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The effect of particle shape on simple shear flows

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Abstract

Simple shear flows, (without gravity force and implemented using periodic boundary conditions or in Couette flow configurations with gravity) have been the subject of study using DEM simulation for more than two decades. Earlier studies explored the effect of attributes such as shear rate, particle size and domain scale on the distribution of the particles in the flow, velocity profiles and the stress distributions. These studies were conducted using simple shapes for the particles such as spheres. In recent years, the importance of particle shape on flow has been recognized in a range of industrial application including mixing, comminution, hopper discharge and chute flows. In this paper, we return to the simple shear flows and quantitatively explore the effect of particle shape on velocity, volume fraction, granular temperature and stress distributions across the channel. Particle shape is found to sharply increase the strength of the material making it stronger and harder to shear. The generation of particle spin throughout the flow of non-circular particles leads to high granular temperatures, dilative pressures and lower solid fractions in the core of the flow. For aspect ratios between 0.6 and 0.5, a transition in the effective behaviour of the wall boundary conditions is identified. The connections of shape to spin, to granular temperature, to bulk flow changes are elaborated.

Keywords: Shear cell; Couette; DEM; Shape; Granular temperature; Super-quadric

1. Introduction

Granular materials are by their nature discrete and flows are determined by the interaction of discrete collision events. The detailed behaviour of these flows is best modelled at the grain scale. The computational methods used to model such discrete flows are typically called Discrete Element Methods (DEM), see Campbell [1,2] for reviews of the fundamental issues and Cleary [3] for application to industrial and geophysical flows. DEM encompasses a broad variety of methods; soft particle methods as initiated by Cundall and Strack [4]; and event driven or hard particle methods [5]. There are also variants of the contact force models and many types of coupled physics. DEM, as a class of computational methods, is now a powerful tool for modelling granular materials and flows. But it is inherently limited by the number of particles that can be included in the model. Currently models with up to 10 million can be simulated in reasonable times on single processor computers. This is sufficient for modelling many applications. But for fine powders (10–100 μm) this represents less than 1 cm^3 and compared to a stock pile with 10^{12}–10^{15} particles, the current capacity of DEM is dwarfed. So with DEM one could model a whole pharmaceutical tablet, but certainly not the bulk mixing process (typically performed in tonnes).

For these large systems there is ultimately little choice but to adopt a continuum method. This involves averaging over some length scale that is much larger than the particle scale and removing all the direct discrete interactions from the model system and replacing them with a series of conservation equations involving constitutive laws for continuum properties such as stress, granular temperature and pressure. The strength of this approach is that it can handle any volume of material and is not restricted by the particle numbers. The disadvantage (and a huge one) is that all the detailed micro-mechanics are replaced by constitutive laws whose form needs to be determined and whose parameters must be fitted from somewhere. Localisation in shear bands also means that the averaging scales can be comparable to or smaller than the key physical process length scales so models based on homogenisation are then not valid.

An early and popularly adopted class of models based on kinetic theory was developed by Savage and co-workers [6–10]. Many extensions of this model have been explored and used, see Campbell [1] for a review of these. The basic model is formally valid only for spherical mono-sized particles under restricted

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conditions (but is commonly used in circumstances far beyond its range of validity). Efforts to include even the simplest additional physics require significant theoretical and computational development. Kinetic theories have been extended to binary mixtures [10] but extension to arbitrary continuous size distributions are a major challenge. The inclusion of a representative particle size with corresponding particle rotations leads to higher order continua theories, such as micro-polar and Cosserat models [11,12]. The more general constitutive laws tend to have very large numbers of adjustable parameters that must be tuned to a specific system. Conversely, many constitutive laws are quite simplified and apply in only restricted circumstances. Within their areas of validity, these can be powerful tools with which to explore the behaviour of granular systems. Often though they are used outside these valid ranges with unpredictable consequences — one should certainly not expect a priori quantitative accuracy from such models when used in this way.

So the ongoing challenge is to develop continuum models that capture increasingly broad amounts of the micro-mechanical detail in their constitutive laws while having less free parameters to fit. This is a popular but extraordinarily difficult problem with many people working on it. Progress to date has been restricted. One approach sometimes adopted is to use DEM to model simple systems from which constitutive behaviour can be extracted. This can assist in the construction of continuum models with suitable rheology and appropriate boundary conditions [1,13]. Key continuum components of such models are flow velocities, volume fractions, granular temperature and stresses.

Flow dynamics and the form of the stress tensor for rapid granular shear flows have been explored using the Discrete Element Method (DEM) for around two decades. Early work focused on the effect of boundary roughness, volume fraction and particle friction in both two and three dimensions. A reasonably clear understanding of the flow dynamics was established for small simple shear cells [14,15] and for Couette shear flows driven by oppositely moving walls [16–19].

At a micro-mechanical level, particle shape has been shown to have a very important effect on flow dynamics. Mixing rates and quality is strongly affected by shape [20,21], material strength which determines when solid granular material failure will occur is heavily shape dependent [22,23] and the flow pattern within hoppers is dominated by the shape of the particles [24]. The impact of particle shape on continuum flow properties has not yet been explored. So in this paper, we re-visit the granular plane Couette flow and use continuum averaging of DEM predictions to explore the effect of particle shape variation on the velocity, volume fraction, stress tensor and the granular temperature distributions. The aim is to better understand the quantitative impact of the shape variation on these continuum flow characteristics, so as to better understand the issues that need to be addressed by continuum granular flow models.

2. DEM method

Discrete element modelling (DEM) of granular flows involves following the trajectories, spins and orientations of all the particles and predicting their interactions with other particles and with their environment. These methods are now well established and are described in review articles by Campbell [1], Barker [25] and Walton [26]. The DEM code used here has been successfully applied to many industrial and mining applications by Cleary [3,24,27,28].

In DEM, the particles are allowed to overlap and the amount of overlap Δx, and normal v_n and tangential v_t relative velocities determine the collisional forces. There are a range of possible contact force models available that approximate the collision dynamics to various extents. A conventional linear spring dashpot model is used in these simulations.

The normal force :

$$F_n = -k_n \Delta x + C_n v_n, \tag{1}$$

consists of a linear spring to provide the repulsive force and a dashpot to dissipate a proportion of the relative kinetic energy. The maximum overlap between particles is determined by the stiffness k_n of the spring in the normal direction. Typically average overlaps of 0.1–1.0% are desirable, requiring spring constants of the order of 10^4–10^7 N/m (in two dimensions). The normal damping coefficient C_n is chosen to give a required coefficient of restitution ε (defined as the ratio of the post-collisional to pre-collisional normal component of the relative velocity), and is given in Cleary [27].

The tangential force is given by:

$$F_t = \min\left\{\mu F_n, k_t \int v_t \mathrm{d}t + C_t v_t\right\}, \tag{2}$$

where the integral of the tangential velocity v_t over the collision behaves as an incremental spring (with stiffness k_t) that stores energy from the relative tangential motions and represents the elastic tangential deformation of the contacting surfaces. The dashpot (with strength C_t) dissipates energy from the tangential motion and models the tangential plastic deformation of the contact. The total tangential force (given by the sum of the elastic and plastic components) is limited by the Coulomb frictional limit at which point the surface contact shears and the particles begin to slide over each other. Here μ is the dynamic friction coefficient.

Traditionally particles are modelled as discs in two dimensions. The central theme of this paper is the exploration of particle shape effects on flow, so a more complex shape description is needed. Here we use super-quadrics, with general form:

$$x^N + \left(\frac{y}{A}\right)^N = s^N, \tag{3}$$

to describe non-circular particles. Here, the power N determines the blockiness of the particle (with the shape smoothly changing from a circle to a square as N increases) and A is the aspect ratio of the particle with semi-major axis s. Super-quadrics have previously been used to describe particle shapes [29,3,21–24]. Super-quadric particle shapes are able to capture the most essential elements of real particle shape and greatly extend the range of applicability of DEM with only moderate computational cost. In our implementation aspect ratios of up to 20:1 and