Advanced Powder Technology xxx (2017) xxx–xxx

Contents lists available at ScienceDirect

Advanced Powder Technology

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

Original Research Paper

Numerical simulation of flow behavior of particles in a liquid-solid stirred vessel with baffles

Shuyan Wang [*], Xiaoxue Jiang, Ruichen Wang, Xu Wang, Shanwen Yang, Jian Zhao, Yang Liu

School of Petroleum Engineering, Northeast Petroleum University, Daqing 163318, China

ARTICLE INFO

Article history:
Received 12 October 2016
Received in revised form 5 February 2017
Accepted 4 April 2017
Available online xxxx

Keywords:
Two-fluid model
Liquid-solid
Stirred vessel
Numerical simulation

ABSTRACT

Flow behavior of particles is simulated by means of two-fluid model combining with kinetic theory of granular flow in a liquid-solid stirred vessel with baffles. The Huilin-Gidaspow drag model is used to obtain interphase interaction of liquid and solids phases. The virtual mass force is considered in simulations. The moving reference frame is applied to the rotation of numerical domain. Predictions are compared with experimental data measured by Pianko-Oprych et al. (2009) in a liquid-solid stirred vessel. This comparison shows that the present model can capture the liquid-solid flow in a liquid-solid stirred vessel. The distributions of velocity and solids volume fraction are predicted at the different heights. The effects of particle density on flow behavior of particles are generally scarce using CFD. Simulations indicate the stirred vessel consists of three regions based on distributions of velocity and turbulent kinetic energy, they are blade circulation region, conical induced region and near-wall region. As an increasing of the impeller speed, the turbulence kinetic and solids phase velocity rise, and the particles fluctuation is intensified.

1. Introduction

Stirred vessels and reactors have wide applications in the chemical and process industries, such as crystallization operations, liquid-liquid extractions, biological fermentations, and heterogeneous catalytic reactions, etc [1]. Reasonable understanding the hydrodynamic behavior is the key to design, operate and control over this equipment. As for a liquid-solid stirred vessel, the solids volume fraction, particle and liquid turbulent behavior, turbulent diffusivity etc., are fundamental concepts and parameters to investigation on the fluid dynamics. The flow behavior of stirred vessels is very complex due to these parameters interrelating to each other, in particular, the distribution of solids volume fraction is a rather complex function of stirred velocity, turbulence properties and liquid-particle interactions, hence some literature works focused on this field [2]. Pinelli et al. (2004) obtained the solids distribution, axial dispersion coefficient of solids phase and particle settling velocity from experiments. They proposed axial dispersion coefficient as an empirical parameter, was associated with flow macromixing features and local turbulent behavior [3]. Soos et al. (2008) illustrated the effect of stirring speed and solids volume fraction on aggregation and breakage of aggregates produced from polymer particles under turbulent conditions in a stirred vessel. The aggregate structure and shape were independent on the stirring speed under certain conditions [4]. Ibrahim et al. (2015) studied the effects of particle size, solids loading and impeller clearance on the suspension of fine particles in a stirred tank with experiments. The particle size influenced on the settling velocity, and smaller particles required less specific energy for suspension [5]. Kee et al. (2004) investigated the impact of particles on impeller blades during solid-liquid mixing processes. The impact velocities were close to the linear speed of the blade at the impact radius, and the velocity closing to the blade tip is the largest. The highest impact rates also occurred at the blade tip, and below the disk of the Rushton turbine [6]. A novel experimental method, steady cone radius method, is proposed by Brucato et al. (2010) to determine the just-suspension agitation speed in top-cover stirred tank without baffles. The agitation speed depended on solids volume fraction and density, while a negligible dependence on particle diameter was observed [7]. Busciglio et al. (2014) measured the dispersion dynamics of particles over a vertical section of the stirred vessel. They confirmed the existence of two well defined, partially segregated, zones that give rise to a double mixing dynamics behavior [8]. Lei Yang (2013) studied the hydrodynamics character in a dished-bottom stirred tank with multiple impellers using experimental method. The effects of particle size, impeller speed, solids holdup, feed position and energy input had been considered [9].

---

[*] Corresponding author. Fax: +86 459 5967161.
E-mail address: wangshuyan@nepu.edu.cn (S. Wang).

http://dx.doi.org/10.1016/j.apt.2017.04.004
0921-8831/

Please cite this article in press as: S. Wang et al., Numerical simulation of flow behavior of particles in a liquid-solid stirred vessel with baffles, Advanced Powder Technology (2017), http://dx.doi.org/10.1016/j.apt.2017.04.004

Table 1
Closure relations for solids phase.

1. Stress tensor of liquid phase	$\tau_l = \mu_f\left[\nabla \boldsymbol{u}_l + (\nabla \boldsymbol{u}_l)^T\right] - \frac{2}{3}\mu_f(\nabla \cdot \boldsymbol{u}_l)\boldsymbol{I}$	(T1-1)
2. Solids stress	$\tau_s = \mu_s\left\{\left[\nabla \boldsymbol{u}_s + (\nabla \boldsymbol{u}_s)^T\right] - \frac{2}{3}(\nabla \cdot \boldsymbol{u}_s)\boldsymbol{I}\right\} + \xi_s \nabla \cdot \boldsymbol{u}_s \boldsymbol{I}$	(T1-2)
3. Particle pressure	$p_s = \varepsilon_s \rho_s \theta + 2\rho_s(1+e)\varepsilon_s^2 g_0 \theta$	(T1-3)
4. Solids shear viscosity	$\mu_s = \frac{4}{5}\varepsilon_s^2 \rho_s d_s g_o (1+e)\sqrt{\frac{\theta}{\pi}} + \frac{10\rho_s d_s \sqrt{\pi\theta}}{96(1+e)\varepsilon_s g_o}\left[1 + \frac{4}{5} g_o \varepsilon_s (1+e)\right]^2$	(T1-4)
5. Solids bulk viscosity	$\xi_s = \frac{4}{3}\varepsilon_s^2 \rho_s d_s g_0 (1+e)\left(\frac{\theta}{\pi}\right)^{1/2}$	(T1-5)
6. Conductivity of granular energy	$k_s = \frac{25\rho_s d_s \sqrt{\pi\theta}}{64(1+e)g_o}\left[1 + \frac{6}{5}(1+e) g_o \varepsilon_l\right]^2 + 2\varepsilon_s^2 \rho_s d_s g_o (1+e)\left(\frac{\theta}{\pi}\right)^{1/2}$	(T1-6)
7. Rate of kinetic energy dissipation	$\gamma_s = 3(1-e^2)\varepsilon_s^2 \rho_s g_o \theta\left(\frac{4}{d_s}\sqrt{\frac{\theta}{\pi}} - \nabla \cdot \boldsymbol{u}_s\right)$	(T1-7)
8. Rate of energy exchange	$D_{ls} = \frac{d_s \rho_s}{4\sqrt{\pi\theta} g_o}\left(\frac{18\mu_l}{d_s^2 \rho_s}\right)^2 \lvert \mathbf{u}_l - \mathbf{u}_s \rvert^2$	(T1-8)
9. Radial distribution function	$g_0 = \left[1 - \left(\frac{\varepsilon_s}{\varepsilon_{s,\max}}\right)^{1/3}\right]^{-1}$	(T1-9)
10. Drag model	$\beta = (1-\varphi)\beta_E + \varphi\beta_{WY}$	(T1-10)
	$\varphi = \frac{\arctan\left[150 \times 1.75(0.2-\varepsilon_s)\right]}{\pi} + 0.5$	(T1-11)
	$\beta_E = 150\frac{(1-\varepsilon_l)^2 \mu_l}{(\varepsilon_l d_s)^2} + 1.75\frac{\rho_l (1-\varepsilon_l)\lvert \mathbf{u}_l - \mathbf{u}_s \rvert}{\varepsilon_l d_s} \quad \varepsilon_l \leqslant 0.8$	(T1-12)
	$\beta_{WY} = \frac{3}{4} C_d \frac{\rho_l (1-\varepsilon_l)\lvert \mathbf{u}_l - \mathbf{u}_s \rvert}{d_s}\varepsilon_l^{-2.65} \quad \varepsilon_l > 0.8$	(T1-13)
11. Boundary conditions	$u_{t,w} = -\frac{6\mu_s \varepsilon_{s,\max}}{\pi\phi\rho_s \varepsilon_s g_o \sqrt{3\theta}}\frac{\partial u_{s,w}}{\partial n}$	(T1-14)
	$\theta_w = -\frac{k_s \theta}{\chi_w}\frac{\partial \theta_w}{\partial n} + \frac{\sqrt{3}\pi\phi\rho_s \varepsilon_s u_s^2 g_o \theta^{3/2}}{6\varepsilon_{s,\max}\chi_w}$	(T1-15)
	$\chi_w = \frac{\sqrt{3}(1-e_w^2)\pi\varepsilon_s \rho_s g_0 \theta^{3/2}}{4\varepsilon_{s,\max}}$	(T1-16)

Guida (2010) studied the turbulence liquid-solid suspensions with the technique of positron emission particle tracking in a stirred vessel. The trajectory, velocity and spatial phase distribution were obtained. The criterion had been used to describe the uniformity of the suspension with the solids volume fraction [10]. Carletti (2014) analyzed the solids distribution in a stirred vessel by electrical resistance tomography. Big particle size and solids loading can lower the solids distribution homogeneity. The particle size influenced the shape of interface [11]. Montante et al. (2012) investigated the effects of the dispersed phase on mean velocity and turbulence levels of the continuous phase and the local solid-liquid slip velocity in a turbulence stirred vessel by Particle Image Velocimetry. The liquid velocity fluctuations were depended on the particle size. The turbulence level variations were more pronounced at increasing solids contents [12]. Indeed, all of these results from experiments indicate that the flow behavior and performance of liquid-solid stirred vessels are related to the operating parameters, geometric structural parameters and solids and liquid physical properties, etc.

As regards to mathematical modeling, computational fluid dynamics (CFD) of hydrodynamics in stirred vessels gives very detailed information about the local of values of volume fraction and their spatial distributions where measurements are either difficult or impossible to obtain. Such information can be useful in the understanding of the transport phenomena in stirred vessels. Hongliang Zhao et al. (2014) investigated the flow behavior in a baffled tank stirred with an improved intermig impeller using computational and experimental analyses. The results indicated that special baffles sloped was benefit to solids circulation in axial, which promoted the suspension of solid particles at the bottom [13]. Santos-Moreau et al. (2012) investigated the liquid flow field in a stirred reactor by means of CFD-RANS simulations, coupling with a Realizable k–ε model. The velocities were maximal near the impeller and decreasing along with radial direction, as well as, the velocities were lower and in the opposite direction above and below the impeller [14]. Tamburini (2014) simulated two different baffled tanks stirred by Rushton turbines using an Eulerian-Eulerian two fluid model. Gidaspow's model can capture the flow of dense particle at high impeller speeds [15]. Wadnerkar et al. (2012) studied the effect of drag model on the solid suspension in stirred tanks with Eulerian–Eulerian model. The modified drag was a function of particle diameter to Kolmogorov length scale ratio. It is observed that high turbulence can increase the drag coefficient as high as forty times when compared with a still fluid [16]. Tamburini et al. (2011) simulated the flow of dense solid-liquid partial suspensions in baffled stirred tanks at different agitation speeds with an Eulerian-Eulerian model coupled with a standard k–ε turbulence model for the liquid phase. Different turbulence corrections to the fluid-particle drag correlation were considered. The influence of the impeller motion treatment can be negligible [17].

To date, hydrodynamic characteristics of the stirred vessels such as volume fraction, stirred speed, velocities of liquid and solids phases in stirred vessels have been experimentally and modeled investigated, and certain correlations developed on some hydrodynamic characteristics are provided. Our present work has shown that the majority of investigations focused on particle distribution, solids and liquid velocities, and the turbulence. The studies related to effects of particles density and impeller speed on flow behavior of particles are generally scarce using CFD. That is to say, a comprehensive parameter study on the influence of operational parameters on mixing performance of liquid and solids phases is still not available in a liquid-solid stirred vessel. This indicates the quantitative understanding by means of numerical simulations is still needed to describe the flow behavior of liquid-solid stirred vessels. In this study, an attempt has been made to interpret hydrodynamics in a stirred vessel. The modeling is based on a three-dimensional Eulerian-Eulerian approach in combination with kinetic theory of granular flow. The moving reference frame is applied to model the rotation of numerical domain. The effects of particles density and impeller speed on distributions of concentration, velocity and turbulence are predicted in a liquid-solid stirred vessel. The fluctuating kinetic energy of particles based on the granular temperature is evaluated. The knowledge of these characteristics is fundamental question to the design and improvement of stirred technology in this field.

2. Liquid and solids two-fluid model

The two-fluid method normally requires much less computational resources compared to the Eulerian–Lagrangian method (DEM), therefore, it can be used to model and study pilot scale and industrial scale reactors [18,19]. In the present work, the Eule-

Please cite this article in press as: S. Wang et al., Numerical simulation of flow behavior of particles in a liquid-solid stirred vessel with baffles, Advanced Powder Technology (2017), http://dx.doi.org/10.1016/j.apt.2017.04.004