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CFD simulation of bubble in flow field: Investigation of dynamic interfacial behaviour in presence of surfactant molecules

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ABSTRACT

This work presents the results of numerical simulation of liquid flow on a static bubble. Velocity and surfactant concentration profiles of the liquid around a bubble exposed in flow field were estimated via unsteady CFD solution. Governing equations are the Navier-Stokes and conservation of mass in the liquid bulk and at the interface. Resulted profiles of surfactant concentration and velocity in the liquid bulk are used to determine the dynamic surface tension data via two adsorption isotherms of Langmuir and Frumkin. Data of dynamic surface tension were validated via experimental data of “bubble in flow field” protocol. Surface concentrations of surfactants were also numerically estimated. At longer flow times, surface concentration increases due to adsorption and accumulation of surfactants at the interface. The rate of mass transfer is increased by development of velocity profile around the bubble surface. Steady state was reached about 36 s after flow starts.

1. Introduction

Multiphase flow occurs in a wide variety of engineering applications [1–3]. One of the most important issue in many industries is understanding the behavior of multiphase mixtures in different processes [4–6]. Bubbly flows are of great importance in the chemical and process industries. A number of processes, such as absorption, fermentation, coal liquefaction and waste-water treatment, operate under bubbly-flow conditions to attain larger interfacial areas for heat and mass transfer. Although a number of recent studies have examined bubbly flows [7–10], many important complications have not been resolved [11,12]; these include complications associated with presence of surfactants in liquid mediums [13–15]. Along with the physical properties of continuous liquid phase, interfacial properties can significantly affect the motion of bubbles through a liquid medium [16]. Surfactants, which can be present as impurities or added deliberately, can change interfacial properties and affect multiphase flow behavior. In bubbly flows, the presence of even small traces of surfactants can considerably affect rising-bubble hydrodynamics [17–19].

Generally, the transport of surfactants from continuous liquid phase to the surface of rising bubbles takes place over several stages [20,21]: (1) convection-diffusion in the liquid medium, characterized by bulk velocity and concentration; (2) the adsorption stage, at which surfactant molecules emerge from the liquid bulk very near the interface to the bubble surface; and (3) convection-diffusion at the gas-liquid interface [21–24]. The convection-adsorption mechanism is well suited for investigating high-velocity regimes with lower bulk diffusivity of surfactants; while low-velocity systems with higher bulk diffusivity of surfactants are more accurately described by the diffusion-adsorption mechanism [25].

Hadamard and Rybczinski [26,27] presented a fundamental theory for bubbles rising in highly purified liquid and in cases of low Reynolds numbers. The surface of rising bubble is assumed to be fully mobile in this theory, and viscous friction was ignored. Thus the rising velocity is higher than that of a solid sphere with the identical diameter and density. However, the velocity of rising bubbles in surfactant solutions is considerably less than in pure liquids [21,28–30]. The rear stagnant cap (RSC) theory is well established [19,31,32] for describing the effect of surfactants on the velocity of rising bubbles. According to RSC theory for rising bubbles, the convection and diffusion of surfactants leads to non-uniform surface coverage and surface-tension gradients [30]. As a result, the mobility of the bubble surface declines, and viscous drag increases due to creation of Marangoni stresses [24].

Previous numerical investigations have been performed to study the adsorption and desorption of surfactants to and from the surface of rising bubbles. These studies were conducted by solving the full Navier–Stokes equation and mass-conservation equations in the bulk and at the interface [21,33]. The results revealed that surfactant

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adsorption at the rear pole of the bubble would be higher than at the leading pole, and that the difference in local adsorption rate increased with increasing Reynolds number. However, hydrodynamic conditions were simplified in these previous models, and in some cases there was no direct validation of the experimental data. The effects of the adsorption and desorption of surfactants on the shear-induced lift force exerted on the surface of rising bubbles have also been studied [34]. While predictions of these models were in accordance with RSC theory, the lift coefficients were found to be greater than those predicted by the RSC model.

Many theoretical and experimental studies have examined the dynamics of rising bubbles [7,35,36]; however, there are some uncertainties about the effect of surfactant transport on rising velocity. The persistence of most of the questions in this area can be attributed to the lack of a relevant model that recognizes the rate-limiting step in convective-diffusion kinetics [24]. Diffusion, convection and adsorption cannot be comprehensively described by the simulation of rising bubbles due to the lack of validation evidence [21]. One of the important parameters that might be used as a predictive quantity is the dynamic surface tension. Although there are various methods to measure dynamic surface tension, the measurement of instant values of surface tension as a bubble rises in liquid medium remains an important challenge [27,37,38]. These measurements require having the ability to instantly access and monitor the moving interface, which is nearly impossible. Hence, it is a helpful alternative to develop a procedure that simulates the state of rising bubbles. Lotfi et al. introduced an experimental protocol that provides instant measurements of surface tensions for a stationary bubble exposed in various liquid flows; they named it "bubble in flow field". This protocol incorporates the flow field in oscillating drop and bubble analyzer (ODBA) technique [24]. These experiments were carried out for freshly formed and pre-aged bubbles in surfactant solutions. A significant decrease in dynamic surface tension was observed for freshly formed bubbles. However, the results for pre-aged bubbles showed no significant differences to the results for the zero-flow condition.

The surface tension vs. time data for the bubble in flow field technique provides evidence that can be used to validate a model-oriented approach. Such a model could be used to investigate the impact of a flow field on the surface concentration gradient of surfactants. For this purpose, a computational model was introduced in this study to investigate the mass transfer of surfactants in a system involving a stationary bubble under flow conditions. A novel approach was used to apply a monophasic CFD simulation to the liquid bulk. The result for the monophasic solution was then applied to solve an ordinary differential equation at the interface. The model was then used to predict the surface concentration of the surfactant at various flow times. The simulation was conducted for non-ionic surfactant C_{12}DMPO (dodecyl dimethyl phosphine oxide) and ionic surfactant CTAB (cetyl trimethyl ammonium bromide). The main novelties of the proposed model include: introducing the first mathematical model for the bubble in flow field protocol that could be validated using experimental data for dynamic surface tension; predicting the surface concentration of surfactant; and determining the rate-limiting step in the mass transfer of surfactant from the liquid bulk to the bubble surface.

2. Description of the bubble in flow field protocol

It is difficult to instantly measure dynamic surface tension data for interface with rising bubbles. However, experimental procedures that simulate the situation of rising bubbles would be suitable alternatives for studying the flow effects on surface properties of such a system. Lotfi et al. [24] investigated the effects of a flow field on a bubble surface in surfactant solutions using the bubble in flow field protocol. This method is incorporates liquid flow in oscillating drop and bubble analyzer (ODBA) techniques (Fig. 1a). ODBA is one of the most accurate methods for measuring dynamic surface tension; more details of this technique are given in [39]. This technique has been used as a conventional tensiometery method for measuring dynamic interfacial tension. In the bubble in flow field protocol, some changes have been done on ODBA equipment (Fig. 1a), which provides liquid flow to the bubble surface. The operational conditions were capillary tip geometry, liquid flow rate, bubble size and distance of the flow outlet to the bubble pole. The experiments were carried out for pure water and for freshly formed and pre-aged bubbles in surfactant solutions. For freshly formed bubbles, flow started about 5 or 10 s after bubble formation, for which the adsorbed layer at the bubble surface was far from the equilibrium state. For pre-aged bubbles, flow started about 120 s after bubble formation, for which the bubble surface approached the equilibrium adsorption state. Significant effects of the liquid flow field were observed on freshly formed bubbles rather than pre-aged bubbles.

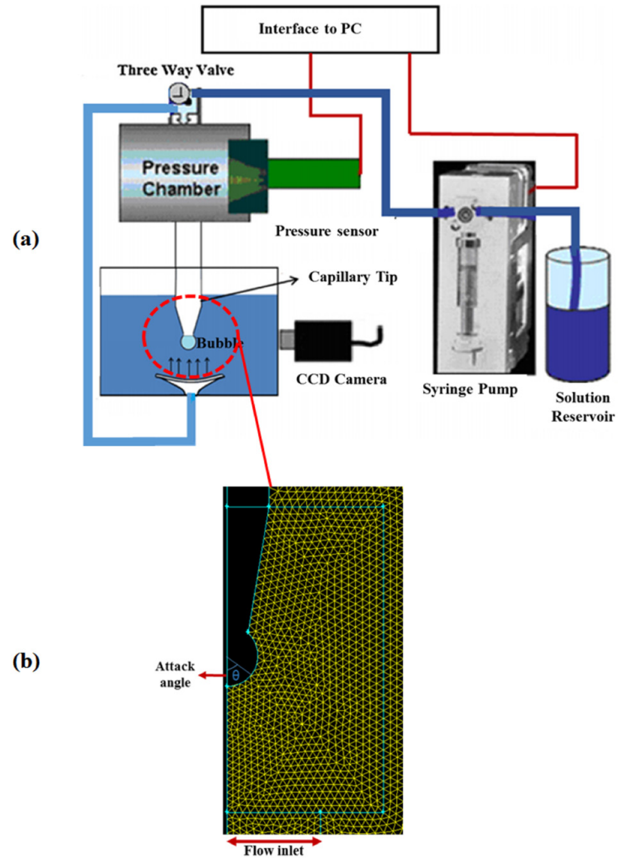

Fig. 1. a: Schematic of the bubble in flow field setup designed by Lotfi et al. [24] and b: 2D geometry and mesh configuration.

3. Methodology

This study was done to clarify some uncertainties about the rate-limiting step of the surfactant transport from flowing liquid bulk to the bubble surface. For this purpose a novel approach was introduced to simulate the bubble in flow field protocol. The model predicts the data for dynamic surface tension, which could be validated using experimental data. The surface concentration of the surfactant could be predicted at various flow times, and the rate-limiting step in the mass transfer of the surfactant from the liquid bulk to the bubble surface could be determined.

3.1. Computational geometry and domain

Lotfi et al. observed no significant shape deformation for bubbles in the presence of liquid flow [16]. Thus the modeling of the bubble in