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Short communication

On continuum modeling using kinetic–frictional models in high shear granulation

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ABSTRACT

This short communication demonstrates why extreme caution has to be taken when applying conventional kinetic–frictional closures to continuum modeling of high shear granulation (HSG). Conventional models refer to closure laws where the kinetic and frictional stresses are summed up to obtain the total stress field. In the simple, dense, and sheared system of a Couette shear cell, the effect of the lack of scale separation on the model predictions is examined, both quantitatively and qualitatively. It is observed that the spatial resolution has a significant effect on the magnitude of the kinetic and frictional contributions to the solid phase stresses. With this new investigation and previous studies of HSG, it is concluded that conventional kinetic–frictional models are inadequate for continuum modeling of HSG.

1. Introduction

High shear granulation (HSG) is a common process in the pharmaceutical industry. A better understanding of the flow conditions of powders and granulates in large-scale HSG equipment is crucial for constructing predictive models. The staggering amount of particles in the HSG process makes the use of continuum flow models highly attractive. Large regions of the flow are similar to fluidized beds, with rapid and dispersed flow, and where continuum models based on the kinetic theory of granular flow have proven useful (van Wachem, Schouten, Krishna, & van den Bleek, 1999). The kinetic–frictional models have been adapted to modify the stress field and extend the use of continuum models to systems where sustained particle contacts occur. The frictional stresses are simply added to the stress field in an ad hoc way (Campbell, 2006). Granular flows typically suffer from a weak or non-existent separation of characteristic length scales between that of the flow and that of the particles (Goldhirsch, 1999). A possible exception is when contacts between particles are close to elastic. As a consequence, it has been shown that the stress tensor field of the particulate phase is scale-dependent (Glasser & Goldhirsch, 2001). The latter fact implies that all the transport coefficients within the kinetic–frictional framework have a pronounced resolution dependence. The flow in HSG equipment contains very dense regions that are close to the packing limit, located near the walls and close to the impeller blades. These regions are of great importance for the flow field since they dictate the input of momentum to the system. Darelius, Rasmuson, van Wachem, Niklasson Björn and Folestad (2008) and Ng, Ding, and Ghadiri (2009) used kinetic–frictional closures to model HSG equipment. They modeled the stress tensor as a sum of three contributions: collisional, translational, and frictional parts. The collisional and translational stresses were modeled according to the kinetic theory of granular flow, and their sum here is referred to as the kinetic contribution to the solid-phase stresses. Both of the above researches concluded that the model underestimated the frictional stress in the dense sheared regions near the walls and the impeller. Their simulations also showed the importance of the dense regions for modeling high shear granulators. The relation between the kinetic and frictional stress contributions has been investigated by Ng, Ding, and Ghadiri (2008), showing that a 25–50% relative increase in the frictional contribution may improve model predictions.

The aim of this study is to discuss the use of kinetic–frictional models for HSG modeling. Using the simple, dense, and sheared system of a Couette shear cell, the present work qualitatively and quantitatively inspects the effect of the spatial resolution on model predictions. Comparing with previous attempts to model the flow in HSG equipment using continuum models, the result demonstrates that applying simple frictional models to deal with the dense regions of the flow is inadequate.

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Table 1
Properties of the meshes used in this study.

Mesh notation	Radial cell dimension (mm)	Total number of cells
$12d_p$ – 6 mm	6	4005
$8d_p$ – 4 mm	4	7789
$4d_p$ – 2 mm	2	31,603
$2d_p$ – 1 mm	1	125,347
$1d_p$ – 0.5 mm	0.5	57,021

2. Method

The modeled system in this study is an annular Couette shear cell. The geometry and data for the system were taken from Ng et al. (2008). The inner cylinder had a diameter of 58.5 mm and a rotational frequency of 1 Hz. The outer cylinder had a diameter of 75 mm. The sheared material consisted of glass beads of a 0.5 mm diameter with a particle–particle restitution coefficient of 0.9 and a density of 2600 kg/m^3, a bulk density of 1500 kg/m^3 and a tapped density of 1590 kg/m^3.

The governing equations for the mass and momentum transfer for both phases were written according to Anderson and Jackson (1967). The momentum exchange between the phases was modeled as described by Wen and Yu (1966). The transport equation for the granular temperature was the one formulated in Ding and Gidaspow (1990) with the assumption of local equilibrium between the production and dissipation of granular energy. The dissipation rate of granular energy due to collisions was modeled according to Lun, Savage, Jeffrey, and Chepurneiy (1984). The radial distribution function used was that of Lun and Savage (1986). The bulk viscosity and solid pressure were modeled as given by Lun et al. (1984). The solid pressure was modeled with an additional friction contribution according to Johnson and Jackson (1987). Dynamic viscosity was modeled as the sum of three contributions, translation, collision and friction, as given by Eq. (1):

$$\mu_s = \mu_{s,\text{collision}} + \mu_{s,\text{translation}} + \mu_{s,\text{friction}} \tag{1}$$

The stresses from particle collision and translation, modeled according to Syamlal, Rogers, and O'Brien (1993), are dependent on granular temperature, as described by the kinetic theory of granular flow framework. The frictional model was a semi-empirical equation based on the Coulomb friction law, containing the frictional pressure, P_f, modeled according to Schaeffer (1987). The full set of equations can be found in Darelius et al. (2008) or Ng et al. (2009).

In this study, the equations were solved in a transient form with a first-order implicit temporal discretization. The segregated solver for pressure and momentum was used with the PC-SIMPLE algorithm for pressure velocity coupling, and the first-order upwind scheme was used for interpolation of the cell face values. The no-slip boundary condition was used for both phases at the walls. The time step was set to 10^{-4} s for all simulations except for the finest mesh (see Table 1), where 5×10^{-5} s was used because of the fine resolution. The convergence of the simulations was determined by monitoring the velocities at three points: two close to the inner wall and one at the center of the gap, until the readings became stable.

A uniform mesh size was used for all the meshes except for the finest mesh, where the computational time was determined unnecessarily long for a uniform mesh to be used. A finer boundary mesh was thus implemented close to the inner cylinder with a refinement in the radial direction. The boundary layer had a constant cell size that was applied five millimeters into the channel. Table 1 presents detailed information on all the meshes used. The meshes were termed after the radial cell dimension measured in particle diameters and in millimeters. Initially the spatial resolution was set several times larger than the particle length-scale, where the use of averaged particle properties within the cell was adequate. The mesh was then refined all the way down to the particle length-scale. Note that in the latter case, the rules for representative averaging in obtaining field equations were clearly disobeyed which, as a consequence, can provide misleading results. By doing this we aimed at illustrating that even such radical refinement of a mesh cannot compensate for the effects of the lack of scale separation in highly dense flows.

The simulations have been compared to the available experimental data on the non-dimensionalized tangential velocity in different Couette configurations. Ng et al. (2008) presented the velocity data from several experimental investigations. They observed that many of the data sets collapsed on a Gaussian expression, as seen in Eq. (2). In this study, this expression is used for comparison with simulations.

$$\frac{u_t^p}{u_t^w} = 0.925 \exp\left(-0.284\frac{l}{d_p} - 0.0534\left(\frac{l}{d_p}\right)^2\right), \tag{2}$$

where u_t is the tangential velocity and the superscripts p and w refer to the particles and the inner wall, respectively, l is the distance from the inner wall and d_p is the particle diameter.

3. Results and discussion

We have investigated the effects of the spatial resolution of simulations on the distribution of stresses in the particulate phase by examining the ratio between frictional and kinetic viscosities (here termed as the viscosity ratio) and the frictional viscosity. In addition to these variables, the solid volume fraction and the dimensionless tangential velocity (non-dimensionalized by the inner wall velocity) have also been studied. Fig. 1 shows the mentioned variables plotted vs. the dimensionless distance from the inner wall, non-dimensionalized by the particle diameter.

The viscosity ratio plot shows that there is a redistribution between the frictional and kinetic stresses as the size of the computational cell is reduced (Fig. 1(a)). The change in the viscosity ratio between the $12d_p$ – 6 mm and the $1d_p$ – 0.5 mm cases was 5.0 ± 0.4% between the dimensionless distances 2 and 4. The same difference became less than 1% for all the resolutions used after a dimensionless distance of 5. The stresses were redistributed toward the lower frictional contributions two particle diameters from the inner wall, but with a sharper gradient that resulted in a higher value of the viscosity ratio in the region 2–5 particle diameters from the inner wall. Fig. 1(b) shows a clear increase in frictional viscosity as the simulations were carried out with a finer resolution. The expression for frictional viscosity illustrates a strong dependence on the solid volume fraction throughout the solid pressure, and that small changes can have a large effect (van Wachem, Schouten, van den Bleek, Krishna, & Sinclair, 2001). The plot of the solid volume fraction shows an increase in value in the region beyond two particle diameters from the inner wall with a finer spatial resolution (Fig. 1(c)).

The redistribution of the stresses is also reflected when studying the dimensionless tangential velocity (Fig. 1(d)), where an increase in frictional stresses gives a sharper velocity gradient. When compared to Eq. (2), it is clear that the velocities do not converge to the experimental data as the spatial resolution