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Computational Fluid-Dynamic modeling of the pseudo-homogeneous flow regime in large-scale bubble columns

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ABSTRACT

An understanding of the fluid dynamics and the transport phenomena in bubble columns (in the homogeneous and heterogeneous flow regimes) is of fundamental importance to support the design and scale-up methods. In this respect, multiphase Computational Fluid-Dynamics (CFD) simulations in the Eulerian multi-fluid framework are particularly useful to study the fluid dynamics in large-scale reactors; in particular, this study concerns the modeling of the fluid dynamics in bubble columns within the boundaries of the homogeneous flow regime. Reliable predictions of the homogeneous flow regime with this approach are, however, limited up to now. One important drawback is that usually the needed closure models for the interphase forces, turbulence and coalescence and break-up are selected case-by-case, which hinder improvement of the predictive value. A set of closure relations has been collected at the Helmholtz-Zentrum Dresden-Rossendorf that represents the best available knowledge and may serve as a baseline model for further investigations. In this paper, the validation of this set of closure relations has been extended to the pseudo-homogeneous flow regime—characterized by a wide spectrum of bubble sizes and typically associated with the large sparger openings used in industrial applications—in large-scale bubble columns, thus establishing a first step towards the simulation of industrial-scale reactors. To this end, the benchmark considered is a comprehensive dataset obtained for a large-scale bubble column, which has been built accordingly with the well-known scale up criteria (large-diameter, high aspect ratio and large sparger openings). The numerical approach has been tested in its fixed-poly-dispersed formulation (considering the two- and four-classes approaches to represent the dispersed phase) and considering the coalescence and break-up closures. The results suggest that the correct simulation of the fluid dynamics in the bubble column requires the definition of coalescence and break-up closures. 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 basis for future studies.

1. Introduction

Bubble columns are multiphase reactors in which a gas phase is dispersed into a continuous phase (a liquid phase or a suspension) by means of a sparger. Bubble columns can be designed to work either in semi-batch mode or in continuous mode (with the continuous phase moving with or counter the dispersed phase). In this paper we focus on gas-liquid bubble columns operated in the batch mode, which are widely used in the chemical, petrochemical and biochemical industries because of a number of advantages they provide in both design and operation. Unfortunately, despite the simple column arrangement, the interactions between the phases inside the reactor are extremely complex, making their design and scale-up very difficult (Leonard et al., 2015; Rollbusch et al., 2015). Furthermore, in most industrial applications, internal devices are added to control heat transfer, to increase bubble break-up or to limit liquid phase back-mixing: these elements can highly influence the multiphase flow inside the bubble column (Besagni and Inzoli, 2016c). The understanding of the fluid dynamics, the interactions between the phases, and the transport phenomena involved is essential to support the design and scale-up methods (Shaikh and Al-Dahhan, 2013); in this respect, there is a growing attention towards Computational Fluid-Dynamics (CFD) to predict the fluid dynamics in bubble columns. Indeed, the correct design, operation and scale-up of bubble columns rely on the proper prediction of the global as well as the local fluid dynamic properties—i.e., the gas holdup (ε_G) and the bubble size distribution (BSD). The gas holdup is a dimensionless parameter defined as the volume of the gas phase divided by the total volume of the dispersed phase. It determines

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Nomenclature

Acronyms

BSD Bubble Size Distribution
CFD Computational Fluid Dynamics
CFL Courant Friedrichs Lewy number
CLD Chord Length Distribution
GVF Gas Volume Fraction
HZDR Helmholtz-Zentrum Dresden-Rossendorf
iMUSIG Inhomogeneous Multiple Size Group
RANS Reynolds Averaged Navier Stokes
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

$C_{\varepsilon B}$ - Bubble-induced turbulence coefficient in Eq. (4).
C_μ - Constant in Eq. (7).
C_D - Drag coefficient in Eq. (11).
C_L - Lift coefficient in Eq. (16).
C_{TD} - Turbulent dispersion coefficient in Eq. (23).
C_{VM} - Virtual mass force coefficient in Eq. (24).
C_{WL} - Wall force coefficient in Eq. (20).
d_{23} mm Sauter mean bubble diameter
d_b mm Bulk bubble diameter in Eq. (5).
d_{eq} mm Bubble equivalent diameter
$d_\perp$ mm Maximum horizontal dimension of the bubble
d_c mm Diameter of the column
d_o mm Diameter of the column sparger openings
d_{cr} mm Bubble equivalent diameter for the change of sign of the lift force
f - Class relative frequency
$Eo_\perp$ - Eötvös number considering the maximum horizontal dimension of the bubble $d_\perp$
F_D kg m^{-2} s^{-2} Drag force
F_L kg m^{-2} s^{-2} Lift force
F_{TD} kg m^{-2} s^{-2} Turbulent dispersion force
F_{VM} kg m^{-2} s^{-2} Virtual mass force
F_{WL} kg m^{-2} s^{-2} Wall force
M_I kg m^{-2} s^{-2} Momentum exchanges
$\vec{n}_w$ - Unit normal to the wall pointing toward the fluid
g m s^{-2} Acceleration of gravity
h m Distance from the sparger
U_G m s^{-1} Gas superficial velocity
k m^2 s^{-2} Turbulent kinetic energy
p Pa Pressure
S^k kg m^{-1} s^{-3} Source term for the turbulent kinetic energy (bubble induced turbulence contribution) – Eq. (3).
S^ε kg m^{-1} s^{-3} Source term for the turbulent energy dissipation (bubble induced turbulence contribution) – Eq. (4).
S^ω kg m^{-1} s^{-3} Source term for the specific dissipation (bubble induced turbulence contribution) – Eq. (6).
t s Time
u m s^{-1} Velocity in governing equations
v_b m s^{-1} Bubble velocity
y m Distance to the wall

Greek letters

α - Volume fraction
ε_G - Gas holdup
$\varepsilon_{G,\ Local}$ - Local void fraction
μ kg m^{-1} s^{-1} dynamic viscosity
ρ kg m^{-3} density
σ N m^{-1} surface tension
γ - Volume fraction contribution (Eq. (26))
σ_{TD} - Schmidt number in Eq. (23).
$\bar{\tau}$ kg m s^{-2} viscous and Reynolds stresses
τ s^{-1} Time scale

Superscripts

$\rightarrow$ Vector quantity
turb Turbulent quantity
mol Physical quantity
eff effective value (turbulent and physical)

Subscripts

|| Component of the vector parallel to the wall
cap-bubble Cap-shape bubble
ellipse Ellipse-shape bubble
large large bubble gropus
small small bubble group
sphere Spherical-shape bubble
j j-th dispersed phase in governing equations
k k-th Continuous phase in governing equations
z Generic phase in governing equations
liquid-phase Term included in the governing equations for the liquid phase

Turbulence quantities

k m^2 s^{-2} Turbulent kinetic energy
ε m^2 s^{-3} Turbulent dissipation rate
ω s^{-1} Specific dissipation rate

the mean residence time of the dispersed phase and, in combination with the BSD, the interfacial area for the rate of interfacial heat and mass transfer (and, thus, the reactor scale, for given heat and mass transfer requirements). It is important to observe that the global and local fluid dynamic properties are related to the prevailing flow regime: in a large-diameter bubble column—accordingly with the "*large-diameter*" definition of Besagni et al. (Besagni et al., 2016b)—the prevailing flow regimes can be distinguished in (i) the homogeneous and (ii) the heterogeneous flow regimes. A complete discussion of the characteristics of these flow regimes have been firstly proposed by Besagni et al. (Besagni et al., 2016c) and further elaborated and formalized in the subsequent study by Besagni et al. (Besagni et al., 2017); in the following, the main concepts are outlined, for the sake of clarity within this work. The homogeneous flow regime—associated with small superficial gas velocities, U_G—is referred as the flow regime where only "*non-coalescence-induced*" bubbles exist (e.g. as detected by the gas disengagement technique, ref. (Besagni and Inzoli, 2016b)). The homogeneous flow regime can be further distinguished into "*pure-homogeneous*" (or "*mono-dispersed homogeneous*") flow regime and "*pseudo-homogeneous*" (or "*poly-dispersed homogeneous*" or "*gas maldistribution*") flow regime: the former is characterized by a mono-dispersed BSD (and, generally, has a flat local void fraction