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Mass transfer of a rising spherical bubble in the contaminated solution with chemical reaction and volume change

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ABSTRACT

In the present study, a systematic numerical study is conducted to investigate the mass transfer of a slightly contaminated spherical bubble under the effect of chemical reaction with the consideration of volume change of the bubble. The numerical approach is first validated by the benchmark tests, i.e., the dissolutions of a static bubble and a rising bubble. The numerical results are compared with the results from literatures and show very good agreements. Afterwards, the numerical method is utilized to study the chemical absorption process of a rising spherical CO_2 bubble in the alkaline solution of NaOH. The shrinkage of the bubble and the decrease of bubble velocity during the chemical absorption process are taken into account, and the accumulation of the contamination on the bubble surface is also considered based on the stagnant cap model. The profiles of species concentration are presented in detail, and it can be found that the cap angle and the flow separation significantly influence the distribution of the concentration layers. The local mass transfer rate and reaction rate around the bubble surface are studied quantitatively, and the local mass transfer is found to be dominated by the chemical reaction directly. In additional, the supplement of the hydroxyl ion significantly affects the mass transfer which is mainly determined by the local velocity.

1. Introduction

The mass transfer occurring between the bubble and external flow is very important for understanding the transport phenomena in multiphase systems in both chemical engineering and biochemical engineering progresses, i.e., the sewage treatment and the petroleum refining, etc. Herein, the presence of contaminants is of major importance in the practical situations and significantly influences the bubble motion and mass transfer [1,2]. For example, it has been concluded that a bubble in the slightly contaminated water changes from behaving like a fluid sphere to a solid particle with the increase of contaminant [3]. Such phenomenon has been proved to be related to the presence of surface contaminants which tend to accumulate on the bubble surface, and the contaminants attaching to the bubble change the condition of fluid on bubble surface, i.e., slip, no-slip, or partial slip. In order to explain the change of bubble surface condition caused by the contaminants, a stagnant cap model has been proposed [4]. The adsorbed contaminant molecules are assumed to be dragged toward the rear of the bubble by the adjacent liquid, and thus the rear surface of the bubble is considered to be immobile (no-slip). As shown in Fig. 1, a stagnant cap angle is introduced to distinguish the slip region and no-slip region on the bubble surface. Therefore, the bubble surface in slip region ($\theta \leq \theta_{cap}$) can move with the liquid whereas the contaminated zone ($\theta > \theta_{cap}$) behaves as stagnant cap (no-slip surface).

By implementing the stagnant cap model with appropriate cap angle, Mclaughlin [5] successfully predicted the rising velocities of the bubbles in tap water and the dilute solution of Triton X100, and the results agreed very well with the experimental results. Bel Fdhila and Duineveld [6] presented an experimental and numerical study of the rising spherical bubble in quiescent contaminated solutions. They found a rapid decrease of bubble rising velocity when there was contaminant, which was due to dramatic increase of the shear stress on the leading surface coated by contaminants. They also confirmed that the stagnant cap assumption and the hypothesis of contaminant adsorption reasonably described the observed physical phenomena. Another decisive effort has been made by Sadhal and Johnson [7] that a closed analytical form for the variation of the drag coefficient as a function of the cap angle θ_{cap} was developed for creeping flow. The method can directly estimate the influence of the stagnant cap angle on the bubble motion, and it has been widely used in the numerical studies of bubble motion and mass transfer in quiescent contaminated solutions.

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Nomenclature

A	surface area, m^2
c	molar concentration of species, $kmol/m^3$
C_D	drag coefficient, –
D	diffusive flux, mol/m^2 s
d	bubble diameter, m
g	gravity acceleration, m/s^2
H	the Henry's coefficient, $kmol/m^3$ bar
h_m	mass transfer rate, m/s
I	ionic strength, mol/m^3
k	reaction rate constant, $m^3/kmol$ s
M	molecular weight, kg/mol
$\dot{m}$	mole transfer rate, mol/s
P	pressure, Pa
Pe	Peclet number, ul/Γ
r	r coordinate, m
R	bubble radius, m
Re	Reynolds number, ul/ν
Sc	Schmidt number, ν/Γ
t	time, s
T	temperature, K
u	velocity, m/s
U	velocity vector, m/s
V	volume, m^3
Y	the mass fraction, –

Greek symbols

γ	mass transfer parameter of contaminant, –
Γ	diffusion coefficient, m^2/s
η	valence, –
θ	angle, °
μ	dynamic viscosity, Pa s
ν	kinematic viscosity, m^2/s
ρ	density, kg/m^3
ϕ	angle, °
Φ	the chemical reaction rate, $kmol/m^3$ s
φ	scalar, –

Subscripts

B	bubble
cap	cap
C	clean bubble
D	drag
F	fully contaminated bubble
gas	gas
i	the i-th species
$initial$	initial
int	interface
l	liquid
m	mass
w	pure water

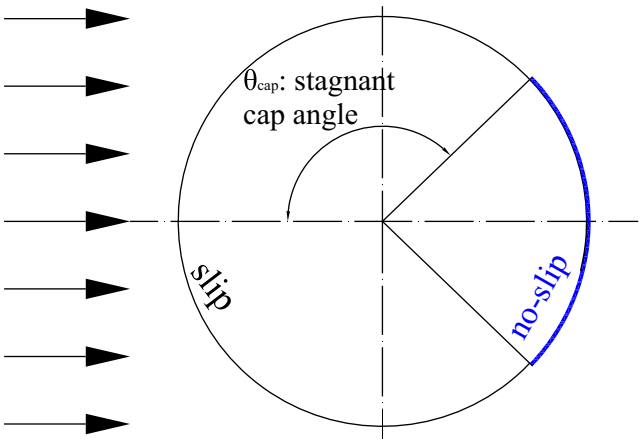

Fig. 1. The schematic of the stagnant cap model.

Ryskin and Leal [8] presented a finite-difference method to study the axisymmetric bubble motion and an adaptive grid technique was used to track the bubble surface, in which the bubble was assumed to be a void and the motion of the bubble was predicted accurately. Based on their work, Mclaughlin et al. [9,10] developed a method to consider the bubble deformation and the effect of contamination at high and moderate Reynolds numbers. The numerical results successfully predicted the flow separation and the existence of the wake behind the bubble when the contaminant existed. The effect of contaminant on the mass transfer coefficient of bubbles was also discussed in their studies, and the correlations for mass transfer rate of the bubble in presence of contaminants were reported.

Apparently, the contamination is considered important for the gas dissolution process of the free rising bubble, because it influences both the rising velocity [2,4,5] and the mass transfer rate. This topic has also been of interests to the researchers in past two decades [11–21]. Cuenot et al. [11] presented a systematic numerical study of the dissolution of a contaminated moving bubble with constant velocity. The stagnant cap model was proved to work well in describing the fluid flow with slightly soluble contaminants around the bubble, and the contaminant diffusion from the liquid bulk was found to play a significant role. Saboni et al. [12,13] presented a systematic study of the bubble motion and dissolution considering the effect of contaminant. It was interesting that the internal circulation within the bubble was taken into consideration, and the influence of the ratio of gas viscosity to liquid viscosity on the bubble motion and mass transfer rate was presented. Vasconcelos et al. [14,15] carried out a lot of experimental studies of the bubble dissolution in both clean water and contaminated aqueous solutions, and the mass transfer coefficients were obtained and compared with the numerical results. It was found that the gas-liquid mass transfer coefficient decreased as the bubble rose along the column, and the value was closer to that of fluid sphere with mobile surface on the bottom of the column, while it was closer to rigid particle on the top of the column with completely immobile surface. Moreover, the transition of mobile bubble to rigid bubble was successfully interpreted and modeled in terms of the kinetics of the accumulation of contaminants onto the bubble interface. Tomiyama and the co-authors [16–18] presented both experimentally and numerically the systematic studies on the mass transfer of rising bubbles within the contaminated solution in vertical pipes. The bubble shapes and velocities as well as the mass transfer rates were obtained from the precise visualization results. It was found that the contaminant decreased the mass transfer rate with the increase of the surfactant concentration. Interestingly, they managed to obtain the distribution of the contaminant on the bubble surface numerically by solving the partial differential equation along the moving interface, and the predicted bubble shapes agreed well with the experiment results. They also showed that considerably higher mesh resolution