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Discrete element modelling of flexible fibre packing

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ABSTRACT

This paper presents Discrete Element Model simulations of packing of non-cohesive flexible fibres in a cylindrical vessel. No interstitial fluid effects are modelled. Each fibre-particle is modelled as a series of connected sphero-cylinders. In an initial study each particle is modelled a single rigid sphero-cylinder; 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 angular velocity. 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 is developed to include flexibility by connecting sphero-cylinders as sub-elements to describe a particle. Some basic tests are shown for the joint model that connects the sub-elements. The simulation results show similar trends to the rigid particle results with increased packing fraction. The effects of number of sub-elements, joint properties and contact friction are examined. The model has the potential for predicting packing of fibrous particles and fibre bundles relevant to the preparation of preforms for the production of discontinuously-reinforced polymer, ceramic and metallic matrix composites.

1. Introduction

Modelling of the packing of fibres is of high interest to the fabrication of discontinuously-reinforced composite materials. For the example of metal matrix composites, their preparation can be affected by the pressure-assisted 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 will dictate both the processing conditions required for successful infiltration but also the structure and properties in the final composite part. Fig. 1 shows an example of a metal matrix composite made by infiltration of a preform of discontinuous carbon fibres as well as the typical architecture of a "mat" made from carbon fibres.

Altering the aspect ratio of the fibre is one of the simplest ways in which the packing fraction might be varied and means that through appropriate chopping or milling, 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 effective load transfer to the reinforcement [1]. Examples of applications of metal matrix composites are described in [2,3] and a commercial example is shown at <http://www.cmt-Ltd.com/index.html>.

Simple geometrical models, such as that by Parkhouse and Kelly [4], 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.

Section 2 summarises the DEM technique which is widely used to model granular flow and packing [5–8]. 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, and also flexible fibres modelled by connected sphero-cylinders.

Section 3 describes an initial study which modelled each particle as a single rigid sphero-cylinder with aspect ratios up to 30 [9]. This posed some modelling challenges in terms of stability which

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were overcome by imposing limits on the particle angular velocity. Model results are compared with theory and experiments.

Section 2.4 describes how the model is developed to include flexibility by connecting sphero-cylinders as sub-elements to describe a particle, and shows some basic tests for the joint model. Section 4 shows the results of packing fraction dependent on particle properties for the flexible particles. Section 5 summarises the conclusions.

2. Discrete Element Model (DEM)

2.1. DEM sphere method

The Discrete Element Method applied to spheres is well established as a reasonably realistic tool, in a wide range of engineering disciplines, for modelling packing and flow of granular materials; Asmar et al. [8] describes the fundamentals of this method as applied by code developed in-house at Nottingham; since these are widely documented the details are not reproduced here, simply a summary. It applies an explicit time stepping approach to numerically integrate the translational and rotational motion of each particle from the resulting forces and moments acting on them at each timestep. The inter-particle and particle wall contacts are modelled using the linear spring–dashpot–slider analogy. Contact forces are modelled in the normal and tangential directions with respect to the line connecting the particles centres. Particle elastic stiffness is set so sphere "overlap" is not significant and moderate contact damping is applied. Particle cohesion can also be modelled but is assumed to be negligible in the current 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. Near-neighbour lists are used to increase the computational efficiency of determining particle contacts and a zoning method is used each time the list is composed; that is the system is divided into cubic regions, each particle centre is within one zone, and potential contacting particles are within the same or next-door neighbour zones. Full details are given in Asmar et al. [8].

Rolling friction is often modelled as an angular torque arising from the elastic hysteresis loss or viscous dissipation [10], this enables more realistic rolling behaviour in DEM spheres (but is not applied here to the fibres described later). Further useful references which consider determination of contact parameters for DEM and scaling laws are in [11,12].

2.2. DEM for non-spherical particles

Developing DEM to model non-spheres is a significant issue. Various methods are used as reviewed in [5] and briefly in [7]. These include sphero-cylinders, super-quadrics, sphero-discs, polyhedra and combined finite–discrete element (FEM/DEM) methods. These studies show that particle shape can be very significant. For fibre shaped particles the following references are particularly noted.

Cruz Hidalgo et al. [13] models rods in an experimental and numerical study of stress propagation in granular packings; the contact force distribution is affected by particle aspect ratio. Hidalgo et al. [14] investigate the effect of particle cohesion in packing simulation of rods in 2D; the cohesion tends towards more open packing and breaks up the horizontal alignment of non-cohesive packings. Using clumped spheres is another method and has the advantage of simplicity and versatility. For example Nan et al. [15] models packing of long rigid fibres, straight and curved; the packing structure is investigated for different aspect ratio and

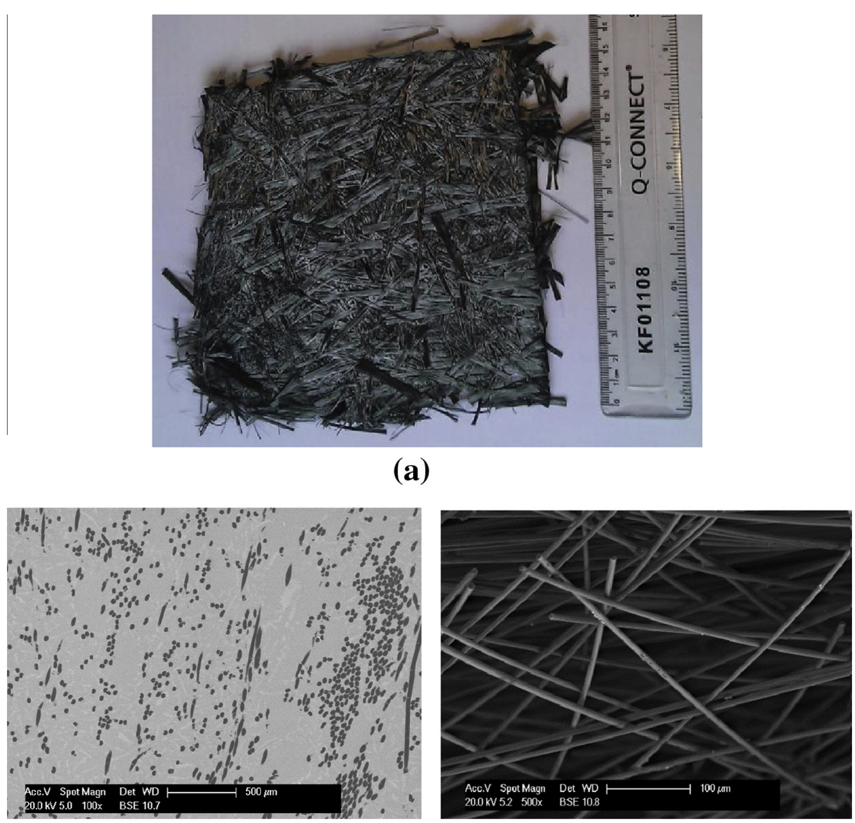

Fig. 1. (a) Example of directed carbon fibre preform; (b) an Al alloy composite containing discontinuous carbon fibres; (c) a preform of carbon fibres.