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Direct numerical simulation of mass transfer from Taylor bubble flow through a circular capillary

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ABSTRACT

In this work mass transfer during a Taylor bubble flow regime has been investigated by a volume of fluid (VOF) based numerical method. The hydrodynamics of Taylor bubble flow through a circular capillary has been simulated in a single unit cell by a moving reference frame. The validity of Taylor bubble hydrodynamics simulation has been checked by comparing the liquid film thickness and the relative bubble velocity obtained from computational fluid dynamics (CFD) simulations with reported empirical correlations and experimental results. The conservation equation of tracer has been solved in whole of flow domain for simulating mass transfer from Taylor bubble to surrounding liquid. The tracer concentrations in the cells that are either completely or partially filled with the gas phase are assigned the equilibrium concentration by employing the concept of internal boundary condition. By this concept an artificial diffusion of tracer has been appeared in the simulations. In order to eliminate this artificial diffusion, the advection scheme in the tracer conservation equation has been modified by using the two film mass transfer model. The simulation of mass transfer from a single bubble has been validated by comparing the CFD results with reported experimental data. Afterwards, the effects of capillary number, unit cell length and capillary diameter variation on mass transfer from Taylor bubble has been investigated.

1. Introduction

The use of monolith reactors is becoming increasingly important in view of advantages such as high catalytic surface concentration, high mass transfer rate, low pressure drop, and ease of scale up. These reactors are increasingly considered for multiphase catalytic reactions such as hydrogenations [1], hydrodesulphurization [2], oxidations [3], bioremediation [4] and Fischer–Tropsch synthesis [5]. In multiphase monoliths, the predominant flow pattern is very close to Taylor regime. For simplicity of the numerical solutions, an unsteady, periodic flow of elongated bubbles which are separated by liquid slugs is considered. In this simplification, the bubbles fill almost the entire channel cross-section and travel with the same axial velocity.

For the efficient design of monolith reactors, detailed knowledge of mass transfer between Taylor bubbles and surrounding liquid or solid is of fundamental importance. Optimization of mass transfer in these reactors requires profound understanding of underlying hydrodynamics and mass transport. Here, numerical simulation provides a helpful tool to reduce the usually large experimental expense for reactor design.

The numerical simulation of gas–liquid interphase mass transfer can be done by fundamentally two different methods. In the first method the averaged governing equations for each phase are solved and empirical correlations are used for computing the gas–liquid interphase mass transfer coefficient. The generality of this approach is limited since it always relies on certain assumptions for mass transfer and thus requires appropriate closure models. The second method is direct solution of two phase flow and species conservation equations, in which the motion of interface is considered by means of an interface tracking method. In this approach the two phase flow field which is needed for calculation of convective mass transfer, is obtained by solving the Navier–Stokes equations. There are different surface tracking methods for simulation of multiphase flow such as volume-of-fluid (VOF) [6], level set [7] and marker point [8]. Among these methods, VOF is the most widely used method.

In literatures, the hydrodynamics of Taylor bubble flow regime has been simulated both in entire capillary length and in a single unit cell. Modeling of Taylor bubble flow in entire capillary length is very difficult and needs a high computational cost. Some researchers have modeled the Taylor bubble flow in entire capillary length [9–13]. Modeling of Taylor bubble flow by this method requires only the superficial velocities of two phases as an input and the void fraction, the bubble velocity are calculated as a part of the solution. However, when using such an approach, a long

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Nomenclature

A	surface concentration, m^2/m^3
C^*	non-dimensional tracer concentration
C_L	tracer concentration in liquid, mol/m^3
Ca	Capillary number, $\mu_L U_B/\sigma$
D	binary diffusivity of tracer in the liquid, m/s^2
Dc	capillary diameter, mm
DNS	direct numerical simulation
f_σ	surface tension force, N
g	gravity acceleration, m/s^2
$\mathbf{g}$	gravity vector, m/s^2
$k_L a$	volumetric mass transfer coefficient, s^{-1}
Le	developing length, m
Ls_F	length of liquid slug in front of the bubble, m
Ls_B	length of liquid slug behind of the bubble, m
L_{UC}	unit cell length, mm
p	pressure, Pa
r	normal distance from the interface, m
Pe_L	Peclet number, $Re_L Sc_L$
Re_B	Reynolds number based on bubble velocity, $\rho_L U_B dc/\mu_L$
Re_L	Reynolds number based on superficial liquid velocity, $\rho_L U_{SL} dc/\mu_L$
Re_{TP}	Reynolds number based on total superficial velocity of two phase flow, $\rho_L U_{TP} dc/\mu_L$
Sc_L	Schmidt number, $\mu_L/\rho_L D$
t_{film}	film exposure time, s
t_{cap}	cap exposure time, s
u	velocity, m/s
U_B	bubble velocity, m/s
U_G	superficial gas velocity, m/s
U_{SL}	superficial liquid velocity, m/s
U_{TP}	total superficial velocity of two phase, m/s
U_w	wall velocity, m/s
V	volume, m^3
W	relative bubble velocity

Greeks

α	local phase volume fraction
ε_G	overall gas volume fraction in domain
μ	dynamic viscosity, kg/m s
ρ	density, kg/m^3
σ	surface tension, N/m
τ	residence time, s

Subscripts

cell	computational cell
B	bubble
eq	equilibrium
G	gas
L	liquid
M	mixture quantity
sys	system
UC	unit cell

Superscripts

$*$	dimensionless variable
T	transpose

computational domain is required to obtain fully developed Taylor bubble flow [14]. Moreover, it needs a refined computational grid in order to capture flow features accurately.

Some researchers have modeled fully developed Taylor bubble flow in a single unit cell where liquid flows over the stationary bubble and the moving channel wall [15–18]. This approach not only can reduce significantly the computational complexity, but also requires flow parameters such as the slug length, void fraction and the bubble velocity as input parameters. In this approach, the liquid velocity is initialized at the inlet with an appropriate guess and then iteratively updated until the bubble stays at rest. The side wall velocity is specified as a moving wall which moves with the bubble velocity.

The first volume-of-fluid (VOF) based simulation of interphase mass transfer has been done by Ohta and Suzuki [19]. They studied mass transfer from a rising drop in a solvent extraction process. Davidson and Rudman [20] have used VOF method with mass transfer for studying interphase mass transfer from a drop rising in a liquid column. Schlottke and Weigand [21], Onea et al. [22], and Bothe et al. [23] have also used the VOF method for direct numerical simulation of interphase mass transfer. Hassanvand et al. [24] used VOF method in conjunction with a mass transfer model to investigate process of gasoline evaporation during the splash loading of the fuel tank. Petera and Weatherley [25] investigated the mass transfer from a falling axisymmetric drop using a finite element method. The finite element method was also used by Waheed et al. [26] to compute the mass transfer of single spherical drops by free and forced convection. Comprehensive two-dimensional investigations of the liquid-side mass transfer from single bubbles and bubbles swarms with constant concentration in the bubbles have been performed using a front-tracking method by Koynov et al. [27] and Koynov and Khinast [28].

In contrast to large number of publications for numerical simulation of Taylor bubble flow hydrodynamics, there are up to now only few numerical investigations of mass transfer reported in open literatures for this flow regime. Among the pioneers, Irandoust and Andersson [29] used the finite difference method for modeling of mass transfer from Taylor bubble. van Baten and Krishna [30] have studied the mass transfer from Taylor bubble rising in circular capillaries. In their study they ignored the effect of surface tension on the hydrodynamics behavior and modeled the bubble as a void with a fixed gas–liquid interface (no moving interface). They also assumed the thin liquid film around the bubble corresponds to air–water system (low capillary number). Under these conditions they proposed a correlation for mass transfer coefficient. This correlation is applicable for the cases with low capillary number. However in some processes because of high viscosity of the liquid phase and the two phase superficial velocities the monolith reactor operates at high capillary number.

In this work the mass transfer from Taylor bubble has been simulated by using a VOF based numerical method. To the authors' knowledge, the effect of capillary number variation on mass transfer coefficient of Taylor bubble flow through the capillary tubes has not been studied yet by direct numerical simulation (DNS). The effects of capillary number, unit cell length and capillary diameter variation on mass transfer from Taylor bubble has been investigated.

2. Mathematical modeling

2.1. Hydrodynamics

Fig. 1 depicts the schematic of computational set-up for simulation of Taylor bubble flow in circular capillary. The coordinate system is defined by taking y as axial direction and x as the radial direction. The gravity vector points in the negative y-direction. In present work the VOF model has been used for tracking the