NUMERICAL SIMULATIONS TO INVESTIGATE THE ROLE OF PARTICLE SHAPE ON BULK BEHAVIOR OF PARTICLES IN SILOS

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1 INTRODUCTION

In Discrete Element Modelling (DEM), as an effective tool in the area of particulate materials, a particulate medium is represented by an assembly of discrete model particles. The shape of these particles is arbitrary, but ideally should match the shape of actual particles under consideration. The choice of particle shape representation is critical to the accuracy of the simulation of real particle behaviour, the method used for contact detection and the method of computation of contact forces¹. Although contact detection and computation time are very important, the critical objective in DE modelling is accurate simulation of the behaviour of an assembly of real particles. The influence of particle shape on the predicted behaviour is less well documented than the relationship between shape and the efficiency of contact detection². As a result, the application of the DE method to particular applications has resulted in various methods of particle shape representation. While the earliest DE models were two-dimensional and employed circular elements with a linear contact models, later models have been developed with complex shape representation such as polygon, ellipse, and more recently the combination of primitives, mainly circle³ and sphere⁴. In this study a DE model, based on the Multi Sphere Method of particle generation⁴, has been used to investigate the effect of model particle shape on the bed structure and flow characteristics of particulate assemblies of different shapes. Aspect ratio has been selected as a criterion to compare and describe particles of different shapes.

2 SIMULATION PROCEDURE

A flat bottom hopper of 100cm width has been simulated in 2-D *i.e.* the 3D model particles have been positioned in a single vertical layer. The hopper structure consisted of an upper and lower part. The height of the upper section could be changed so that all model particles have been generated in the hopper without any contact. The orifice has been simulated as a removable wall which has been positioned at the midpoint of the hopper. The particles discharged from the upper box, collected in a chamber beneath the hopper. Four sets of simulations have been performed with particles of the same cross sectional area (each particle comprised of a linear array of mono-sized spheres) with aspect ratios from one to four. The radius of mono-sized element spheres of a non-overlapping multi-sphere model particle of aspect ratio *n* with area equal to the area of a sphere of unit radius is:

$$R_n = \left(\frac{1}{n}\right)^{\frac{1}{2}} \tag{1}$$

where n is the aspect ratio or the number of non-overlapping element spheres in the model particle. These particles are shown in *Fig. 1*.



Figure 1: Particles used in the simulations with the same cross section area but different aspect ratio, ranging form one to four

In the case of non-spherical particles, a random orientation has been given to each particle in the X-Z plane in order to generate random packing of particles. Particles were then allowed to consolidate under the gravity field until particle movement was negligible. To study the effect of particle shape on the bed structure independently of the effect of inter-particle friction, the particle-particle and particle-wall coefficients of friction have been set to zero during the consolidation. This method of particle bed preparation also had the effect of speeding up the consolidation process. At the end of the particle bed generation stage the coefficients of friction have been set to 0.5 and 0.2 for particle-wall and particle-particle respectively.

3 RESULTS AND DISCUSSION

3.1 Packing structure

The effect of particle shape on the prediction of the DE model has been investigated for packing structure of particle beds (the arrangement of particles) at the end of consolidation by comparing the results of simulations in terms of bed height, the distribution of solid fraction through the bed, and particle co-ordination number. The initial bed height and the bed structure in a frictionless condition for the assemblies of particles comprising aspect ratio from one to four are shown in *Fig. 2*. The original bed height increased as the particle aspect ratio became higher due to greater void space among the particles of higher aspect ratio.



Figure 2: Bed height and structure at the end of consolidation for particles of aspect ratio: (a) 1, (b) 2, (c) 3 and (d) 4; (e) Relationship between the average solid fraction of the particle bed and aspect ratio of particles at the end of consolidation.

In the bed of spherical particles, some localized densely packed areas of homogenous particle packing structure have been observed, separated with narrow regions of higher porosity caused by bridging of particles. The size of the homogenous densely packed area was increasingly smaller in beds of particles of higher aspect ratio. There was a greater difference in the size of the area of densely packed particles between beds of particles of aspect ratio one and two (comparing *Fig. 2a* and *Fig. 2b*) than two and three, and from three to four (comparing *Fig. 2c* and *Fig. 2d*). This suggests that the change of particle shape from spherical to non-spherical had a greater effect on the packing structure of the particle bed than an increasing in the aspect ratio of non-spherical particles.

The packing structure has been quantified by solid fraction calculation of the bed. The overall reduction in the average solid fraction was about 8 % as bed particle aspect ratio changed from one to four; however most of this reduction occurred between aspect ratio of two and four. The effect of particle aspect ratio on the packing structure of the particle bed has been investigated by comparing the distribution of the solid fraction. The frequency distribution of solid fraction, which is characterized by skewness and kurtosis, is a particular parameter if the assumption is made that in a normal distribution of the solid fraction there is a wide varieties of voids (different in shape and size) in the bed. A lower skewness and higher kurtosis achieved, indicating a closer distribution to a normal distribution for the beds of particles of higher aspect ratio, implying a wider variety of void shape and size. In contrast, the highly negative skewed for the bed of spherical particles indicates a more uniform distribution of solid fraction for this bed, showing a smaller variation in void size and shape.

Co-ordination number is defined as the average number of contact points per particle in the particulate assembly. This parameter correlates with the degree of dilation of the bed and it can be used as an index for comparison of particle bed structure. *Figure2e* shows the co-ordination number for particle beds of different aspect ratios at the end of consolidation. The final co-ordination number of the beds generally decreased, as the aspect ratio became higher, indicating a looser packing structure for non-spherical particles. The change in the magnitude of co-ordination number was greater (15.1 %) between particles beds of aspect ratios of one and two (spherical and non-spherical) than two and four (11.3 %).

3.2 Flow characteristics of particles

Parameters such as particle track, particle orientation, and particle velocity, have been used to study the effect of particle shape on flow behaviour of the beds. For all particle beds convergent or funnel flow zone has been seen in the lower portion of the hopper. In the plug flow region (upper portion of the hopper) the particles moved downwards without any considerable lateral movement, exhibiting a mass flow with identical behaviour of particles in this region for all particle shapes. However, the transition zone was higher in beds of particles of higher aspect ratio. This can be explained from the rate of interlocking among particle beds of different aspect ratios. In this region, for a bed of spherical particles, a smooth path has been observed for the trajectories of particles, while for non-spherical particles the trajectories were uneven with a sharp change in the direction of particle movement. These indicated a repeated interlocking between elongated particles. In this regard the formation of arching has been also simulated by the DE model. A qualitative correlation between the frequency of arching and aspect ratio has been recognised. More arching occurred as the aspect ratio of particles increased.

It has been observed that while the bed of spherical particles sheared vertically, an inclined shearing observed for the beds of non-spherical particles. Furthermore, spherical particles started to move laterally with a height closer to the bottom of the hopper even for those particles close to the side walls, indicating a flow which was closer to that of mass flow.

In contrast, in non-spherical particle beds, the track of particles showed a relatively concentrated funnel flow which would normally be expected for a flat bottom hopper of real particles of non-spherical shape.

The dynamic behaviour of the beds has been also investigated, by recording the energy ratio, as the ratio of rotational and traslational energy of a particle. Although in all assemblies the rotational energy of particles was lower than their translational energy, the observed rotation, in all parts of the hopper, was much greater for particle of spherical shape than non-spherical particles. In all assemblies the particles in the central part of the hopper had the minimum rotation compared to the sides of the hopper and the evolution of the average energy ratio in the sides of the hopper was almost the same (symmetrical) but higher for spherical particles.

The simulation of the filling process and repose tests for frictional spherical and nonspherical particles showed that the shape of heap could be affected by particle shape, i.e. a steeper heap has been found for non-spherical particles than spherical particles even though the drop height was higher for non-spherical particles.

4 CONCLUSION

Particle discharge from a flat bottom hopper has been performed employing a DE model with MSM particles, in order to investigate the effect of particle shape on bed structure and flow characteristics of particles. The localised densely packed areas have been separated by voids caused by bridging of particles in the beds. There was a distribution of solid fraction within each bed, with the closest distribution to the normal distribution for the beds of elongated particles. It has also been observed that variation in bed structure and co-ordination number between beds of spherical (aspect ratio=1) and non-spherical particles (aspect ratio=2) were much greater than those between elongated particles (aspect ratio \geq 2). It can therefore be concluded that the results obtained from the DEM models with spherical particles cannot be generalised to real material comprising non-spherical particles.

The flow Simulations showed that the behaviour of beds of spherical particles was quite different from that of non-spherical particles. During flow, spherical particles moved individually and rolled over each other, resulting in a lower resistance to shear with a fluid-like flow, whereas elongated particles exhibited a stronger shear due to interlocking between particles, resulting in a flow, like a breaking continuum with a higher transition zone.

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