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Modelling of dense and complex granular flow in high shear mixer granulator—A CFD approach

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ABSTRACT

In the aspect of granulation process control, the numerical simulations appear to be a cost-effective and flexible tool to investigate the flow structure of granular materials in mixer granulators of various configurations and operating conditions. *Computational fluid dynamics* (CFD) is used in this study to model the granular flow in a vertical high shear mixer granulator. The simulation is based on the continuum model of dense-gas kinetic theory [Gidaspow, D., Bezburuah, R., Ding, J., 1992. Hydrodynamics of circulating fluidized beds, kinetic theory approach. In: Fluidization, vol. VII, Proceedings of the 7th Engineering Foundation Conference on Fluidization, Brisbane, Australia, pp. 75–82] with consideration of inter-particle friction force at dense condition [Schaeffer, D.G., 1987. Instability in the evolution equations describing incompressible granular flow. Journal of Differential Equations 66 (1), 19–50]. This study aims to verify this numerical method in modelling dense and complex granular flows, where the solids motion obtained from the simulation is validated against the experimental results of *positron emission particle tracking* (PEPT) technique [Ng, B.H., Kwan, C.C., Ding, Y.L., Ghadiri, M., Fan, X.F., 2007. Solids motion of calcium carbonate particles in a high shear mixer granulator: a comparison between dry and wet conditions. Powder Technology 177 (1), 1–11]. In general, the Eulerian based continuum model captures the main features of solids motion in high shear mixer granulator including the bed height and dominating flow direction (the tangential velocity). However, the continuum based kinetic-frictional model is not capable of capturing the complex vertical swirl pattern. Quantitative comparison shows over-predictions in the tangential velocity and stiff drops of the tangential velocity at the wall region. These results demonstrate the deficiency in transmitting forces in the bed of granular materials which indicate the necessity to improve the constitutive relations of dense granular materials as a continuum.

1. Introduction

Wet massing granulation is one of the most important unit operations in the chemical, food, pharmaceutical, detergent industries for enhancing the flow ability, appearance, strength and other physical/mechanical properties of particulate solids, reducing explosion hazards, and formulation for specific functionality. In this process the dry particles of various components are mixed and a binder liquid is added to the powder mix to form granules. Although there have been significant advances in understanding of the mechanisms of granulation, the granulation process is still difficult to monitor and control as fundamental progress has been inhibited by a lack of understanding of how the motion of the powder within the mixer granulator is induced by the impeller. Previous investigations have shown that the final granule size is a function of breakage and agglomeration which are very sensitive to the flow patterns within the particle bed (Lekhal et al., 2003, 2004). There is potential to improve the design of the mixer granulator to give a better control of product properties which requires an understanding of the motion of materials within granulators and how the granulator interacts with the materials being granulated.

Despite wide interest and more than five decades of investigations, many aspects of the behaviour of flowing granular materials in mixer granulators are still not well understood. With the recent advances in the measurement methods, the internal details of granular flows within mixer granulators start to be unveiled. Various factors, which may have influence on the granular flow in mixer granulators, have been attempted. These include the agitation speed (Bridgwater et al., 1993; Broadbent et al., 1993, 1995; Conway et al., 2005; Hiseman et al., 2002; Litster et al., 2002; Nilpawar et al., 2005; Ramaker et al., 1998; Schutyser et al., 2003; Stewart et al., 2001), fill level (Bridgwater et al., 1993; Broadbent et al., 1993, 1995; Hiseman et al., 2002; Laurent et al., 2000; Stewart et al., 2001), number and

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geometry of blade (Conway et al., 2005; Laurent and Bridgwater, 2002; Lekhal et al., 2006), etc. The findings in the literature are not in agreement and it is extremely difficult to compare and generalise these findings because of the differences in geometries and configurations of granulators, materials and operating conditions. The observations obtained with a particular type of mixer granulator are usually not applicable to the other types. It is always necessary to do measurements in order to understand the solids motions in a particular type of mixer granulator and/or operating conditions.

This is where the numerical simulation comes into play to provide a cost-effective and flexible tool to investigate the flow structure of granular materials in mixer granulators of various configurations and operating conditions. Of many options of numerical tools, the *computational fluid dynamics* (CFD) appears as the primary choice in simulating granular flows in mixer granulators mainly due to its capability in modelling system of complex geometry and to model multiphase systems. The use of CFD in dilute particulate system is well documented in the literature (Benyahia et al., 2000; Ding and Gidaspow, 1990; Li et al., 2006; Neri and Gidaspow, 2000). However, the application of CFD in simulating dense granular flow is poorly reported. Further, there are limited studies compared to the solids motion. Specifically, there is only one open literature reporting the application of CFD to model the high shear mixer granulator (Darelius et al., 2007). In this study, Darelius et al. (2007) compared the simulated bed height and velocity at wall to the PIV measurements. It was found that the bed height could be well predicted whereas the tangential wall velocity was under-predicted.

This study focuses on the overall velocity field and internal flow structure inside a vertical high shear mixer granulator (Cyclomix 5L, Hosokawa Micron B.V. of the Netherlands) by using CFD techniques (Fluent 6.2.16, FLUENT Inc., Lebanon, New Hampshire, USA) and the results were compared to the experimentally measured solids motion for validation purpose. The actual solids motion during the operation was acquired experimentally by using the *positron emission particle tracking* (PEPT) technique at the single particle level (Ng et al., 2007). The configuration and schematic of the granulator can be found in previous communication (Ng et al., 2007).

2. A review of numerical methods for granular flow modelling

Experiments on particulate systems are difficult and show poor repeatability. Comparison between sets of experimental data is often uncertain due to the inability to prepare exact replicas of the physical system and many laboratory experiments accessing the inner behaviours of the real materials rely on the estimation of the macroscopic stress and strain states from measurements at the boundaries, which themselves depend on assumptions made about material behaviour. Due to the difficulties in experiments, numerical simulation has been sourced as a useful tool in studying particulate systems. It represents an interface between laboratory experiments and theory, and can be understood as a "virtual experiment". Numerical simulation has been used for complex geometries, pilot runs, supplement to difficult-to-do experiments, details study of stresses and force network, etc. Numerical simulation is attractive in many cases since it is more cost-effective than physical testing. In addition, the numerical simulation offers precisely description of materials properties, quantifiable results and visualisation of the internal mechanical processes.

In general, the numerical simulation of particulate systems can be grouped into two different categories, the continuum mechanics approach and the discrete method. The main difference between the two approaches is that the former assumes an average of the physics across many particles and thereby treats the material as a continuum, like a fluid, in the simulation while the latter simulates the dynamics of all particles separately.

Numerical simulation is particularly useful for complex particulate systems and it is more cost-effective as compared to physical testing in a majority of cases. The numerical simulation has the advantage to simulate a wide variety of granular flow situations and allows a more detailed study of the micro-dynamics of powder flows. For example, the force networks formed in a granular media can be visualised using data generated with the *discrete element method* (DEM). This is nearly impossible to obtain experimentally with small and many particles.

The use of numerical simulation in particulate systems is not without limitation. The main limitation of numerical simulation is the available computational power. Meanwhile, complex simulations are challenging as well as error-prone. In comparison, both continuum and discrete approach have their own strength and weakness. The main difficulty in continuum approach is to judge the physical meaning of parameters used in the continuum mechanics theory. This leads to difficulties in selecting appropriate experiments to rigorously test a theory. In particular, the flow of granular materials is treated as a fluid flow where solids phase viscosity for the granular materials in flow needs to be defined. The solids viscosity is difficult to measure, if not impossible, in considering the phenomenon of dilation.

Of advantage over the continuum approach, the discrete method only needs to define the physical properties of individual particles, which can often be obtained using single particle tests. However, due to intense computational power requirement, the discrete method is usually confined to small and simple systems. The other drawback of discrete method is the limitation in simulating multiphase systems with fluids which appear to be a standard solver in most commercial codes of continuum approach. Combination of discrete and continuum methods is under intense research and lots of progress has been made (i.e. FLUENT, New Hampshire, USA; Tsuji, Osaka University; Xu, University of Leeds; EDEM, DEM Solutions, Edinburg, etc.).

In general, choosing a numerical scheme for simulating a particulate system is depending on the geometry complexity and the role of the interstitial fluid. Discrete system is suitable for simple and small systems while continuum approach is suitable for large systems with complex geometry and where multiphase is involved, continuum approach is the primary choice. The discrete method is suitable for particulate systems in vacuum condition or where the influence of interstitial fluid is negligible. Due to geometrical complexity of the Cyclomix machines as well as the potential influence of interstitial fluid at high operating shaft speeds, continuum approach was chosen as the primary simulation tool in this study.

3. Model descriptions

The two phases are described by separate conservation equations with a shared pressure term and interaction terms representing coupling between them; the following continuous and momentum equations can be obtained:

$$\frac{\partial \alpha_g \rho_g}{\partial t} + \nabla(\alpha_g \rho_g \vec{u}_g) = 0 \quad (1)$$

$$\frac{\partial \alpha_s \rho_s}{\partial t} + \nabla(\alpha_s \rho_s \vec{u}_s) = 0 \quad (2)$$

$$\alpha_g + \alpha_s = 1 \quad (3)$$

$$\frac{\partial \alpha_g \rho_g \vec{u}_g}{\partial t} + \nabla(\alpha_g \rho_g \vec{u}_g \vec{u}_g) = -\alpha_g \nabla p + \nabla \vec{T}_g + \alpha_g \rho_g \vec{g} + K_{gs}(\vec{u}_s - \vec{u}_g) \quad (4)$$

$$\frac{\partial \alpha_s \rho_s \vec{u}_s}{\partial t} + \nabla(\alpha_s \rho_s \vec{u}_s \vec{u}_s) = -\alpha_s \nabla p - \nabla p_s + \nabla \vec{T}_s + \alpha_s \rho_s \vec{g} + K_{gs}(\vec{u}_g - \vec{u}_s) \quad (5)$$