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DISCRETE ELEMENT MODELLING OF HIGH ASPECT RATIO SPHERO-CYLINDER PARTICLE PACKING

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Abstract. This paper presents Discrete Element Model simulations of packing of rigid sphero-cylinders. The method has been used before but this study considers higher aspect ratios, up to 30. This posed some modelling challenges in terms of stability which were overcome by imposing limits on the particle motion. The results show very good agreement with experimental data in the literature and more detailed in-house experiments for packing volume fraction. Model results on particle orientation are also shown. The model has the potential for predicting packing of fibrous particles and fibre bundles relevant to the preparation of preforms for the production of polymer and metallic matrix composites. Future model developments will include adding flexibility by connecting sphero-cylinders as sub-elements to describe a particle.

1 INTRODUCTION

Modelling of the packing of fibres is of high interest to the fabrication of metal-ceramic composites. For metal matrix composite preparation by the infiltration of a packed ceramic fibre “preform” with a liquid metal, it is of significant benefit to be able to predict the packing behaviour of the fibres (or bundles of fibres) which form a rigid preform and hence which dictates the structure and properties in the final composite part.

Altering the aspect ratio of the fibre is one of the simplest ways to vary the packing fraction and means that through appropriate chopping of the fibres, the volume fraction of fibres in the rigid preform can be tailored to suit the mechanical properties required.

Whilst improved packing, and to some extent easier interspersion of the metal and fibre phases, occurs as the fibre aspect ratio decreases, this is to the detriment of the efficiency of load transfer and hence the final properties. For typical metal-ceramic systems (with 20-50 vol.% reinforcement), a minimum aspect ratio of roughly 20 is targeted to achieve stiffness values that are close to those predicted by the rule of mixtures [1].

Simple geometrical models, such as that by Parkhouse & Kelly [2], have been developed for similar treatments in polymer composite systems and show the interdependence between fibre aspect ratio and packing fraction (for example a packing of 30 vol% of the available space being predicted for fibres with an aspect ratio of 20). Development of these simple models to finite volumes, to incorporate additional friction and cohesion terms and with quantification of the orientation distribution of the fibres in the vessel will greatly enhance the insight that is possible through this modelling approach.

DEM is widely used to model granular flow and packing [3-5]. Most applications model spherical particles but there are an increasing number which model non-spheres such as hemi-spherical ended cylinders. This paper models packing of such sphero-cylinders, but for a large aspect ratio λ up to 30. These are somewhat unstable in the model, but with restrictions on motion the model is shown to give reasonable results.

2 APPLICATION OF DEM TO SPHERO-CYLINDER PARTICLE PACKING

2.1 DEM Method

The DEM technique uses an explicit time stepping approach to numerically integrate the motion of each particle from the resulting forces acting on them at each timestep. The particle flow model here follows a fairly standard DEM approach. The inter-particle and particle wall contacts are modelled using the spring–dashpot–slider analogy. Contact forces are modelled in the normal and tangential directions with respect to the particle surface. Particle cohesion can also be modelled but this is not used in this study. The translational and rotational motion of each particle is modelled using a half step leap-frog Verlet numerical integration scheme to update particle positions and velocities. A zoning method is used to increase the computational efficiency of determining particle contacts.

Developing DEM to model non-spheres is a significant issue. Various methods are used as reviewed in [3] and briefly in [5] . These include super-quadrics, sphero-discs, polyhedra and combined finite-discrete element (FEM/DEM) methods. These studies show that particle shape can be very significant.

2.2 DEM "Sphero-Cylinder" Method

This technique is briefly mentioned in the review by Džiugys & Peters [3]. The particle is described by a cylinder with hemi-spherical ends of the same radius. The advantage of this geometry is that an essentially analytical method can be used to calculate contact location and contact normal force direction. The algorithm below was developed in [4] and has been used in the current study.

- Check for enclosing sphere contact, exit if none
- Calculate the shortest distance pq between the two lines for each cylinder axis
- If p and q lie within the particle line segments, check for cylinder-cylinder contact
- If p or q lie within the particle line segments, check for cylinder-sphere contact
- If neither p or q lie within the particle line segments, check for sphere-sphere contact.

2.3 Application of DEM to fibre packing

The above algorithm for sphero-cylinders is used here to model dropping fibre particles into a cylindrical vessel to estimate the packing fraction. Particle-particle forces are modelled with a linear spring–dashpot–slider analogy. Cohesion and rolling friction coefficients are set to zero and no interstitial fluid is included. Particle-wall forces are similarly modelled. Constant gravity is modelled. A "softened" particle normal stiffness is used as is usual in DEM flow/packing simulations to allow a reasonable simulation timestep. Compared with previous DEM cylinder simulations in the literature, this study models quite large aspect ratios. This poses some modelling challenges in obtaining stability. Both the particle stiffness and damping factors are set proportional to the particle aspect ratio. The principal data used is shown in Table 1 and example figures illustrating filling & packing are shown in Figure 1.

Table 1: Principal DEM data

Parameter	Value
Vessel height (m)	10.
Vessel diameter (m)	0.21, 0.41, 0.61
Number of particles	500, 700, 700
Particle diameter (m)	0.01
Particle aspect ratio	10, 20, 30
Particle solid density (kg m^{-3})	2,700
Contact damping	"moderate"
Contact friction coefficient	0.2
Time modelled (s)	10

In practice the particle would offer some flexure, whereas in this model it does not. The inflexible particles here, even with softened normal interactions, show ill-conditioned interactions due to "amplification" of motion – like a long lever with the fulcrum near one end. This is essentially overcome here by using the softened interaction, but also by limiting the particle angular velocity. In the filling stage the limit is set at 4π rad s^{-1}, and in the settling stage at 0.2π rad s^{-1}. The higher the aspect ratio the more "vulnerable" the system is to instability. Example packings for the largest aspect ratio λ=30 are shown in Figure 2, which show that stability is achieved.

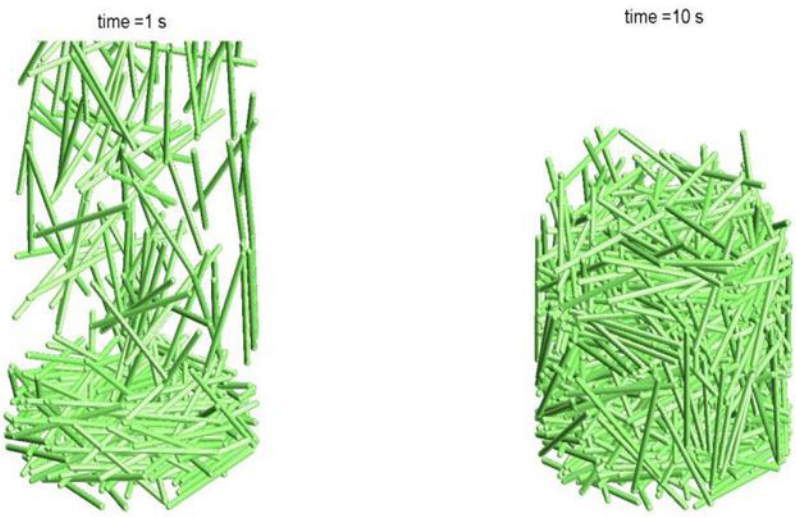

Figure 1: Snapshots of DEM Sphero-cylinder fill & packing

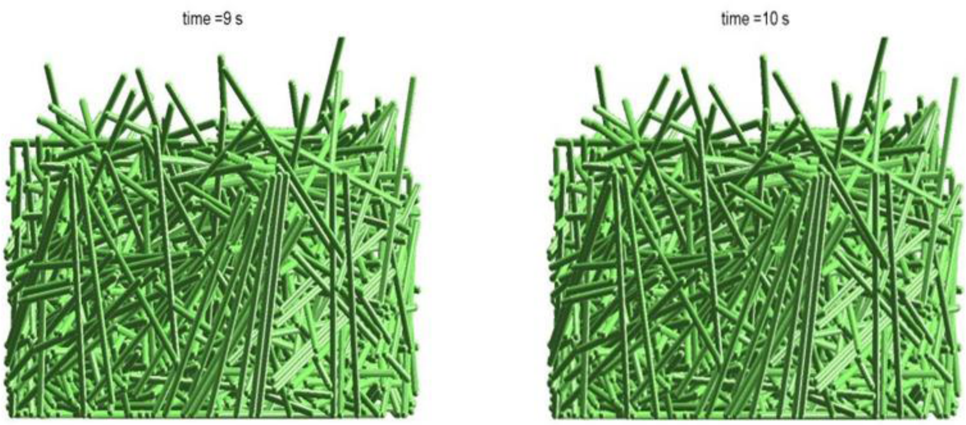

Figure 2:Stability achieved in DEM for λ = 30

2.4 Packing results

The simulation monitors two measures of solid volume fraction V_f (=1-voidage): first on the whole vessel up to the centre of the highest particle; secondly in a cylindrical cellular region inside the packing about half this volume, estimated numerically. The values are close but the latter is taken as more accurate. Parkhouse & Kelly [2] present a plot of V_f v $1/\lambda$ for experimental data points and a theoretical curve; most of the experimental points lie just below the curve but follow its trend. Figure 3 shows results for the DEM simulations for λ=10, 20, 30 and compares with the theory from [2]. These show good agreement. The DEM results are slightly lower than the theory as are most of the experimental cases cited in the reference. Indeed the DEM seems comparable with the experiments. Initial experiments undertaken in-house also show good agreement. These will be shown in a future publication along with sensitivity to particle properties such as friction.

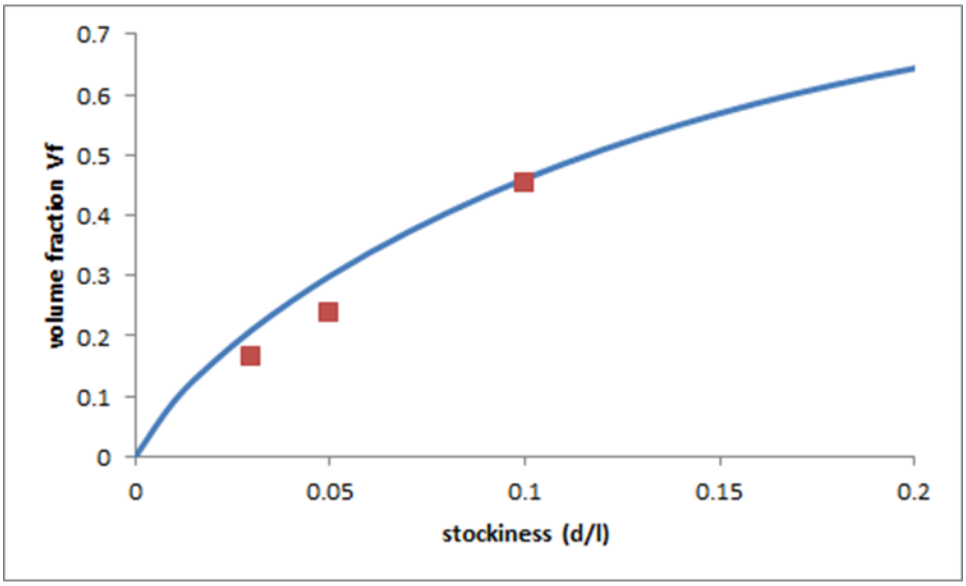

Figure 3: DEM results (squares) for sphero-cylinder packing compared with theory from [2]

2.5 Particle orientation

It is interesting to note the orientation distribution of the settled packings shown in Figure 4 for λ = 20 & 30. These are similar and show that most particles are near horizontal. This indicates that they have not been unduly restricted by the vessel walls during the filling. It would be useful to monitor this experimentally.

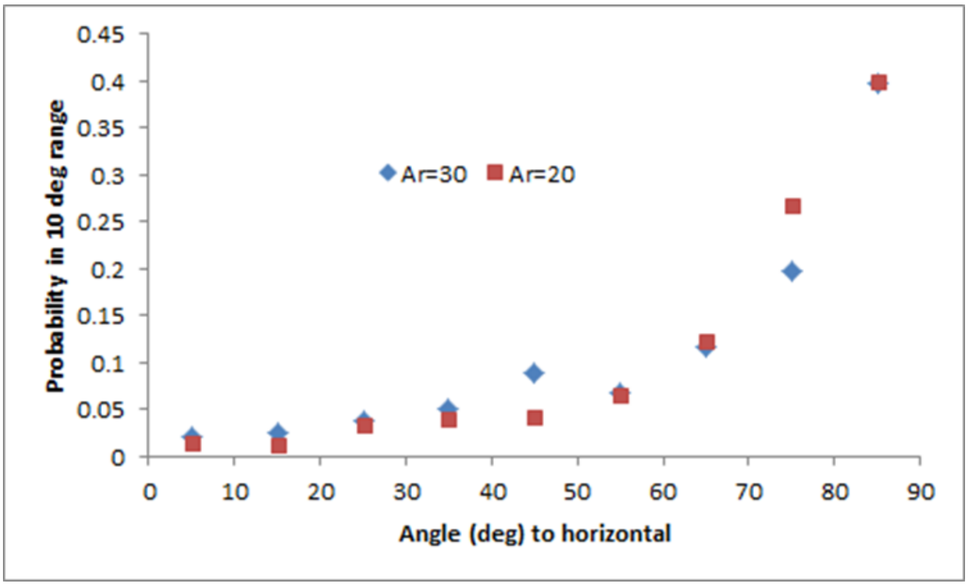

Figure 4: Particle orientation distribution in DEM

3 CONCLUSIONS

- DEM is applied to model packing of sphero-cylinders in a cylindrical vessel. Conventional methods are used with softened interactions. The aspect ratio is quite large for DEM which caused some stability issues. Use of softened interactions as commonly applied to enable a reasonable timestep and limiting angular velocity allowed stable packings up to λ=30.
- DEM results of V_f v λ showed very good agreement with information in the literature, including experimental and theoretical data [2].
- Particle orientation in the DEM showed that most particles are close to horizontal. It would be useful to analyse experimental data on this.
- The model could be developed to include particle flexure by linking sphero-cylinders with rotational stiffness at joints.

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