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Continuum modeling of multi-regime particle flows in high-shear mixing

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ABSTRACT

This article compares and evaluates different approaches for continuum modeling in high shear mixers covering the full range of the solid volume fraction. High shear mixing is considered as the first stage in industrial high shear granulation processes. The study is focused on and compared with experimental data for a MiPro mixer. Different granular flow regimes are located in different regions of the system and suitable models are applied for each region. Accordingly, the dilute regions are modeled with the standard kinetic theory of granular flow (KTGF) model. The dense regions are modeled using a framework developed by Jop et al. [1] which treats dense flows with pseudo-plastic rheology. The transitional region from dilute to dense is either modeled with KTGF or by using modifications to the transport coefficients that describe the solid phase stresses as proposed by Bocquet et al. [2] (the viscosity divergence model). The results using the latter model show significant improvement compared to similar studies in the past. A very good agreement between simulation and experiments is achieved. It should be noted that the proposed modeling frameworks are formulated for the full range of volume fractions and can be applied to various particulate flows. To sum up, this research provides a better description of multi-regime granular flows, particularly the transitional behavior in the intermediate range of volume fractions.

1. Introduction

Granulation is a basic process in pharmaceutical industries for producing tablets [3]. The process consists of a dry mixing stage in which the ingredients are mixed together in a batch process to give a homogeneous dry mixture. This stage is followed by wet mixing in which a binder liquid is added to the mixture, agglomeration commences and the final products in the form of granules with desirable properties are produced [4].

The physics of the granulation process is complex, however, extensive research has increased our fundamental knowledge of the granulation process [5]. One of the remaining problems is to develop accurate continuum models for the particulate flow to be used for the design of real granulators. The dry mixing stage is considered in the present study.

Particle flow in high shear dry mixing is mostly in the dense and transitional regimes. Granular flows generally display various kinds of behavior depending on the local volume fractions and the degree of excitation. Granular flows can behave like a solid in a pile, like a liquid when they are discharged from a container or like a gas in a fluidized bed. Accordingly, granular flows are basically divided into three different categories: solid-, liquid- and gas-like. In a granular solid, a force chain in a network of grains allows the grains to rest on one another and construct a static system [6]. Proper models based on soil mechanics for slow plastic flows have been introduced for this state of granular materials [7]. Dilute granular systems at the opposite extreme resemble gas molecules in that the motions of the grains are uncorrelated, and the mechanisms of momentum transfer are translational and collisional. Consequently, the approach has been to extend the kinetic theory of gases to develop a kinetic theory for collisional rapid flows [8]. Granular liquid or dense granular flow as an intermediate regime is the most complicated flow regime to model and currently there are no unified relations describing such systems [1]. Transitional behavior, which has the characteristics of neither dilute nor dense granular flow, has been observed in the intermediate range of volume fractions. Categorizing and modeling the mentioned flow regime as either of the two extremes cause significant errors.

The aim of this study is to implement a new generation of models of dense and transitional granular flows combined with the kinetic theory of granular flows (KTGF) to reach a proper framework for large-scale industrial high-shear mixers. The models are implemented in computational fluid dynamics (CFD) to assess the velocities and volume fraction profiles of the system. The results are compared with experimental data for a MiPro high-shear mixer.

2. Theory

The various flow regimes have been divided into three categories: dilute, intermediate and dense. There are relatively well defined modeling frameworks for the two extremes (dilute and dense) whereas for the behavior of the intermediate regime there is no unified modeling strategy. Accordingly, the dilute regime has been modeled by KTGF and the dense regime was modeled using a framework developed by

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Jop et al. [1] which treats dense flows with pseudo-plastic rheology. However, the intermediate range of the volume fraction, which shows a transitional behavior from dilute to dense, has been modeled either by prolonging KTGF into the intermediate regions (Model I), similar to previous studies [9,10], or using modifications to the transport coefficients (Model II) that describe the solid phase stresses, as proposed by Bocquet et al. [2]. This transitional behavior is discussed specifically. A brief description of the models is given below.

2.1. Kinetic theory of granular flow

In developing a continuum approach to granular flows, Bagnold [11] has formulated the dependence of the stress field on the strain rate, and, consequently, an equation for kinetic energy [12]. Savage et al. have considered the equivalence of random particle motions to the classical molecular motions which initiate the kinetic theory approach [13]. Following this, a complete form of KTGF has been proposed by Lun et al. [14] and Johnson et al. [15]. In order to extend the continuum models to dense systems, where sustained particle contacts occur, kinetic-frictional models have been adopted by other studies. The frictional terms added to the stress field were derived by Schaeffer [16]. The stresses were simply added to the stress field [17]. Previous studies show that such an approach may cause large errors, especially for dense systems [3,4,9].

2.2. Viscosity divergence model

According to this model, shear viscosity shows a faster divergence than other transport coefficients [18]. This fact has been observed both experimentally and as a result of discrete element method (DEM) simulations [2,19]. The model formulates the dependency of shear viscosity on the solid volume fraction (Eq. (1)) [2,19] as:

$$\eta_s = \eta_1 \frac{\sqrt{T_g}}{\left(1-\frac{\alpha_s}{\alpha_{s,\max}}\right)^{\beta}} \tag{1}$$

where η_s is the shear viscosity, T_g is the granular temperature, α_s is the local solid volume fraction and $\alpha_{s,\max}$ is the volume fraction at random close packing of solid particles which for uniform spherical particles is equal to 0.63. The values of β and η_1 are experimentally found [2,18]. The model has shown the ability to correctly capture the phase transition and coexistence of solid-like and fluid-like phases in dense granular flows [20].

2.3. Rheology model

A new empirical approach to finding transport coefficients for dense granular flows is to assume that they resemble visco-plastic fluids, considering their similarities on the macro-scale. This approach leads to a local rheology that approximates the transport coefficients for dense granular flows [1,21]. The approach provides a correlation between shear stress and strain rate using a dimensionless number called the inertial number. This model also includes the pressure dependence of the solid phase shear stresses (Eq. (2)).

$$\tau = \mu(I)P \tag{2}$$

The coefficient $\mu(I)$ has been determined from experiments and is dependent on the frictional properties of the particles and the volume fraction of solids in the flow. It is a function of the dimensionless Inertial number I:

$$I = \gamma \frac{d}{\left({}^{P}/_{\rho}\right)^{0.5}}. \tag{3}$$

Here d is the particle diameter, ρ is the particle density and γ is the shear rate. This dimensionless number can be interpreted as the ratio of inertial forces (due to shear) to confining forces (due to pressure). The frictional parameters have been determined from steady hopper flow experiments and stopped flow experiments [1]. The final expression for the shear is given in Eq. (4).

$$\tau = \mu_1 P + \frac{(\mu_2 - \mu_1)P}{{}^{I}/_{I_0} + 1} \tag{4}$$

where μ_1 and μ_2 are the values of the friction coefficient at zero and high shear, respectively, and I_0 is a constant related to the physical properties of the grains. This formulation leads to a rheology model similar to that of Herschel–Bulkley non-Newtonian fluids with pressure dependence for both the yield stress and the strain-rate-dependent parts.

The model contains the volume fraction of solids as a parameter but with a constant value. This approach has shown promising results for treating quasi-static flows [1] and for a disk impeller high-shear granulator [10,22].

3. Experimental

The equipment used was a MiPro high-shear granulator (ProCept, Belgium) with a diameter of 150 mm. This equipment contained a three-bladed beveled impeller. The same equipment was previously used by Darelius et al. [3], however, the present study does not include the liquid distributor and the chopper. The impeller speed could be varied between 50–1350 rpm, but in this study was set to 500 and 750 rpm. These impeller speeds provide a high enough shear and do not impose macro instabilities in the granulator.

Spherical micro glass particles with a diameter of 0.5 ± 0.05 mm (KEBO Lab AB) were chosen since data corresponding to the Rheology model could be found in the literature for this particular particle size [23–25]. 1485 g (1 l) of the particles was loaded into the system.

A high-speed camera with a capacity of 2000 frames per second was used to measure the velocity profiles along the transparent sidewalls. A schematic view of the experimental setup is presented in Fig. 1. Particle image velocimetry (PIV) was performed in MATLAB over the preprocessed images taken with the high-speed camera. The size of the interrogation windows was chosen to be 8 ∗ 8 pixels which gives the proper number of particles in each window to reach the averaged velocity field. A global and a local filtering were applied and the missing values were interpolated. A post processing procedure in MATLAB provided the average velocity profiles and the intensity of the fluctuations on the vertical lines along the sidewalls and at different angular positions.

4. Numerical

Fluent 14.5 (ANSYS Inc., US) was used to perform the simulations. The mesh was imported from a previous case thoroughly reported by Darelius et al. [9]. The geometry was an imported CAD drawing of the original equipment as described in the above section. A sliding mesh was used to resolve the rotation of the impeller. The geometry was divided into two parts as shown in Fig. 2. The Figure shows that a hexahedral mesh was applied in the upper part, for a more stable solution, whereas a tetrahedrone mesh was the only alternative in the bottom part due to the complexity of the geometry imposed by the shape of the impeller blades. The simulations are performed using the Eulerian-Eulerian framework. The impact from the surrounding air phase is found to be negligible.

Two simulation strategies (models) were implemented to account for the solid phase transport coefficients. For both models, the rheology model has been applied to the dense regions. Model I, applies KTGF to the regions at dilute and intermediate levels of volume fractions. Model II replaces KTGF with the Viscosity divergence model. The aim is to compare the abilities of these two modeling frameworks (Model I