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Modeling and simulation of the influences of particle-particle interactions on dense solid–liquid suspensions in stirred vessels

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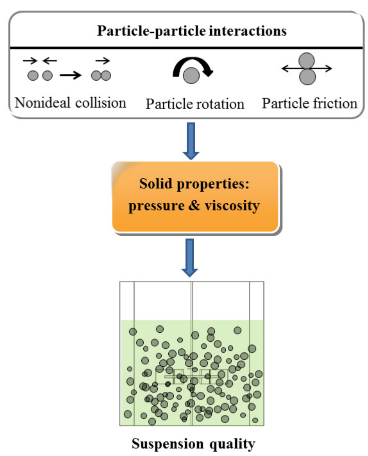
HIGHLIGHTS

- Coupled CFD with a modified KTGF model for describing solid-liquid suspension behaviors.
- Validation of the coupled model using open experiment data.
- Solid particle distribution phenomenon is studied by CFD.
- Investigation of the role of particle-particle interactions.

GRAPHICAL ABSTRACT



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ABSTRACT

Solid–liquid suspensions are commonly encountered in industrial production processes. The dynamics of the solid–liquid suspension behaviors depends on both liquid–particle and particle–particle interactions. In this work, an Eulerian–Eulerian model is used to characterize the suspension dynamics and the role of particle–particle interactions in solid-liquid mixing vessels is studied. The collision and friction of coarse particles are considered by calculating solid pressure and viscosity based on a modified kinetic theory of granular flow (KTGF). The solid phase holdup and the velocity are predicted and compared with semi-empirical models. Effects of several key model parameters are investigated as well. The comparison between computational fluid dynamics simulations and experimental data shows a satisfactory agreement, which validates the robustness of the multi-fluid model. The proposed model is then applied to study the influences of particle size and solid loading for exploring the importance of particle–particle interactions. The obtained simulation results show that particle–particle interactions can influence suspension characteristics in the case of large particle size and high solid loading.

1. Introduction

Solid–liquid suspensions in agitation vessels commonly found in the crystallization, polymerization, catalytic reactions, mineral,

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Nomenclature

a_{ct}, a_{kt}, a_r, a_t	KTGF model parameter, (–)
B	percent solids concentration, (–)
C_1, C_2	KTGF model parameter, (–)
$C_{1\varepsilon}$, $C_{2\varepsilon}$	k-ε model parameter, (–)
C_D	Drag coefficient, (–)
d	diameter of particles (m)
D	impeller diameter, (m)
e_0	fluctuation kinetic energy ($m^2\ s^{-2}$)
e_s	normal restitution coefficient, (–)
E	Drag model parameter, (–)
F_{ls}	inter-phase force ($N\ m^{-3}$)
g	gravitational acceleration ($m\ s^{-2}$)
g_0	radial distribution function, (–)
$G_{k,l}$	k-ε model parameter, (–)
I	unit tensor, (–)
k	turbulent kinetic energy, ($m^2\ s^{-2}$)
k_{dil}	KTGF model parameter, (–)
K	KTGF model parameter, (–)
n	grid number, (–)
N_{js}	just suspended speed, (rpm)
p	pressure, (Pa)
Re	Reynolds number, (–)
S	dimensionless coefficient in Zwietering's correlation, (–)
t	Time, (s)
T	tank diameter, (m)
v	velocity, ($m\ s^{-1}$)

Greek letters

α	volume fraction, (–)
β	tangential restitution coefficient, (–)
β_{ls}	inter-phase drag force coefficient, ($kg\ m^{-3}\ s^{-1}$)
γ_s	collisional dissipation energy, ($kg\ m^{-1}\ s^{-3}$)
ρ	density, ($kg\ m^{-3}$)
$\bar{\bar{\tau}}$	stress tensor, (Pa)
μ	viscosity, (Pa s)
ε	turbulent dissipation rate, ($m^2\ s^{-3}$)
σ_ε	turbulent Prandtl number, (–)
η	KTGF model parameter, (–)
Π	KTGF model parameter, (–)
ξ_b	bulk viscosity, (Pa)
ξ_s	spin viscosity, (Pa)
δ_{ij}	Kronecker's symbol, (–)
κ_s	thermal conductivity coefficient, ($kg\ m^{-1}\ s^{-1}$)

and water treatment processes. Such processes usually require a highly effective contact between solid and fluid phases (Kasat et al., 2008; Shah et al., 2015, 2008; Wadnerkar et al., 2012). A high solid suspension rate is important to strengthen the mass transfer in these processes. Consequently, experimental research (Hartmann et al., 2004; Hosseini et al., 2010a; Montante et al., 2001; Sardeshpande et al., 2010) and computational fluid dynamics (CFD) simulations (Derksen, 2003; Feng et al., 2013; Guha et al., 2008) in the past few decades have been carried out to study the dynamics of solid–liquid mixings.

As an effective and powerful method, CFD simulation has been increasingly used to predict the hydrodynamic characteristics of the solid–liquid two-phase flows, leading to insights on particle concentrations and velocity distributions in reactors. Significant simulation results have been obtained and used for the reliable design and accurate control of solid–liquid mixing apparatus. However, accurately simulating the suspension behaviors in stirred tank reactors is still a challenging task. Especially, for dense solid–liquid systems, the suspension quality is highly dependent on the liquid–particle and particle–particle interactions.

In the Eulerian–Eulerian multi-fluid method, solid particles are considered as continuous phase. Particle–particle interactions can be considered through the introduction of solid properties (i.e., pressure and viscosity), which are calculated with the kinetic theory of granular flow (KTGF) model. Many original KTGF models have been derived for ideal particles: sphere, rigidity, smoothness, and elasticity (Jenkins and Richman, 1985; Jenkins and Savage, 1983; Lun et al., 1984). Meantime, many types of extensions have been proposed to characterize realistic particles. Several investigations have aimed at studying the effects of particle friction by using the employed roughness or friction coefficient (Abu-Zaid and Ahmadi, 1990; Chialvo and Sundaresan, 2013; Jenkins and Zhang, 2002; Kesava et al., 2008; Lun and Savage, 1987; Wang et al., 2016; Yang et al., 2016). Research shows that the roughness of particles exerts a significant effect on stress. In addition, the collision of frictional particles results in particle rotation (Goldshtein and Shapiro, 1995; Lun, 1991; Wang et al., 2012; Yang et al., 2016; Zhao et al., 2013). Other studies dealt with non-ideal particle–particle collisions, which are modeled based on the restitution coefficient (Chou and Richman, 1998; Goldshtein and Shapiro, 1995; Kesava et al., 2008; Lun and Savage, 1987; Sun et al., 2009; Walton, 1994). Most of the proposed KTGF models were incorporated into CFD models for the numerical simulations of hydrodynamics in gas–solid systems (Ding and Gidaspow, 1990; Gelderbloom et al., 2003; Huilin and Gidaspow, 2003; Iddir and Arastoopour, 2005; Igci et al., 2008; Johansson et al., 2006; Lindborg et al., 2007; Reuge et al., 2008). Several models were also applied in solid–liquid suspension systems (Roy et al., 2014; Shi et al., 2009; Wang et al., 2014, 2016; Yan et al., 2011; Zhang et al., 2012). The obtained predictions quantitatively agreed with experimental data.

In fact, for solid–liquid suspension systems, the prediction results of the hydrodynamic characteristics rely on the descriptions of the particle–particle and particle–fluid interactions. The progress on the selection of appropriate models for solid–liquid mixing is far from being fully understood. Despite the difficulties involved in this process, significant efforts have been devoted to comprehending the dispersion phenomena effectively. Brucato et al. (1998) and Ranade's group (Khopkar et al., 2006; Sardeshpande et al., 2010) evaluated the role of turbulent dispersion in predicting solid–liquid suspension quality. In their work, turbulence became important for stirred tank systems at a high Reynolds number, especially when the particle size was smaller than the turbulent eddies. Feng et al. (2013) developed an explicit algebraic stress model (EASM) for simulating liquid–solid two-phase turbulent flow in stirred reactors. The EASM predictions showed good agreement with the experimental data. Hosseini et al. (2010b) developed a CFD model to investigate the solid–liquid mixing quality under different conditions. Several CFD predictions were consistent with the experimental data (Hosseini et al., 2010a). Montante et al. (2001, 2003) and Montante and Magelli (2007) simulated the dilute solid re-suspension in stirred reactor with multiple impellers. The simulated particle axial concentration profiles were in agreement with the experimental data. But, in this