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Development of a discrete element model with moving realistic geometry to simulate particle motion in a Mi-Pro granulator

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ABSTRACT

This paper presents the implementation of a methodology incorporating a 3D CAD geometry into a 3D Discrete Element Method (DEM) code; discussing some of the issues which were experienced. The 3D CAD model was discretised into a finite element mesh and the finite wall method was employed for contact detection between the elements and the spherical particles. The geometry was based on a lab scale Mi-Pro granulator. Simulations were performed to represent dry particle motion in this piece of equipment. The model was validated by high speed photography of the particle motion at the surface of the Mi-Pro's clear bowl walls. The results indicated that the particle motion was dominated by the high speed impeller and that a roping regime exists. The results from this work give a greater insight into the particle motion and can be used to understand the complex interactions which occur within this equipment.

1. Introduction

Discrete Element Method (DEM) is a particle modelling technique which allows all the particles within the system to move individually and interact at contact points. The advantage of the technique is that all the data for every particle is accessible at any stage of the simulation. The limitation of the technique is the number of particles which can be modelled or the length of a simulation. This is due to the small time steps and large number of calculations performed. The DEM technique resolves contacts over several time steps. In a given time step it is assumed that disturbances of a particle can propagate no further than its immediate neighbours. If this condition is satisfied then at any given time the resultant force acting on a particle is determined entirely by the interactions with its neighbour particles, which are in contact with it. DEM was initially proposed by Cundall and Strack (1979) for studying soil mechanics. Since then it has been applied to industries such as mining (Cleary, 2000; Djordjevic et al., 2004), pharmaceutical (Kwan et al., 2005; Moreno-Atanasio and Ghadiri, 2006), agricultural (Tijskens et al., 2003), food (Raji and Favier, 2004), and chemicals (Kaneko et al., 1999).

DEM has being used extensively to study particle flow in vertical shaft mixers and granulators. The majority of this work has focussed on simple paddle mixers with flat or inclined blades (Stewart et al., 2001; Kuo et al., 2004; Sato et al., 2008; Remy et al., 2010; Remy et al., 2011; Hua et al., 2013). However, more complex geometries such as the three bladed VG-01 (Terashita et al., 2002) have also being studied. Some of these models were validated using either Particle Emission Positron Tracking (PEPT) (Stewart et al., 2001; Kuo et al., 2004) or high speed photography (Remy et al., 2010). In addition to particle flow the DEM has also being used to investigate mixing in vertical shaft mixers (Sinnot and Cleary, 2003; Zhou et al., 2003; Zhou et al., 2004; Chandratilleke et al., 2012; Radl et al., 2010) and has been used to study certain aspects of the granulation process (Nakamura et al., 2013 and Hassanpour et al., 2013).

A major issue within any discrete element model is how the geometry is represented. Especially as most models are representative of real-life systems, with complex geometries. The more complex the geometry incorporated the more difficult the contact detection process between the particles and the geometry becomes, affecting the simulation time. Three techniques exist to represent complex geometries: Mathematical representation; discrete element mesh and constrained spherical particles. Mathematical

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representation is the simplest but is only suitable for very basic geometries such as squares and cubes. Representing the geometry as attached spheres makes the contact detection process simpler but does not allow for the detail of the geometry to be recreated accurately and affects the validity of the model. Therefore discrete element meshes are the most accurate and commonly used method for representing geometries.

The purpose of the mesh is to represent a continuum, in this case surface area, with a series of small discrete elements. These elements recreate the continuum and are easier to incorporate numerically into a DEM model. Contact between the discrete triangular elements and the spherical particles can be determined by the finite wall method of Kremmer and Favier (2001a). These authors also described how to incorporate moving parts into DEM models (Kremmer and Favier, 2001b). Although finite element meshes allow for representation of very complex geometries and can handle movement of internal parts, the drawback is computational expense. New algorithms must be included to detect contacts between particles and triangular wall elements, as well as the original particle–particle contacts. Particle-triangle contacts are more complicated to detect, as contact can occur on the surface of the triangle or on one of the edges or vertices. An important issue when constructing finite element meshes is the number of elements used. The more elements used the more accurately the continuum is recreated, but with the cost of an increased simulation time.

If the DEM model requires motion of the geometry, to represent an impeller in a mixer or the belt of a moving conveyor this can be performed using the mesh data. At each time step the nodes at the vertices of the element can be moved from their current location to the new location according to the set motion. Finite element meshes have been used in DEM models of industrial granular flows (Cleary and Sawley, 2002), and high shear mixers (Terashita et al., 2002).

This work will discuss how a 3D geometry was incorporated into an existing DEM code and the techniques developed for contact detection and motion of the impellor. How simulation parameters such as spring stiffness and simulation time step were calculated will also be presented. The code was then validated using high speed photography and used to simulate particle motion in a Mi-Pro lab scale granulator. These granulators are used to investigate granulation at a small scale (Gamble et al., 2009 and Cavinato et al., 2013). They utilise an impeller with three blades inclined backwards at 45°. As this equipment has a nonstandard geometry it is important to understand the particle flows within them. The DEM model developed in this work was then used to investigate the complex particle flow patterns and particle contacts which exist in this equipment. The results from this modelling study can then be used to develop a deeper understanding understand how granulation will occur in these types of devices.

2. Discrete element method

The DEM technique uses Newton's second law of motion to calculate the acceleration of a particle due to all of the forces acting on it. Integration of the acceleration twice produces the particle's displacement. A particle can have two types of motion, translational and rotational. The translation motion can be calculated from:

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_{j=1}^{k_i} \left(\mathbf{f}_{c,ij} + \mathbf{f}_{d,ij} \right) + m_i \mathbf{g} \tag{1}$$

Where m_i and $\mathbf{v}_i$ are the mass and velocity of particle i respectively. k_i is the number of particles in contact with particle i. $\mathbf{f}_{c,ij}$ and $\mathbf{f}_{d,ij}$ are the contact force and viscous damping contact force respectively between particles i and j. The final term $\mathbf{g}$ in Eq. (1) is the force due to gravity. This model assumes that no other non-contact forces are acting on the particle. It is possible to include non-contact forces such as cohesive liquid forces in DEM models (Xu et al., 1999). The rotational motion of the particle can be calculated from:

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_{j=1}^{k_i} \left(\mathbf{T}_{ij} + \mathbf{M}_{ij} \right) \tag{2}$$

Where I_i is the moment of inertia of the spherical particle i given by:

$$I_i = \frac{2}{5} m_i r_i^2 \tag{3}$$

Where $\boldsymbol{\omega}_i$ is the angular velocity of particle i. $\mathbf{T}_{ij}$ is the torque generated by the contact between particles i and j and $\mathbf{M}_{ij}$ is the rolling friction. The particle i has radius r_i. The DEM modelling technique has three stages: contact detection; evaluation of contact forces; summation of forces to calculate particle motion. Contact detection is concerned with identifying if a contact has occurred between two particles, or a particle and any equipment geometry which may exist in the system. Evaluation of contact forces calculates the forces resulting from a single contact using an appropriate contact model. The resultant force is calculated by resolving all forces acting on a particle, including gravitational effects. Once this is determined Newton's second law of motion can be used to calculate the particle acceleration.

Rolling friction is responsible for bringing rolling objects to a rest. It is important to incorporate rolling friction into DEM especially if the particles are spherical. Rolling friction results from the elastic hysteresis loss as the rotating particle contacts other objects or as a result of any time dependent surface deformation it may experience (Tabor, 1952). Rolling friction has been successfully included in DEM contact models, such as Zhou et al. (1999) in simulation of sand pile formation. This work utilises the methodology of Xu et al. (2001) to include rolling friction. In this model the magnitude of the rolling friction torque, $\mathbf{M}_{ij}$, in Eq. (4) is calculated by shifting the location of the normal contact force $\mathbf{f}_{cn}$ a distance $\boldsymbol{\delta}$ away from the contact point.

$$\mathbf{M}_{ij} = \mathbf{f}_{cn} \times \boldsymbol{\delta} \tag{4}$$

For a spherical particle contacting (and overlapping) a horizontal surface $\boldsymbol{\delta}$ is the horizontal distance between the centre of the particle and the where one side of the particle contacts the surface.

The selection of the numerical scheme used to calculate the particles' translational and rotational motion is important in the DEM. A balance must be found between computationally efficient and numerically accurate schemes. The original work of Cundall and Strack (1979) used an explicit time integration scheme. This explicit scheme is simple to implement and computationally efficient. However, the main drawback is that contacting particles' overlaps are not calculated until a time step has been completed. This requires small time steps to be used to ensure that particle overlaps are not over estimated and fictitious elastic energy during contacts are stored (Xu and Yu, 1997).

3. Model development

The DEM model used for this research was developed from an existing 2D code used to study particle behaviour in fluidised beds (Xu and Yu, 1997). The code was updated to a 3D version and further developed during this work to include geometry representation via a finite element mesh and moving boundaries. The contact model used for this code is a linear spring dashpot model in the normal direction. An additional slider is incorporated in the tangential direction. There are many other nonlinear contact models available such as the Hertz (1882) and elastic-plastic models (Walton and