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Computational fluid-dynamic modeling of the mono-dispersed homogeneous flow regime in bubble columns

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ABSTRACT

Two-phase bubble columns are equipment used to bring one or several gases into contact with a liquid phase. Despite the simple system design, bubble columns are characterized by complex fluid dynamic phenomena at different scales; for this reason, their correct design, operation and scale-up rely on the precise estimation of global and local fluid dynamics properties. In this respect, multi-phase Computational Fluid Dynamics (CFD), in the Eulerian multi-fluid framework, is particularly useful to study the fluid dynamics in multi-phase reactors. Within this approach, the accurate prediction of the fluid dynamics depends on the correct modeling of (a) the momentum exchange between the phases, (b) the effects of the dispersed phase on the turbulence of the continuous phase, and (c) the bubble coalescence and break-up phenomena. Furthermore, the global and the local fluid dynamic properties are related to the prevailing flow regime, i.e., the homogeneous flow regime and the heterogeneous flow regime. This paper mainly focuses on the homogeneous flow regime, which can be classified as "*pseudo-homogeneous*" or "*mono-dispersed homogeneous*", depending on the prevailing bubble size distribution. The numerical modeling of the "*pseudo-homogeneous*" flow regime has been discussed in our previous papers (i.e., modeling closures and suitable boundary conditions); conversely, this paper contributes to the existing discussion on the modeling closures by investigating the "*mono-dispersed homogeneous*" flow regime in "*small-scale*" and "*large-scale*" bubble columns. To this end, two test cases have been considered: (a) a "*small-scale*" bubble column (a test case taken from the previous literature); (b) a large-scale bubble column (a test case experimentally studied within this paper by image analysis, optical probe and gas holdup techniques). In particular, this paper studies the effects of the interfacial forces and bubble induced turbulence modeling within the Eulerian two-fluid approach. Three-dimensional transient simulations have been performed and the numerical results were compared with experimental data (both local and global fluid dynamics parameters). The results have been critically analyzed and the reasons for the discrepancies between the numerical results and the experimental data have been identified and may serve as a basis for future studies. Likewise, recommendations on suitable closures as well as guidelines for future studies have been provided. In conclusion, this paper extends the validation of a previously proposed set of closure relations (validated for the "*pseudo-homogeneous*" flow regime in a "*large-scale*" annular gap bubble column) to the "*mono-dispersed homogeneous*" flow regime in "*small-scale*" and large-scale bubble columns.

1. Introduction

Bubble columns provide a good experimental setup to study the turbulent phenomena in dense bubbly flows and to support the validation of numerical approaches. Indeed, the numerical modeling of the local and the global fluid dynamics in bubble column reactors is a way of supporting the reactor design and scale-up. In particular, among the different numerical approaches, Computational Fluid Dynamics (*CFD*) is a promising method to study the fluid dynamics in bubble columns (See, for example, (Peña-Monferrer et al., 2017)). In this respect, the local and the global fluid dynamic properties are related to the prevailing flow regime: mainly the homogeneous flow regime and the heterogeneous flow regime, if "*large-diameter*" bubble columns are considered (Besagni et al., 2017b). The homogeneous flow regime—generally associated with small gas superficial velocities, U_G—is referred as the flow regime where only "*non-coalescence-induced*" bubbles exist (as defined by Besagni and Inzoli (Besagni and Inzoli, 2016)). The homogeneous flow regime can be classified into the "*mono-dispersed homogeneous*" flow regime and the "*pseudo-homogeneous*" flow regime: the former is characterized by a mono-dispersed bubble size distribution (*BSD*), whereas the latter is characterized by a poly-dispersed *BSD*. The distinction between mono-dispersed and poly-

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Nomenclature

Acronyms

BSD	Bubble Size Distribution
CFD	Computational Fluid Dynamics
CFL	Courant Friedrichs Lewy number
URANS	Unsteady Reynolds Averaged Navier-Stokes

Non-dimensional numbers

$Eo = \frac{g(\rho_k - \rho_j)d_{eq}^2}{\sigma}$	Eötvös number
$Mo = \frac{g(\rho_k - \rho_j)\mu_k^4}{\rho_k^2\sigma^3}$	Morton number
$Re = \frac{\rho_k v_b d_{eq}}{\mu_k}$	Reynolds number

Symbols

A_c	Cross-sectional area of the column
A_{in}	Gas inlet area
C_L	Lift coefficient in Eq. (8)
C_{TD}	Turbulent dispersion coefficient in Eq. (11)
C_{VM}	Virtual mass force coefficient
C_{WL}	Wall force coefficient in Eq. (12)
C_{W1} and C_{W2}	Coefficients in Eq. (13)
d_b	Bubble equivalent diameter (mm)
d_c	Bubble column inner diameter (m)
d_{lift}	Bubble equivalent diameter for the change of the sign in the lift force coefficient (mm)
$d_\perp$	Maximum horizontal dimension of the bubble (mm)
$Eo_\perp$	Eötvös number considering the maximum horizontal dimension of the bubble $d_\perp$
F_D	Drag force ($kg\,m^{-2}\,s^{-2}$)
F_L	Lift force ($kg\,m^{-2}\,s^{-2}$)
F_{TD}	Turbulent dispersion force ($kg\,m^{-2}\,s^{-2}$)
F_{VM}	Virtual mass force ($kg\,m^{-2}\,s^{-2}$)
F_{WL}	Wall force ($kg\,m^{-2}\,s^{-2}$)
M_I	Momentum exchanges ($kg\,m^{-2}\,s^{-2}$)
g	Acceleration of gravity ($m\,s^{-2}$)
H_c	Bubble column height (m)
H_D	Height of the liquid free surface after aeration (m)
H_0	Height of the liquid free surface before aeration (m)
U_G	Gas superficial velocity (m/s)
p	Pressure (Pa)
u	Velocity in governing equations (m/s)
y	Axial distance from the gas sparger (m)
y_W	Distance to the nearest wall in Eq. (13) (m)
$v_{G,in}$	Velocity of the gas phase at the gas sparger, Eq. (6) (m/s)
V	Volume (m^3)

Greek letters

α	Volume fraction
ε_G	Gas holdup
$\varepsilon_{G,Local}$	Local void fraction
μ	Dynamic viscosity ($kg\,m^{-1}\,s^{-1}$)
ρ	Density ($kg\,m^{-3}$)
σ	Surface tension coefficient ($N\,m^{-1}$)
σ_{TD}	Schmidt number in Eq. (11)
$\overline{\tau}$	Viscous and Reynolds stresses ($kg\,m\,s^{-2}$)
τ	Time scale (s^{-1})

Superscripts

$\rightarrow$	Vector quantity

Subscripts

j	j-th dispersed phase in governing equations
k	k-th Continuous phase in governing equations
z	Generic phase in governing equations

Turbulence quantities

ε	Turbulent dissipation rate ($m^2\,s^{-3}$)
ω	Specific dissipation rate (s^{-1})

dispersed BSDs is based upon the change in the sign of the lift force coefficient (See Refs. (Besagni and Inzoli, 2016; Lucas et al., 2015)), which occurs at, approximately, an equivalent bubble diameter of $d_b = 5.8$ mm (considering air-water systems at ambient conditions).

The "*mono-dispersed homogeneous*" flow regime is a good test for numerical codes, to validate models to be applied for the design of "*industrial-scale*" bubble columns, where the "*pseudo-homogeneous*" flow regime and the heterogeneous flow regime are observed at most. Among the available modeling techniques, the Eulerian multi-fluid approach and the Eulerian-Lagrangian approach can be used. The former is the most common approach to simulate bubble columns, as reported in the review of Jakobsen et al. (Jakobsen et al., 2005); conversely, the latter is mostly applied to simulate "*small-scale*" reactors with low gas holdup[1] (Besbes et al., 2015; Buwa et al., 2006; Delnoij et al., 1997; Hu and Celik, 2008; Jain et al., 2013; Lapin and Lübbert, 1994). The Eulerian multi-fluid approach treats each phase as inter-penetrating continua and relies on an ensemble averaging of the multiphase Navier-Stokes equations; for this reason, this approach needs closures for the flow turbulence and the inter-phase exchanges phenomena. The latter have to include (a) the exchange of momentum between the phases, (b) the effects of the dispersed bubbles on the turbulence of the continuous phase, and (c) the effects of coalescence and break-up phenomena. The first two aspects are discussed in the following; for the last point, the reader may refer to Rzehak et al. (Rzehak et al., 2015).

In the Eulerian multi-fluid modeling approach, correlations for inter-facial forces are implemented to model the inter-phase momentum exchanges (i.e., the drag, lift, virtual mass, turbulent dispersion and wall lubrication forces). The drag force has large effects on the macroscopic flow patterns, i.e., gas the gas holdup, axial velocity profiles and local void fraction profiles (Laborde-Boutet et al., 2009; Tabib et al., 2008). The lift force is responsible for the migration of small bubbles toward the column walls in co-current flow, and for the uniform spreading of small bubbles in counter-current flow or in the batch mode. Conversely, a force that can be assimilated to the lift force tends to push large and deformed bubbles towards the center of the column (Lucas et al., 2005; Tomiyama et al., 2002). As a result, correlations for the lift force coefficient usually display a change of sign from negative, for smaller diameter bubbles, to positive, for large diameter bubbles (Tomiyama et al., 2002). The bubble dispersion due to the liquid turbulent fluctuations is taken into account through the turbulent dispersion force; this force has an important role on the gas fraction profiles as it modulates peaks of small bubbles near the walls and spreads out large bubbles from the pipe center (Lucas et al., 2007). Its magnitude is high near the inlets of the gas sparger (Krepper et al., 2007), thus supporting the modeling of bubble dispersion near coarse gas spargers. The wall lubrication force is intended to model the lift force

[1] The gas holdup (ε_G) is a dimensionless parameter defined as the volume of the gas phase divided by the total volume of the system. Th gas holdup is a global fluid dynamic property of fundamental and practical importance. The gas holdup determines the mean residence time of the dispersed phase and, in combination with the size distribution of the dispersed phase, the interfacial area for the rate of interfacial heat and mass transfer.