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CFD simulation of the high shear mixing process using kinetic theory of granular flow and frictional stress models

Anders Darelius[a], Anders Rasmuson[a,*], Berend van Wachem[b], Ingela Niklasson Björn[c], Staffan Folestad[c]

[a]*Department of Chemical and Biological Engineering, Chalmers University of Technology, SE-412 96 Göteborg, Sweden*
[b]*Department of Applied Mechanics, Chalmers University of Technology, SE-412 96 Göteborg, Sweden*
[c]*AstraZeneca Centre of Excellence for Process Analytical Technology, R&D Mölndal, SE-431 83 Mölndal, Sweden*

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Abstract

In order to enhance process understanding and to develop predictive process models in high shear granulation, there is an ongoing search for simulation tools and experimental methods to model and measure the velocity and shear fields in the mixer. In this study, the Eulerian–Eulerian approach to model multiphase flows has been used to simulate the mixer flow. Experimental velocity profiles for the solid phase at the wall in the mixer have been obtained using a high speed camera following the experimental procedure as described by Darelius et al. [2007a. Measurement of the velocity field and frictional properties of wet masses in a high shear mixer. Chemical Engineering Science, 62, 2366–2374]. The governing equations for modelling the dense mixer flow have been closed by using closure relations from the kinetic theory of granular flow (KTGF) combined with frictional stress models. The free slip and partial slip boundary conditions for the solid phase velocity at the vessel wall have been utilized. The partial slip model originally developed for dilute flows by Tu and Fletcher [1995. Numerical computation of turbulent gas–solid particle flow in a 90° bend. A.I.Ch.E. Journal, 41, 2187–2197] has been employed. It was found that the bed height could be well predicted by implementing the partial slip model, whereas the free slip model could not capture the experimentally found bed height satisfactorily. In the simulation, the swirling motion of the rotating torus formed 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 advantage of using the Eulerian–Eulerian approach compared to discrete element methods is that there is no computational limitation on the number of particles being modelled, and thus manufacturing scale granulators can be modelled as well.

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

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, and a step of wet high shear mixing, where binder liquid is added in order to build up agglomerates. Many researchers have focused their work on agglomeration and breakage mechanisms occurring in the high shear mixer, e.g. Iveson et al. (2003) and Reynolds et al. (2005). 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. (2005), Faure et al. (2001) and Niklasson Björn et al. (2005).

The discrete element method (DEM) is shown to be a promising modelling tool for modelling the particulate flow in the mixer (Gantt and Gatzke, 2006; Kuo et al., 2004). In the DEM approach, the motion of every single particle is tracked.

* Corresponding author. Tel.: +46 31 7722940; fax: +46 31 814620.
E-mail addresses: rasmuson@chalmers.se, rasmuson@chemeng.chalmers.se (A. Rasmuson).

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However, the computational power of today allows the flow of less than a million particles to be modelled using DEM, whereas billions of particles are present in the real mixing process. Another approach for modelling multiphase flows is the Eulerian–Eulerian approach where the particles are not followed individually, but instead are treated as a continuous medium with properties derived from closure models. When it comes to papers published in the field of high shear mixing using the DEM or the Eulerian–Eulerian approach, there are numerous publications on DEM but, to the best of the authors' knowledge, no study of high shear mixing where the Eulerian–Eulerian approach is applied has been published. However, for modelling e.g. fluidized beds and hopper flows, this approach is frequently employed. In fluidized beds, the kinetic theory of granular flow (KTGF), where colliding particles are treated similarly as colliding molecules in an ideal gas, is shown to be a promising model for modelling the particle–particle interactions (e.g. van Wachem et al., 2001). For denser flows, e.g. hopper flow, where particles are in sustained contact, the stresses between particles become much larger than those predicted by KTGF. Thus, frictional stress models must be used in combination with the KTGF to describe the much larger stresses associated with enduring particle–particle contact.

The aim of this study is to use computational fluid dynamics (CFD) software to obtain a quantitative picture of the velocities and volume fractions of particles in different regions of the high shear mixer by using the Eulerian–Eulerian approach with KTGF and frictional stress models. As stated above, to understand the local mixing in the different regions of the mixer is necessary in order to develop better agglomeration and breakage models. The local shear rates can be calculated from the velocity field. The frictional stress models are of an empirical nature and experimental data of the flow field is necessary to validate calculations. Validation can be performed using e.g. Laser Doppler Anemometry as described by Darelius et al. (2007b). However, for the particular mixer studied, experimental data are provided using a high speed camera as presented by Darelius et al. (2007a).

2. Mathematical model

2.1. The Eulerian–Eulerian approach

In the Eulerian–Eulerian approach to modelling multiphase flows, the fluid and dispersed phases are averaged over a fixed volume that is large in comparison with the size of the individual particles. The governing equations for momentum and mass for the gas phase in a gas–solid flow can be written as (Anderson and Jackson, 1967):

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

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

where α_g represents the volume fraction of gas, ρ_g is the intrinsic gas density and $\mathbf{u}_g$ is the gas velocity. P is the pressure, $\overline{\overline{\tau_g}}$ is the viscous stress tensor and β is the coefficient for the interphase momentum exchange term, $\mathbf{u}_s$ 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

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

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

with the index s for solid and with P_s as the solids pressure. The sum of the volume fractions should sum to unity,

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

The viscous stress tensor is described for both phases by Newton's law of viscosity as

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

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

$$\overline{\overline{S_k}}=\tfrac{1}{2}(\nabla\mathbf{u}_k+(\nabla\mathbf{u}_k)^{\mathrm{T}}). \quad (7)$$

The bulk viscosity of a fluid is a measure of the difference between the thermodynamic and mechanical pressures and for a Newtonian fluid (e.g. air), the bulk viscosity is set to zero in what is referred to as the Stokes' assumption.

2.2. Interphase momentum exchange

Several models describing the interphase momentum exchange exist in the literature. However, van Wachem et al. (2001) have compared different models and come to the conclusion that the Wen and Yu (1966) model performs well over the range of relevant solid volume fractions. The model for the exchange coefficient is formulated as

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

where D_p represents the particle diameter and C_D is the drag coefficient for a single sphere (Rowe, 1961):

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

The particle Reynolds' number is defined as

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