Chemical Engineering Science 192 (2018) 714–724

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Drag force of bubble swarms and numerical simulations of a bubble column with a CFD-PBM coupled model

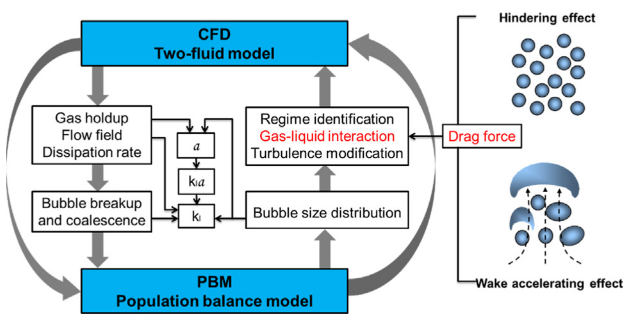
Guangyao Yang, Huahai Zhang, Jiajia Luo, Tiefeng Wang *

Beijing Key Laboratory of Green Reaction Engineering and Technology, Department of Chemical Engineering, Tsinghua University, Beijing 100084, China

HIGHLIGHTS

- Both hindering effect and wake accelerating effect were included in the drag correction.
- Bubble columns (BCs) were simulated by CFD-PBM with the new drag model.
- Drag correction should be based on both local gas holdup and bubble size distribution.
- CFD-PBM with the new drag model can simulate BCs well at complex conditions.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 2 May 2018
Received in revised form 2 July 2018
Accepted 6 July 2018

Keywords:
Bubble columns
Computational fluid dynamics (CFD)
Bubble swarms
Drag force
Gas holdup

ABSTRACT

The underlying mechanism and the generality of the drag correction factor C_D/C_{D0}, which was developed and applied in the simulation of bubble columns at elevated pressure in our recent work, was discussed in detail. With this drag model, numerical simulations of a bubble column were carried out by computational fluid dynamics (CFD) coupled with the population balance model (PBM). The complex variations of the drag correction factor and slip velocity with increasing local gas holdup were well predicted. The results confirmed that the drag correction should be based on the bubble size distribution and local gas holdup, instead of on the superficial gas velocity or overall gas holdup as commonly reported in the literature. The good predictions of the gas holdup and gas-liquid mass transfer in both water and high-viscosity liquids showed that the CFD-PBM model was powerful for the simulation of bubble columns under complex operating conditions.

1. Introduction

Bubble column reactors are widely used in a variety of chemical processes, such as Fischer-Tropsch synthesis, hydrocracking of petroleum residue and partial oxidation of ethylene to acetaldehyde, due to their good heat and mass transfer characteristics and ease of operation (Chilekar et al., 2010; Krishna and Sie, 2000; Shaikh and Aldahhan, 2013). Although extensive experimental and numerical studies have been carried out on bubble column reactors over the past decades (Esmaeili et al., 2015; Krishna et al., 2001; Lau et al., 2004; Wang et al., 2006), their complex hydrodynamic behaviors are still not fully understood. Computational fluid dynamics (CFD) offers the capability of simulating and designing the reactors with some fundamental parameters, without the need of constructing experimental facilities. However, the CFD model requires closure equations for the gas–liquid interphase forces, including the drag, lift, virtual mass, turbulent dispersion and wall lubrication forces (Buffo et al., 2016; Tabib et al., 2008; Wang et al., 2006). Among these interphase forces, the drag force is undoubtedly the most important in determining the gas holdup and affecting the gas-liquid volumetric mass transfer rate, because it

* Corresponding author.
E-mail address: wangtf@tsinghua.edu.cn (T. Wang).

https://doi.org/10.1016/j.ces.2018.07.012
0009-2509/© 2018 Published by Elsevier Ltd.

Notations

a	gas-liquid interfacial area, m^{-1}
$b(v)$	bubble breakup rate, s^{-1}
$c(v, v')$	bubble coalescence rate, $m^3 \cdot s^{-1}$
C_{D0}	drag coefficient of single bubble, dimensionless
C_D/C_{D0}	drag correction factor of bubble swarms, dimensionless
C_L	lift force coefficient, dimensionless
C_{TD}	turbulent dispersion force coefficient, dimensionless
C_{VM}	virtual mass force coefficient, dimensionless
C_W	wall lubrication force coefficient, dimensionless
d_b	diameter of the mother bubble, m
d_{bH}	maximum horizontal dimension of the bubble, m
d_c	critical bubble size for distinguishing large bubbles and small bubbles, m
d_s	bubble Sauter diameter, m
D	bubble column diameter, m
D_L, D_l	diffusion coefficient, $m^2 \cdot s^{-1}$
Eo	Eötvös number, $g(\rho_l - \rho_g)d_b^2/\sigma$, dimensionless
Eo'	modified Eötvös number, $g(\rho_l - \rho_g)d_{bH}^2/\sigma$, dimensionless
$f_{a,j}$	area fraction of node j in the total area, dimensionless
$f_{b,large}$	fraction of large bubbles, dimensionless
f_i	volume fraction of bubble group i in the gas holdup, dimensionless
F_L	transverse lift force, $N \cdot m^{-3}$
F_{TD}	turbulent dispersion force, $N \cdot m^{-3}$
F_{VM}	virtual mass force, $N \cdot m^{-3}$
F_W	wall lubrication force, $N \cdot m^{-3}$
$k_{b,large}$	model parameter accounting for wake accelerating effect of large bubbles, dimensionless
$k_{b,small}$	model parameter accounting for hindering effect of small bubbles, dimensionless
k_l	gas-liquid mass transfer coefficient, m/s
PDF	probability density function, mm^{-1}
Re	Reynolds number, dimensionless
U_g	superficial gas velocity, m/s
u_{slip}	bubble slip velocity, m/s
v	bubble volume, m^3

Greek letters

α	phase holdup, dimensionless
$\beta(v, v')$	daughter bubble size distribution function, dimensionless
ε	turbulent energy dissipation rate, $m^2 \cdot s^{-3}$
μ	liquid viscosity, mPa·s
ν_l	liquid dynamic viscosity, $m^2 \cdot s^{-1}$
$\eta_{i,k}$	transfer coefficient between bubble groups due to bubble breakup, dimensionless
$\eta_{i,jk}$	transfer coefficient between bubble groups due to bubble coalescence, dimensionless
σ	surface tension, $N \cdot m^{-1}$

determines the terminal velocity and residence time of bubbles in a bubble column.

The rising behavior of single bubbles is well understood and several typical correlations have been reported to calculate the drag coefficient or terminal velocity of single bubbles (Clift et al., 1978; Dijkhuizen et al., 2010; Rastello et al., 2011; Tomiyama et al., 1998). However, the drag coefficient of bubble swarms is very different from that of single bubbles due to the complex bubble interactions (Ishii and Zuber, 1979; Jakobsen, 2001; Roghair et al., 2011; Simonnet et al., 2007). Two effects of bubble swarm have been reported: the hindering effect of small bubbles (Behzadi et al., 2004; Rusche and Issa, 2000; Zenit et al., 2001) and the wake accelerating effect of large bubbles (Acuña and Finch, 2010; Krishna et al., 1999; Vassallo and Kumar, 1999).

Ishii and Zuber (1979) studied the drag force for a wide range of dispersed phase fraction and Reynolds number, and proposed correlations based on extensive experimental data. Although these correlations are applicable to both the homogeneous and heterogeneous flows, an average gas holdup is used and the critical value for the flow regime transition must be specified. Kashinsky and Timkin (1999) and Guet et al. (2004) measured the local bubble slip velocity for the homogeneous regime, and pointed out that it was necessary to correlate the slip velocity with the local gas holdup. Wang et al. (2006) proposed a drag model containing the wake accelerating effect of large bubbles based on the volume fraction of large bubbles and local gas holdup, while the hindering effect of small bubbles was ignored. Simonnet et al. (2007) investigated the variation of drag coefficient with the local gas holdup and proposed an empirical correlation based on experimental data obtained in an air-water system. This drag model was further used for CFD simulations of a bubble column, but a given bubble size was used and the effect of bubble size distribution was not considered (Simonnet et al., 2008). Roghair et al. (2013) studied the bubble swarm effects by front-tracking simulations, neglecting the effects of coalescence and breakup, and proposed two correlations of the drag coefficient of bubble swarms for the air-water and air-viscous liquid systems. They found that the drag coefficient increased with increasing local gas holdup and decreased with increasing bubble diameter. Mcclure et al. (2014a, 2014b) proposed that no hindering effect appearance for bubbles larger than 7 mm, and a modified drag model of Simonnet et al. (2007) was used in their CFD simulations. They also experimentally investigated the bubble swarm effects at high superficial velocities and found that the correction factor depended on both the bubble size distribution and local gas holdup (Mcclure et al., 2017). Liang et al. (2016) simulated a bubble column using the CFD-PBM coupled model with modified drag model and concluded that only the PBM-customized drag model with wake acceleration could reproduce the measured flow field. In summary, both the hindering effect of small bubbles and the wake accelerating effect of large bubbles exist in bubble swarms, and the drag coefficient should be correlated with both the bubble diameter and local gas holdup.

A drag correction factor for the hindering effect and wake accelerating effect was developed and applied in the simulation of bubble columns at elevated pressure in our recent work (Yang et al., 2017), however the underlying mechanism and the generality of this correction factor has not been discussed in detail. In this work, we made systematical comparison of our drag model with several classical models in the literature by numerical simulations of the bubble columns using the CFD-PBM coupled model. An important conclusion was that the drag correction should be based on the bubble size distribution and local gas holdup, instead of on the superficial gas velocity or overall gas holdup as commonly reported in the literature. The reliability and generality of this drag correction was validated by the good agreement of the calculated and experimental C_D/C_{D0} and the good predictions of the bubble column operated in a wide range of liquid viscosities.

2. Modeling and simulations

The numerical simulations were carried out with the CFD-PBM coupled model, which was similar to that in our previous work