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Discrete particle simulations of bubble-to-emulsion phase mass transfer in single-bubble fluidized beds

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ABSTRACT

A classical Euler–Lagrangian model for gas–solid flows was extended with gas component mass conservation equations and used to obtain fundamental insights into bubble-to-emulsion phase mass transfer in bubbling gas–solid fluidized beds. Simulations of injected single rising bubbles under incipient fluidization conditions were carried out, using Geldart-A and -B particles. Phenomena observed in the simulations and those of various theoretical models used to derive phenomenological models were compared to challenge the assumptions underlying the phenomenological models. The bubble-to-emulsion phase mass transfer coefficients calculated for the simulations using Geldart-B particles were in a good agreement with predictions made using the Davidson and Harrison (1963) model. The bubble-to-emulsion phase mass transfer coefficients for Geldart-A particles were, however, much smaller than the predictions obtained from theoretical models (e.g. Chiba and Kobayashi (1970)). The newly developed model allows a detailed analysis of various hydrodynamic aspects and their effects on the mass transfer characteristics in and around rising bubbles in fluidized beds.

Introduction

Gas–solid fluidized bed reactors are often used in process industries owing to their excellent mixing and heat transfer characteristics. It is well known that bubbles prevail in these beds and their dynamics are responsible for the agitation of solids and the accompanying favorable heat and mass transfer characteristics of fluidized beds. An important foundation for a rational design of fluidized bed reactors is a thorough understanding of the mass transfer processes in fluidized beds, specifically the bubble-to-emulsion phase mass transfer. This phenomenon occurs via the combined effects of gas diffusion, coherent gas flow and solids motion carrying adsorbed gas atoms (Davidson & Harrison, 1963; Kunii & Levenspiel, 1991).

Single-bubble fluidized beds and freely bubbling fluidized beds have been used in past decades to study the bubble-to-emulsion phase mass transfer, both experimentally and numerically (a.o. Dang, Kolkman, Gallucci, & van Sint Annaland, 2013; Deshmukh, van Sint Annaland, & Kuipers, 2007; Hernández-Jiménez, Gómez-García, Santana, & Acosta-Iborra, 2013; Patil, van Sint Annaland, & Kuipers, 2003; Pavlin et al., 2007). Phenomenological models, used for the design of industrial-scale reactors, can only provide reliable predictions when accurate mass transfer coefficients are used. Until now, most correlations for these coefficients have been based on (i) analytical considerations and (ii) experiments using invasive measurement techniques. Several problems arise when using phenomenological models. First, various assumptions are made to reduce the mathematical analysis, but the scope of their validity has not yet been analyzed in detail. Second, the invasive experimental techniques may disturb the flow and are limited to point measurements. Noninvasive optical techniques (e.g., Dang et al., 2013; Müller et al., 2006; Pavlin et al., 2007 Roels & Carmeliet, 2006) have been developed in the meantime, but detailed understanding of the underlying mechanisms remains out of reach particularly owing to difficulties in measuring the gas concentration in the emulsion phase (Dang et al., 2013).

Numerical simulations (i.e., computational fluid dynamics) can shed more light on the detailed process of interphase mass transfer. Patil et al. (2003) and Hernández-Jiménez et al. (2013), for instance, employed a two-fluid model (TFM, employing the Euler–Euler technique) for fluidized beds comprising Geldart-B particles. Patil et al. (2003) found that the Davidson and Harrison (1963) model predicted the mass transfer for single injected bubbles reasonably well, but their results gave a bubble size evolution and tracer gas con-

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Nomenclature

A	Area (m^2)
c	Number of species
d	Particle diameter (m)
D_b	Bubble diameter (m)
D	Diffusion coefficient (m^2/s)
e	Coefficient of restitution
f	Volume fraction
$\mathbf{F}_{contact,a}$	Contact force of particle a (N)
$\mathbf{g}$	Gravitational acceleration (m/s^2)
I	Moment of inertia ($kg\ m^2$)
k	Spring stiffness (N/m)
K	Mass transfer coefficient (s^{-1})
m_a	Particle mass (kg)
M	Molar mass (kg/mol)
N_p	Particle number
P	Pressure (Pa)
R	Gas constant (J/mol K)
$\mathbf{S}_p$	Particle drag source term (N/m^3)
t	Time (s)
T	Temperature (K)
$\mathbf{u}_g$, $\mathbf{v}_a$	Gas and solid velocities (m/s)
U	Velocity (m/s)
V	Volume (m^3)
x	Mole fraction
y	Mass fraction

Greek symbols

β	Inter-phase momentum exchange coefficient ($kg/m^3\ s$)
ε	Volume fraction
η	Damping coefficient
μ	Gas phase shear viscosity (Pa s)
μ_f	Friction coefficient
ρ	Density (kg/m^3)
τ	Stress tensor (Pa)

Subscripts

a, p	Particle
b	Bubble
bc	Bubble-to-cloud
be	Bubble-to-emulsion
ce	Cloud-to-emulsion
A, B	Gas component
g	Gas
i, j	Component
mb	Minimum bubbling fluidization condition
mf	Minimum fluidization condition
n	Normal direction
t	Tangential direction
w	Wake
inj	Injection
diff	Diffusion

Acronyms

CFD	Computational fluid dynamics
DPM	Discrete particle model
TFM	Two-fluid model

centration that were inconsistent with the results of experiments conducted by Dang et al. (2013). Hernández-Jiménez et al. (2013), meanwhile, obtained results that were in good agreement with the Davidson and Harrison (1963) model for single-injected bubbles but found that the mass transfer coefficients were more than twice those predicted when using freely bubbling fluidized beds.

It will be possible to identify the most important aspects of the interphase mass transfer with models offering greater detail. While the TFM makes various assumptions to describe the rheology of the emulsion phase, the particle–particle interactions are taken into account deterministically in a discrete particle model (DPM, employing a Euler–Lagrange technique). The DPM model can therefore provide more detailed insight into the prevailing phenomena than the TFM model and allows the simulation of smaller particles (e.g., Geldart-A particles). Geldart-A particles are often used in industrial fluidized beds (typically fluid catalytic cracking catalyst) and are of interest in the design of microfluidized beds (e.g., Tan, Roghair, & van Sint Annaland, 2014, 2016).

The present work uses a state-of-the-art DPM model extended with gas component conservation equations to characterize the interphase mass transfer processes in gas–solid fluidized beds comprising Geldart-B and Geldart-A particles. The model will be used to simulate single injected bubbles that rise through an incipiently fluidized bed, analogous to the experiments carried out by Patil et al. (2003) and Dang et al. (2013), but without the specific limitations inherent to their techniques. Additionally, the tracer gas concentration in the emulsion phase is not neglected but analyzed for the computation of the mass transfer coefficient.

This section continues with a short overview of the available correlations for the bubble-to-emulsion phase mass transfer coefficient, which will be used in the comparison with simulation results. In the following three sections, the DPM model is then outlined and a detailed analysis of mass transfer processes in Geldart-B and subsequently Geldart-A particles is described. A discussion and conclusions are finally presented.

Phenomenological models for bubble-to-emulsion mass transfer

Several correlations have been reported in the literature for the prediction of the mass transfer coefficients. The derivation of these correlations usually assumes a gas cloud between a bubble and the emulsion (bulk) phase, originally deemed as a thin region surrounding the bubble with a relatively high solids holdup compared with the bulk emulsion. Davidson first suggested the existence of the gas cloud in gas–solid bubbling fluidized beds (Rowe, Partridge, & Lyall, 1964). The pioneering model of Davidson and Harrison (1963) has been widely used in phenomenological models for large-scale fluidized bed reactors. In their model, the total mass transfer consists of a convective flow from the bubbles to the emulsion phase and diffusion from the bubbles to the cloud. Kunii and Levenspiel (1991) followed their approach and proposed an extension considering two consecutive transfer steps, namely the transfer from the bubble to the cloud and that from the cloud to the emulsion. According to the stream function derived by Murray (1965) and Chiba and Kobayashi (1970) assumed that the gas composition in the cloud and bubble is uniform and that the mass transfer limitation is largely governed by diffusion through the surface between the cloud and emulsion phases. Table 1 summarizes the equations used to estimate the bubble-to-emulsion mass transfer coefficient for the most popular phenomenological models, together with the main assumptions use

Numerical method

Extended discrete particle model

The soft-sphere DPM employed in this study is based on the pioneering work of Tsuji, Kawaguchi, and Tanaka (1993) and was originally developed by Hoomans, Kuipers, Briels, and Van Swaaij

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