Chemical Engineering Journal 164 (2010) 418–424

Contents lists available at ScienceDirect

Chemical Engineering Journal

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

Fluid dynamics simulation of the high shear mixing process

Anders Darelius[a,1], Johan Remmelgas[c], Anders Rasmuson[a,*], Berend van Wachem[b], Ingela Niklasson Björn[c]

[a] Department of Chemical and Biological Engineering, Chalmers University of Technology, SE-412 96 Göteborg, Sweden
[b] The Department of Mechanical Engineering, Imperial College London, Exhibition Road, London SW7 2AZ, United Kingdom
[c] AstraZeneca Centre of Excellence for Process Analytical Technology, R&D Mölndal, SE-431 83 Mölndal, Sweden

ARTICLE INFO

Article history:
Received 7 July 2009
Received in revised form 6 December 2009
Accepted 14 December 2009

Keywords:
Fluid mechanics
Kinetic theory of granular flow
Frictional stress models
Powder technology
Granulation
Multiphase flow

ABSTRACT

The Eulerian–Eulerian two-fluid approach for modelling multiphase flows is used to simulate the flow in a high shear mixer. The results are compared with experimental velocity profiles for the solids phase at the wall in the mixer obtained using a high speed camera (Darelius et al. Chem. Eng. Sci. 62 (2007) 2366).

The governing equations are closed using relations from the Kinetic Theory of Granular Flow (KTGF) combined with a frictional stress model due to Johnson and Jackson and Schaeffer and inter-phase drag due to Wen and Yu. In addition, calculations are presented for a model with a constant particle phase viscosity (CPV). Free slip and partial slip boundary conditions for the solid phase velocity at the vessel wall and the impeller have been utilized.

The results show that the bed height could be well predicted by the partial slip model, whereas the free slip model could not capture the experimentally found bed height satisfactorily. For the KTGF model, the swirling motion of the rotating torus that is formed by the moving powder bed was over-predicted and the tangential wall velocity was under-predicted, probably due to the fact that the frictional stress model needs to be further developed, e.g. to tackle cohesive particles in dense flow. The CPV model gave predictions in good agreement with the experiments for a solids viscosity of 0.1 Pa s and a wall slip parameter of 0.005 m/Pa s. However, for a very low or very high value of the particle phase viscosity and for a high value of the wall slip parameter the agreement with experiments was poor. Interestingly, values of the viscosity that are commonly employed for fluidized beds seem applicable also in the present case.

1. Introduction

Granulation in high shear mixers is an important unit operation often used in the development and manufacturing of tablets in the pharmaceutical industry. The process comprises a dry mixing step, where the active substances and excipients are mixed together in order to form a homogeneous mixture, followed by a wet mixing step, where binder liquid is added in order to build up agglomerates. Many researchers have focused on agglomeration and breakage mechanisms in the high shear mixer, e.g. Iveson et al. [1] and Reynolds et al. [2]. However, a better understanding of the local mixing and the flow pattern in the granulator is necessary in order to implement the agglomeration and breakage models and to develop quantitative process models that enable predictive scale-up and process optimization. This is highlighted by several authors, e.g. Cameron et al. [3], Faure et al. [4] and Niklasson Björn et al. [5].

The aim of this study is to obtain a quantitative understanding of the flow behaviour of particles in a high shear mixer via fluid mechanics calculations based upon the two-fluid model. The calculated results are compared to the experimental data obtained by Darelius et al. [8] using a high speed camera. In the simulation of fluidized beds, the kinetic theory of granular flow (KTGF), where colliding particles are treated in a similar fashion to colliding molecules in an ideal gas, has been shown to be a promising model for modelling particle–particle interactions (see e.g. van Wachem et al. [6]) and this model is therefore employed here as well. However, for the present flow it is expected that particles will be in sustained contact to a greater extent than in a fluidized bed so that the stresses between particles becomes larger than what is predicted by KTGF. Thus, a frictional stress model is used in combination with KTGF.

2. Mathematical model

2.1. The Eulerian–Eulerian approach

In the Eulerian–Eulerian two-fluid approach for modelling multiphase flows, the fluid and dispersed phases are averaged over a

* Corresponding author. Tel.: +46 31 7722940; fax: +46 31 7723035.
E-mail address: rasmuson@chalmers.se (A. Rasmuson).
[1] Present address: Epsilon Utvecklingscentrum Väst, Lindholmspiren 9, SE-417 56 Göteborg, Sweden.

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doi:10.1016/j.cej.2009.12.020

fixed volume that is large in comparison with the size of the individual particles. The conservation equations for momentum and mass for the gas phase in a gas–solid flow can be written as (Anderson and Jackson [9])

$$\frac{\partial(\alpha_g\rho_g\mathbf{u}_g)}{\partial t} + \nabla\cdot(\alpha_g\rho_g\mathbf{u}_g\mathbf{u}_g) = -\alpha_g\nabla P + \nabla\cdot\left(\alpha_g\overline{\overline{\tau_g}}\right) - \beta(\mathbf{u}_g-\mathbf{u}_s)+\mathbf{F} \quad (1)$$

$$\frac{\partial(\alpha_g\rho_g)}{\partial t} + \nabla\cdot(\alpha_g\rho_g\mathbf{u}_g) = 0 \quad (2)$$

where α_g is the volume fraction of the gas, ρ_g is the gas density, $\mathbf{u}_g$ is the gas velocity, P is the pressure, $\overline{\overline{\tau_g}}$ is the viscous stress tensor for the gas phase, β is the inter-phase momentum exchange coefficient, $\mathbf{u}_s$ is the solid phase velocity and $\mathbf{F}$ represents all external forces acting on the system. For the solid phase, the corresponding equations are expressed as

$$\frac{\partial(\alpha_s\rho_s\mathbf{u}_s)}{\partial t} + \nabla\cdot(\alpha_s\rho_s\mathbf{u}_s\mathbf{u}_s) = -\alpha_s\nabla P - \nabla P_s + \nabla\cdot\left(\alpha_s\overline{\overline{\tau_s}}\right) + \beta(\mathbf{u}_g-\mathbf{u}_s)+\mathbf{F} \quad (3)$$

$$\frac{\partial(\alpha_s\rho_s)}{\partial t} + \nabla\cdot(\alpha_s\rho_s\mathbf{u}_s) = 0 \quad (4)$$

where α_s is the volume fraction of the particle phase, ρ_g is the density of the particles, τ_s is the particle phase viscous stress tensor, and P_s is the solids pressure. The volume fractions sum to unity, i.e.

$$\sum_{k=1}^{n}\alpha_k = 1 \quad (5)$$

For both phases, the viscous stress tensor is described by Newton's law of viscosity as

$$\overline{\overline{\tau_k}} = \left(\lambda_k - \frac{2}{3}\mu_k\right)(\nabla\cdot\mathbf{u}_k)\bar{\bar{I}} + 2\mu_k\overline{\overline{S_k}} \quad (6)$$

where λ_k is the bulk viscosity, μ_k is the dynamic viscosity and $\overline{\overline{S_k}}$ is the strain rate tensor for phase k. The strain rate tensor describes the deformation of a fluid element and is defined as

$$\overline{\overline{S_k}} = \frac{1}{2}\left(\nabla\mathbf{u}_k + (\nabla\mathbf{u}_k)^T\right) \quad (7)$$

The bulk viscosity of a fluid is a measure of the difference between the thermodynamic and mechanical pressures.

For the gas phase, the dynamic viscosity is assumed to be 1.789×10^{-5} Pa s while the bulk viscosity is set to zero in what is referred to as the Stokes' assumption. For the solids phase, the dynamic and bulk viscosities are modelled using either the kinetic theory of granular flow (KTGF Model) as described by Darelius et al. [17] or using a model with a constant particle phase viscosity (CPV Model). In the former case, the total shear viscosity is the sum of the viscosity calculated based upon the kinetic theory of granular flow and a frictional viscosity, as described below.

2.2. Inter-phase momentum exchange

Several models describing the inter-phase momentum exchange exist in the literature. van Wachem et al. [6] have compared different models and shown that the Wen and Yu [10] model performs well over the range of relevant solid volume fractions. The model for the exchange coefficient is formulated as

$$\beta = \frac{3}{4}C_D\frac{(1-\alpha_s)\alpha_s\rho_g\left|\mathbf{u}_g-\mathbf{u}_s\right|}{D_p}(1-\alpha_s)^{-2.65} \quad (8)$$

where D_p is the particle diameter and C_D is the drag coefficient for a single sphere (Rowe [11]):

$$C_D = \begin{cases} 24\dfrac{(1+0.15((1-\alpha_s)Re_p)^{0.687})}{Re_p(1-\alpha_s)} & \text{if } Re_p(1-\alpha_p) < 1000 \\ 0.44 & \text{if } Re_p(1-\alpha_p) \geq 1000 \end{cases} \quad (9)$$

The particle Reynolds' number is defined as

$$Re_p = \frac{D_p\rho_g\left|\mathbf{u}_g-\mathbf{u}_s\right|}{\mu_g} \quad (10)$$

2.3. Closures

Further modelling is needed to provide closures for the particle momentum equations in terms of the solids pressure and the solids phase viscosity. It has been shown by van Wachem et al. [6] that the kinetic theory of granular flow (KTGF), in conjunction with a frictional stress model, works well for moderate to dense gas–particle flows. The KTGF model is an extension of the model for molecular motion in a dense gas that takes into account non-ideal particle–particle interactions (Chapman and Cowling [12]). Numerous studies on KTGF have been published; a detailed derivation is given by, e.g. Gidaspow [13] or Peirano and Leckner [14]. The KTGF model assumes particle–particle interactions to be binary and instantaneous. However, at a high solids volume fraction sustained particle–particle contacts occur, resulting in much higher particle stresses. Hence, an additional frictional contribution must be added to the solids pressure and dynamic solids viscosity. These extra contributions constitute parts of the modelling framework known as frictional stress models, which are used frequently in, e.g. the field of soil mechanics to model avalanches, landslides, etc.

In this work, the extra solid particle pressure, i.e. the frictional pressure, is modelled using the semi-empirical model proposed by Johnson and Jackson [15], namely:

$$P_f = Fr\frac{(\alpha_s-\alpha_{s,\min})^n}{(\alpha_{s,\max}-\alpha_s)^q} \quad (11)$$

where $\alpha_{s,\min}$ is the minimum volume fraction above which frictional forces are important, and Fr, n, and q are empirical constants. The frictional dynamic viscosity that is added to the solid dynamic viscosity is related to P_f through the linear law in an expression derived by Schaeffer [16]:

$$\mu_f = \frac{P_f\sin\varphi}{2\sqrt{I_{2D}}} \quad (12)$$

where φ is the angle of internal friction and I_{2D} is the second invariant of the strain rate tensor $\overline{\overline{S_s}}$ (Eq. (7)). It should be noted that this expression is valid for cohesion-less materials only and it is expected that cohesion will even further increase the particle–particle stresses. Further details are provided by Darelius et al. [17].

Calculations are also carried out also for a model with constant particle viscosity (CPV) in which the solids pressure is modelled using the expression due to Bouillard et al. [24]. For this latter model a compaction modulus of 20 and a reference modulus of elasticity of 1 Pa is assumed based upon previous studies of fluidized beds.

2.4. Boundary conditions

The continuous phase (air) is assumed to obey the no slip boundary condition at the wall and on the impeller. The word wall includes both vessel walls and the impeller hereinafter. For the solid phase, different boundary conditions can be found in the literature. Free slip is used by numerous authors for modelling the solid phase wall velocity in fluidized beds, e.g. van Wachem et al. [6]. Johansson