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A numerical investigation of the void structure of fibrous materials

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Abstract

The void structure of particulate solids has been studied with the aid of a numerical packing algorithm based on the minimisation of an energy potential. This algorithm has been used to form densely packed assemblies of spherical and fibrous particles. The void space within these materials has been characterised using an algorithm that finds chains of voids that pass through the assemblies. The tortuosity (as defined by Carman [P.C. Carman, Fluid flow through granular beds, Trans. Instn. Chem. Engrs., v15 pp 150–166, 1937.]) and mean diameter of these chains have been determined and examined as important parameters that are relevant to the permeability of these materials. Tortuosity was approximately constant in the spherical particle assemblies, while the void size varied with the particle size. In general, the spherical particle assemblies showed much smaller void sizes (relative to the particle diameter) and lower tortuosity than the fibrous materials. The tortuosity of the fibrous materials was found to be a function of both the aspect ratio of the fibres, and the packing efficiency of the assembly.

Keywords: Tortuosity; Numerical simulation; Fibrous particles; Void size; Permeability

1. Introduction

The permeability of porous materials is dependant upon both the amount and structure of the voids within the material. The amount of voidage can be expressed using well defined measures such as the void ratio, or solid fraction, while the 'structure' tends to be defined in more equivocal ways. Features that relate to the structure of the voidage include the size, location and connectivity of the voids. Many of these features are very difficult to characterise by simple measures.

One measure that is often used is the 'tortuosity' of the pore structure. This parameter was first introduced by Carman [1], and is defined by the ratio of the distance travelled by a fluid particle permeating through the material to the overall distance travelled in the direction of the pressure gradient. Obviously this is an important (although difficult to determine) parameter that has an influence on the permeability of a material. Of the two most widely known equations for predicting the permeability of granular materials (Ergun [2], and Kozeny-Carman [3]), only the Kozeny-Carman equation explicitly uses this measure. This would imply that the Ergun equation implicitly assumes that all granular materials have a constant tortuosity, or that the tortuosity is uniquely determined (and included in the correlation) from the void ratio, or particle size.

While the tortuosity is explicitly used in the Kozeny-Carman equation, very little guidance is given as to suitable values. From his experimental work, Carman observed that the path a fluid takes in a random packing of mono-size spherical particles is approximately at an angle of 45 degrees to the superficial flow direction. This tends to suggest that a value of $\sqrt{2}$ is acceptable for mono-size spherical assemblies. The lack of other relevant data has tended to mean that this value is used almost as a default for any granular material regardless of its morphology or size distribution. While this may be accurate enough for many granular materials, care must be taken when the equation is applied to highly irregular particles, or, as-is the focus of this paper, fibrous materials.

An approach that has previously been used to investigate the structure of the void space inside spherical particle assemblies is the use of Delaunay empty spheres [4]. A Delaunay empty sphere [5] is a sphere that is tangent to at least four particles in

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the assembly without overlapping any other particle. Remond et al. [4] investigated the tortuosity of spherical assemblies by determining all of the Delaunay empty spheres within numerically simulated packings. An algorithm was then used to link together the Delaunay empty spheres to find pathways through the assembly. These pathways were used to characterise the tortuosity of the assemblies. This approach was applied to disordered and partly ordered packings, and it was shown that the tortuosity of disordered packings was approximately 1.38 for dense random packing (64% packing efficiency).

In this paper we are focused on examining the void structure within assemblies of spherical and fibrous particles using a similar method to Remond et al. Our approach will differ in that we will use an algorithm that directly forms chains of connected empty spheres. We will begin with a short explanation of the packing algorithms we have used to form the simulated assemblies.

2. Numerical particle packing algorithm

The method that we have used to build numerical assemblies of spherical and fibrous particles has previously been detailed elsewhere [6], and so only a brief review of the method will be presented here.

2.1. Spherical particles

The simulation of random packing of spherical particles was achieved using the optimisation (minimisation) of an energy potential. The energy potential is made up of a gravitational component together with a Hertz contact strain component. The assembly is built up by the sequential addition of individual particles subject to this potential. All other particles in the assembly are frozen in space during the addition of a new particle.

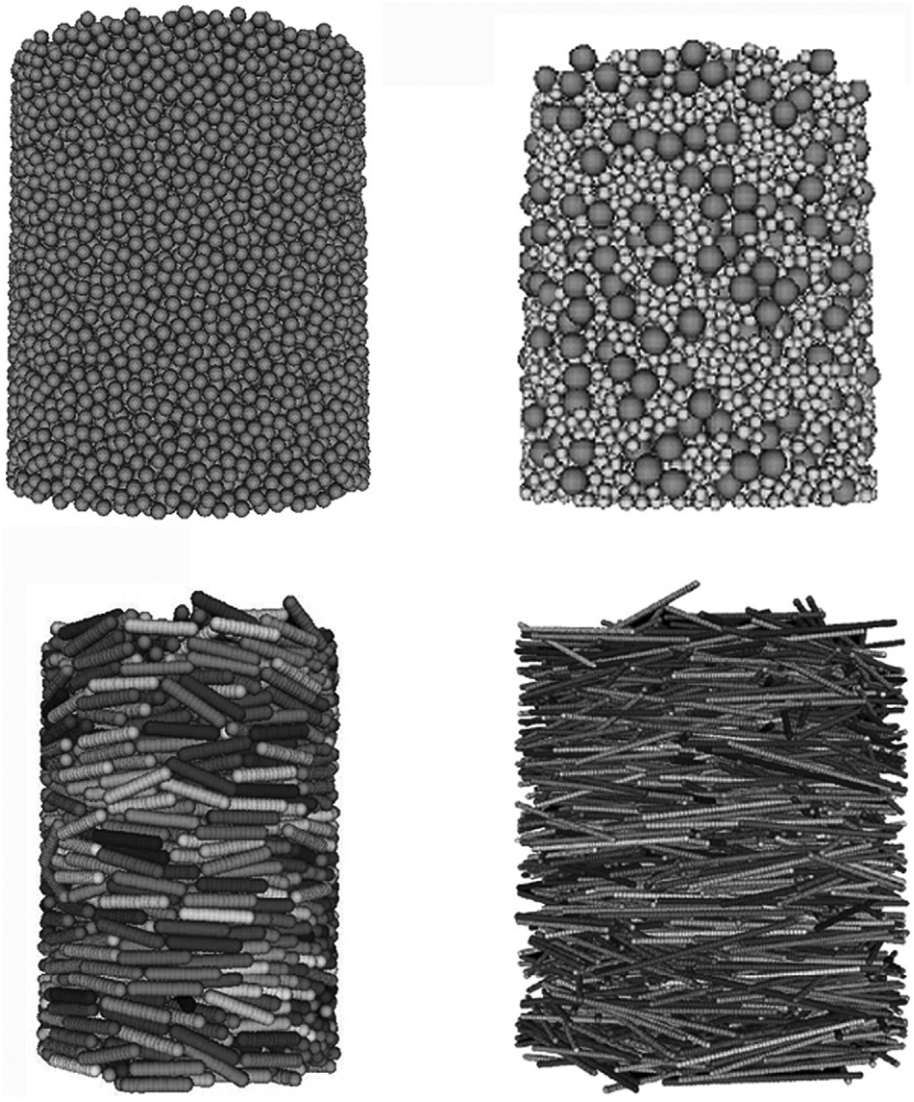

Fig. 1. Examples of the simulated packings used to investigate the void structure of spherical and fibrous materials. Clock-wise from the top-left; monosizes spherical particles, a 2:1 binary spherical system, straight fibres with an aspect ratio of 30, and straight fibres with and aspect ratio of 5.