Particuology xxx (2017) xxx–xxx

Contents lists available at ScienceDirect

Particuology

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

Counter-current three-phase fluidization in a turbulent contact absorber: A CFD simulation

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ARTICLE INFO

Article history:
Received 10 June 2016
Received in revised form 14 October 2016
Accepted 30 October 2016
Available online xxx

Keywords:
Multiphase
Counter-current
Computational fluid dynamics (CFD)
Fluidization
Turbulent contact absorber

ABSTRACT

A computational fluid dynamics study of three-phase counter-current fluidization occurring in a turbulent contact absorber was performed. A two-dimensional, transient Eulerian multi-fluid model was used, in which the dispersed solid phase was modeled employing a kinetic theory of granular flow. The grid independence of the model, the effect of wall boundary conditions, the choice of granular temperature model, the effects of order of discretization scheme and drag models were studied for a base case setting. The results of simulations were validated against experimental results obtained from the literature. Once the model settings were finalized, simulations were performed for different gas and liquid velocities to predict the hydrodynamics of the absorber. Computed bed expansion and pressure drop were compared with experimental data. Good agreement between the two was found for low velocities of gas and liquid.

Introduction

In the past few decades, three-phase operations have been applied extensively in process industry (Blum & Toman, 1977; Brenner, 2013; Epstein, 1981; Martinez, Sánchez, Ancheyta, & Ruiz, 2010; Reese, Silva, Tang, & Fan, 1999; Schügerl, 1997; Soung, 1978; Wright & Raper, 1996; Xu, Zhong, Jin, & Wang, 2014). However, most of the systems investigated have been operated in concurrent-up mode (Cho, Song, Kim, Kang, & Kim, 2001; Larachi, Belfares, Iliuta, & Grandjean, 2001; Miura, Takahashi, & Kawase, 2001; Nikov, Grandjean, Carreau, & Paris, 1990; Szlemp, Janecki, & Bartelmus, 2001). Kielback (1960) was among the pioneers in using counter-current contacting mode for gas scrubbing. This type of device has been referred to in the literature as a turbulent bed contactor, floating bed scrubber, fluidized bed scrubber, turbulent bed cooling tower, and fluidized packing contactor (Haq, 2012; Muroyama & Fan, 1985). Generally, to enhance mass transfer rates, a turbulent contact absorber (TCA) employs light packing as fluidization medium for the counter-current contact of gas and liquid. The gas flows through the device as a continuous phase whereas liquid falls as a dispersed medium. A TCA can be employed for particulate removal, cooling of process air, humidification and dehumidification, absorption and desorption, flue gas desulphurization, and several other areas. TCA type devices do have some disadvantages. For example, back mixing can occur in the liquid phase, damaging packing material with excessive movement and periodic bed pulsing. These effects are more pronounced in large and deep beds (Haq, 2012; Muroyama & Fan, 1985; Reese et al., 1999).

The first attempt to theoretically investigate the hydrodynamics of three-phase turbulent contactors was made by O'neill, Nicklin, Morgan, and Leung (1972). Several attempts to model and simulate hydrodynamics of TCA have been made since then (Bruce, Balasubramanian, Sai, & Krishnaiah, 2006; Chen & Douglas, 1968; Cho et al., 2001; Guerriere, Fayed, & Matchett, 1998; Vunjak-Novakovic, Vukovic, & Littman, 1987). Operating regimes for the TCA can be broadly divided into two categories, namely Type-I and Type-II (Vunjak-Novaković, Vuković, Obermayer, & Vogelpohl, 1980). The former is characterized by operations without flooding conditions, whereas the latter regime is governed by operations under flooding. A comprehensive discussion on this classification can be found in the literature (Muroyama & Fan, 1985; Vunjak-Novaković et al., 1980). For both types, there is a consensus among researchers that liquid holdup increases with liquid velocity and is independent of packing diameter. Furthermore, the pressure drop is not affected significantly by gas velocity; however, it is strongly dependent upon liquid flow rate, packing density, and column diameter. These findings were verified on a pilot-scale set-

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http://dx.doi.org/10.1016/j.partic.2016.10.008
1674-2001/

Please cite this article in press as: Gillani, S. S. J., et al. Counter-current three-phase fluidization in a turbulent contact absorber: A CFD simulation. *Particuology* (2017), http://dx.doi.org/10.1016/j.partic.2016.10.008

Nomenclature

A_i	Area of the *i*th component, m^2
C_D	Drag coefficient
D_c	Diameter of column, m
d_p	Diameter of solid particle, m
e	Restitution coefficient
g	Gravitational acceleration, m/s^2
g_0	Radial distribution function
H_0	Static bed height, m
H_c	Height of column, m
K	Interphase momentum exchange coefficient
L	Grid size, mm
Re	Reynolds number
U	Inlet superficial velocity, m/s
W_s	Weight of solid phase, kg
v	Real velocity, m/s
Greek symbols	
ΔP	Pressure drop, Pa
γ	Collisional dissipation energy, J/(m^3 s)
λ	Solid bulk viscosity
μ	Viscosity, Pa s
φ	Specularity coefficient
ρ_i	Density of the *i*th phase
τ	Stress tensor, Pa
θ	Granular temperature, m^2/s^2
ε	Volume fraction
I	Unit tensor
k_θ	Granular conductivity
Subscripts	
0	Initial
g	Gas phase
l	Liquid phase
p	Particle
r	Radial direction
s	Solid phase
w	Wall
y	Axial direction
col	Collisional
fric	Frictional
kin	Kinetic

up installed at Pakistan Institute of Engineering & Applied Science (PIEAS). In the work of Haq, Inayat, Zaman, and Chughtai (2010) correlations for predictions of liquid holdup and pressure drop across the bed were developed based on data from an in-house TCA. The predictions of the correlation proposed therein agree qualitatively with other literature (Lyashuk & Berengarten, 2001; Vunjak-Novakovic et al., 1987).

CFD modeling of the fluidized beds can be performed by either the Euler–Lagrange approach or Euler–Euler approach (Benyahia, Syamlal, & O'Brien, 2007; Gidaspow, 1994; Li & Zhong, 2015; Mitra-Majumdar, Farouk, & Shah, 1997; Sivaguru, Begum, & Anantharaman, 2009; Ullah, Hong, Chilton, & Nimmo, 2015). System size, time-step size, and lack of accurate particle–particle closures limit the use of the Euler–Lagrange approach (Chen & Wang, 2014; Deen, Annaland, van der Hoef, & Kuipers, 2007; Hamidipour, Chen, & Larachi, 2012). Researchers have used multi-fluid Eulerian approach to model both two- and three-phase fluidized beds successfully with relatively low computational overhead (Chang, Zhang, Meng, Wang, & Wei, 2012; Cornelissen, Taghipour, Escudié, Ellis, & Grace, 2007; Grace & Li, 2010; Hamidipour et al., 2012; Hartge, Ratschow, Wischnewski, & Werther, 2009; Nikolopoulos et al., 2013; Panneerselvam, Savithri, & Surender, 2009; Peng, Dong, Li, Wang, & Lin, 2013; Sivaguru et al., 2009).

Given the presence of the three phases, the multi-fluid model (MFM) or three-fluid model considers the three fluids as interpenetrating continua. All the phases interact with each other in all the cells of the computational domain. The flow and pressure fields are shared among all the phases in accordance with the corresponding volume fraction. A recent thorough review of different aspects of the CFD modeling of three-phase reactors has been presented by Pan, Chen, Liang, Zhu, and Luo (2016). Generally, empirical correlations are used to describe the interphase couplings and kinetic theory of granular flow (KTGF) is used to close the solid-phase stresses. Panneerselvam et al. (2009) performed MFM CFD simulations that included a turbulence model to predict the overall performance of a gas–liquid–solid fluidized bed. Schallenberg, Enß, and Hempel (2005) used the Eulerian approach to successfully simulate three-phase bubble column hydrodynamics. Rampure, Buwa, and Ranade (2003) performed three-phase Eulerian simulations to study the effects of solids loading in a cylindrical bubble column.

In the Eulerian framework, the phase interaction is one of the more complex phenomena, which has to be modeled through appropriate correlations. Interphase interaction comprises several forces, the dominant being drag (Pan et al., 2016). For gas–liquid interaction, Schiller and Naumann (1935) correlation remains the most popular for spherical bubbles. However, because of continuous coalescence and breakup, bubbles are not always spherical. Therefore, other models such as that of Ishii and Zuber (1979) may be used. The coupling between solid particles and fluids, i.e., gas or liquid is generally achieved by modeling drag by the widely used Wen and Yu or Gidaspow model (Gidaspow, 1994). In the Eulerian approach, the particle–particle interaction is generally accounted for using a value for the coefficient of restitution. If the three-phase operation involves heat and mass transfer, they will also play a significant role in determining the interphase momentum transfer. Therefore, a detailed analysis of the effects of physical, chemical, and thermal properties of the three phases must be determined before an industrial scaling up of such three-phase reactors (Kim & Kang, 1997). To summarize, interphase coupling in three-phase fluidized systems is quite complex because of multiple interaction forces, such as drag, lift, the added mass force, and the Basset force. Apart from drag, the dominant of the forces, the degree to which the other forces affect the hydrodynamics, as well as the heat and mass transfer characteristics, of a three-phase fluidized bed, is still an open area for research.

Most of the modeling and simulation studies of three-phase fluidization have been performed for co-current-type systems. Comprehensive modeling of the counter-current fluidized beds such as TCA is still awaited. The present work is a step in this direction. This manuscript is organized such that initially a brief description of the experimental set-up used for simulations is presented. In the sections to follow, the multi-fluid Eulerian modeling approach adopted for the simulation of the hydrodynamics of an in-house counter-current TCA is presented. The results of grid independence, the effect of wall boundary conditions, and the choice of granular temperature model and drag law are all used to simulate hydrodynamics of the TCA for different operating conditions. The results obtained are presented and discussed in light of the available experimental data. The paper concludes with recommendations for further work.

Experimental set-up

Fig. 1 shows a schematic of the experimental set-up of the TCA at PIEAS developed and investigated by Haq (2012). The cylindrical

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