.e., 1-pentanol, 3pentanol and Triton X-100, and BFC simulations of spherical bubbles under the same conditions as the experiments. The simulation confirmed that the surfactant distribution at the interface and the interfacial velocity strongly depend on the adsorption and desorption properties of surfactant. Only two-dimensional axisymmetric bubbles were dealt with in the above studies. Fukuta et al. (2008) and Takagi et al. (2009) carried out three-dimensional BFC simulations of contaminated spherical bubbles in linear shear flows to investigate the effects of surfactant on the lift force. These BFC methods did not solve the flows inside bubbles. On the other hand, Tukovic and Jasak (2008) developed a three-dimensional BFC method solving the flows both inside and outside a bubble. A front tracking method for simulating bubbles contaminated with soluble surfactant was proposed by Muradoglu & Tryggvason (2008). They validated their method through several benchmark tests, e.g., a spherical bubble expanding at a constant speed, bubble migration due to the Marangoni force, and free rising bubbles in contaminated liquids at low Reynolds numbers. As for an Eulerian approach, Alke and Bothe (2009) proposed a volume-of-fluid (VOF) method for simulating contaminated bubbles. They simulated a spheroidal bubble in a vertical pipe and obtained a surfactant distribution corresponding to a stagnant cap model.

Only spherical or slightly deformed bubbles were dealt with in the above studies, and there are no studies on the detailed surfactant motion on bubbles with large shape deformation such as Taylor bubbles.

In this study, an interface tracking method is, therefore, developed to predict the motions of contaminated Taylor bubbles. The Eulerian approach may be suitable for bubbles with large shape deformation. A level set method is, therefore, utilized for tracking the interface. An extrapolation method proposed by Xu and Zhao (2003) is adopted to facilitate the evaluation of the surface gradient of the surface surfactant concentration on Eulerian grids. The adsorption-desorption kinetics is accounted for by using the Frumkin–Levich model. The developed method will be validated through simulations of small air bubbles rising through stagnant water contaminated with soluble surfactant. Then effects of surfactant on Taylor bubble shape and velocity will be investigated for a wide range of  $Eo_D$ . This study focuses on Taylor bubbles in a low Morton number system.

## 2. Field equations

The continuity and momentum equations for incompressible Newtonian fluids based on the one-fluid formulation are given by:

$$\nabla \cdot \boldsymbol{V} = \boldsymbol{0} \tag{1}$$

$$\frac{\partial \boldsymbol{V}}{\partial t} + \boldsymbol{V} \cdot \nabla \boldsymbol{V} = -\frac{1}{\rho} \nabla P + \frac{1}{\rho} \nabla \cdot \boldsymbol{\mu} \Big[ \nabla \boldsymbol{V} + (\nabla \boldsymbol{V})^T \Big] + \boldsymbol{g} \\ + \frac{1}{\rho} [\sigma \kappa \boldsymbol{n} + \nabla_s \sigma] \delta$$
(2)

where **V** is the velocity, *t* the time, *P* the pressure, **g** the acceleration of gravity,  $\sigma$  the surface tension,  $\kappa$  the curvature, **n** the unit normal to the interface,  $\nabla_S (=\nabla - \mathbf{nn} \cdot \nabla)$  the surface gradient operator,  $\delta$ the delta function, which is non-zero only at the interface, and the superscript *T* denotes the transpose. The last term,  $(\nabla_S \sigma)\delta$ , is the surface tension force tangent to the interface and is the cause of the Marangoni effect. The transport equation of surfactant in the continuous phase and that at the interface are given by (Levich, 1962; Stone, 1990; Cuenot et al., 1997)

$$\frac{\partial C}{\partial t} + \boldsymbol{V} \cdot \nabla C = \nabla \cdot D_C \nabla C \tag{3}$$

$$\frac{\partial \Gamma}{\partial t} + \nabla_{S} \cdot \Gamma \boldsymbol{V}_{S} = \nabla_{S} \cdot D_{S} \nabla_{S} \Gamma + \dot{S}_{\Gamma}$$

$$\tag{4}$$

where *C* is the surfactant concentration in the continuous phase,  $\Gamma$  the surfactant concentration at the interface,  $D_C$  and  $D_S$  are the diffusion coefficient in the continuous phase and that at the interface, respectively, and  $V_S$  the tangential component of V. The source term  $\dot{S}_{\Gamma}$  is the molar flux from the continuous phase to the interface due to the adsorption and desorption, i.e.,  $\dot{S}_{\Gamma} = -D_C(\mathbf{n} \cdot \nabla C|_{int})$ , and is evaluated by using the Frumkin and Levich model (Frumkin and Levich, 1947; Levich, 1962):

$$S_{\Gamma} = k[C_{S}(\Gamma_{\max} - \Gamma) - \beta\Gamma]$$
(5)

where k and  $\beta$  are parameters for the adsorption and desorption kinetics, respectively,  $\Gamma_{\text{max}}$  the saturation value of  $\Gamma$ , and  $C_S$  the molar concentration of the continuous phase in the vicinity of the interface.

The interface is tracked by solving the following level set equation (Sussman et al., 1994):

$$\frac{\partial \phi}{\partial t} + \boldsymbol{V} \cdot \nabla \phi = \boldsymbol{0} \tag{6}$$

where  $\phi$  is the level set function, and the interface is given by the zero-level set,  $\phi = 0$ . The unit normal and the curvature are given by:

$$\boldsymbol{n} = \frac{\nabla \phi}{|\nabla \phi|} \tag{7}$$

$$\kappa = -\nabla \cdot \frac{\nabla \phi}{|\nabla \phi|} \tag{8}$$

#### 3. Numerical method

#### 3.1. Method for solving continuity and momentum equations

Several methods for evaluating the normal component of the surface tension force,  $\sigma \kappa \delta \mathbf{n}$ , are available, e.g., the continuum surface tension force (CSF) model (Brackbill et al., 1992), the ghost fluid method (GFM) (Kang et al., 2000) and the immersed interface method (IIM) (LeVeque and Li, 1994). The IIM is the most accurate but not computationally efficient because of the necessity of jump conditions for high order derivatives of physical quantities. On the other hand the CSF model is the simplest but causes large spurious currents. The simplicity and accuracy of the GFM are in-between. The GFM is adopted to evaluate the normal component of the surface tension force in this study.

The momentum equation without the pressure gradient and the normal component of surface tension force is solved to obtain a temporary velocity,  $V^*$ , for the velocity:

$$\boldsymbol{V}^{*} = \boldsymbol{V}^{n} + \Delta t \left[ -\boldsymbol{V} \cdot \nabla \boldsymbol{V} + \frac{1}{\rho} \nabla \cdot \boldsymbol{\mu} \left[ \nabla \boldsymbol{V} + (\nabla \boldsymbol{V})^{T} \right] + \boldsymbol{g} + \frac{(\nabla_{S} \boldsymbol{\sigma}) \delta}{\rho} \right]^{n}$$
(9)

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