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Powder Technology 174 (2007) 10 – 13

POWDER TECHNOLOGY

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Validation of a digital packing algorithm in predicting powder packing densities

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Abstract

DigiPac is a particle packing algorithm based on a digital approach to represent particle shape, packing space and particle movements. It is capable of packing particles of arbitrary shapes and sizes in a container of arbitrary geometry. A number of case studies have been performed to validate this digital approach, some of which are reported in this paper to show that with DigiPac shape factors used by many traditional models for predicting packing density become redundant. It also demonstrates that for polydisperse mixtures of non-spherical particles, a single size distribution measured using conventional means (e.g. light scattering) is inadequate for the purpose of predicting packing properties.

Keywords: Non-spherical; Particle packing; Powder technology

1. Introduction

Although it has long been recognised that particle shape as well as size has a strong effect on the packing characteristics of granular materials, most computer simulation models for particle packing assume a spherical shape. The effects of particle size and size distribution on the packing of particles have been extensively investigated based on the packing of spheres (e.g., [6]), but the study of shape effects is very limited and focused on identical particles with simple analytical geometries such as cylinders or disks [4], ellipsoids [10] and parallelepipeds [2].

The main reason for this is the inherent complexity of representing and handling geometries of asymmetric particles using vector based approaches. The shape of a non-spherical particle may be represented by a sphere-composite. In principle, sphere-composite method may be used for arbitrary shapes to any predefined accuracy. In practice, the immense effort required to construct arbitrary shapes using small spheres and the subsequent computational costs of the simulations have so far limited its application to only a few relatively simple shapes. Using a polygonal mesh to map over the surface of a solid object is another possible way to represent irregular shapes. This surface presentation is widely adopted in 3D computer graphics to render photo-realistic scenes and has also been used in particle packing simulations [7]. The main obstacles that prevent its widespread application are the same as for the sphere-composite approach, plus two added difficulties. One lies in collision and overlap detection, the other in the coding effort required to make the simulation program robust and efficient.

Recently, by taking a very different approach from the traditional packing algorithms, a new, digital packing algorithm, called DigiPac [5], is developed that avoids the difficulties associated with the traditional approaches, and makes it easy to pack particles of arbitrary shapes in containers of an arbitrary geometry. Even though in DigiPac, consideration of particle interactions is limited to the geometric constraints, it can be shown to be able to predict the packing characteristics of irregular shaped particles. This is the focus of this paper.

2. Methodology

In DigiPac, shapes are digitised and represented by pixels. 3D pixels are usually called voxels, but for convenience, both 2D and 3D pixels are simply referred to as pixels in this paper. After

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0032-5910/$ - see front matter © 2006 Published by Elsevier B.V.
doi:10.1016/j.powtec.2006.10.013

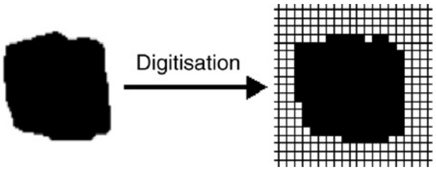

Fig. 1. Schematics of digitisation of particle shape and the packing space.

digitisation, a particle is just a coherent collection of pixels, as shown in Fig. 1. These pixels are stored and manipulated as integers or as bits. In addition, apart from the initial errors in digitisation, the digital algorithm does not suffer from rounding errors as traditional approaches can. The number of pixels to be used for a shape does not depend on the complexity of shape. Because of these features, DigiPac can handle non-spherical particles more efficiently than traditional vector-based methods. Using the pixel representation also means that the real shapes can be taken directly from the digital images of the real particles. There are 3D optical and X-ray scanners that can scan 3D objects and output the structure in digital formats.

In DigiPac, the packing space or the container is also digitised and mapped onto a grid. Thus, a container of arbitrary geometry is easily incorporated into the packing model. Since both particles and the packing space (the container) are digitised, it follows that particles must also move in discrete steps. In other words, particle movements are also digitised. As a result, collision/overlap detection becomes a simple matter of detecting whether two particles occupy the same site(s) at a given time step. The time taken to check overlaps is a linear function of the particle number and does not increase with the complexity of particle shapes. Computationally, this is an important advantage of DigiPac over traditional methods.

In the current version of DigiPac, particles move randomly, one grid cell at a time, on a square lattice. In order to encourage particles to settle, upward moves are accepted with a so-called rebounding probability. This diffusive motion helps the particles to penetrate and explore every available packing space. There are several ways to control how particles are added and how particles move and rotate in the packing space. Rotation usually, but not always, results in denser packing structure since it often increases the chance of a better fit. Particles can be introduced either from a specified point (point source) or randomly across a specified area (rain mode or hopper mode), above the container at a predefined rate. The former results in a heap, the latter fills the container more evenly. The rate of particle addition is adjustable and affects the packing density. Generally, slow addition leads to denser packing structure, and high addition rate leads to a less dense structure. Laterally, the boundaries can be either solid walls or periodical.

3. Case studies

The purpose of this paper is to demonstrate the ability of the DigiPac algorithm to predict correctly and accurately the packing density of non-spherical particles. The case studies reported here form part of the model validation exercise we have been performing over the past few years. We first report several simple yet illustrative case studies involving mono-sized non-spherical objects including tubes, polyhedrons, oblate spheroids, cylinders and spherocylinders. We then report packing results for eight industrial powders and compare them with measured packing densities. For reasons of confidentiality, identities of the powders are withheld and they will simply be referred to as PWD1 to PWD8.

3.1. Packing of plastic beads

Six simple but illustrative case studies were performed using the following three shapes: tube, 16-face-polyhedron and 32-face-polyhedron. The particles are all made of plastics and obtained from toy shops. During each experiment, particles were poured into a container without tapping. Two short cylinders and a small baby food jar were used as containers. The two cylindrical containers had a flat bottom. The number of particles and the particle-container size ratio were the same in both experiments and simulations. The real particles were not exactly identical but had small (<3%) deviations in both dimensions and shape. These differences were ignored in the simulations where each shape is replicated exactly to make up the required number.

Table 1 compares results for the simulated and physical packed beds used in the simple case studies. Some examples are also shown in Fig. 2. Since, geometrically speaking, the particles and containers used for both simulations and physical tests are, within the measurement limits, identical, comparing the heights of the packed beds is equivalent to comparing their mean packing densities. From Table 1, it is clear that the predictions are in good agreement with the measurements.

3.2. Packing of oblate spheroids

Non-spherical particles tend to pack less densely than spheres. However, experiments [3] have shown that small deviations from the perfect spherical shape (e.g., oblate and prolate spheroids) can lead to a higher packing density. This has been tested with DigiPac with oblate spheroids — M and M sweats. The results are given in Fig. 2 and Table 1.

3.3. Packing of cylinders

Packing of cylinders has been investigated by many researchers [1,8,9,11,12]. All studies showed that the packing

Table 1
Summary of packing heights of packed beds

Particles	Height of the packed bed (cm)			
	Cylindrical container		Baby food jar	
	Measured	Simulated	Measured	Simulated
Spheres			5.8	5.3
Short tubes	5.1	5.0	5.6	5.1
16-face polyhedrons	2.6	2.8	3.8	4.3
32-face polyhedrons	5.1	5.2		
M and M candies	8.5	8.8		

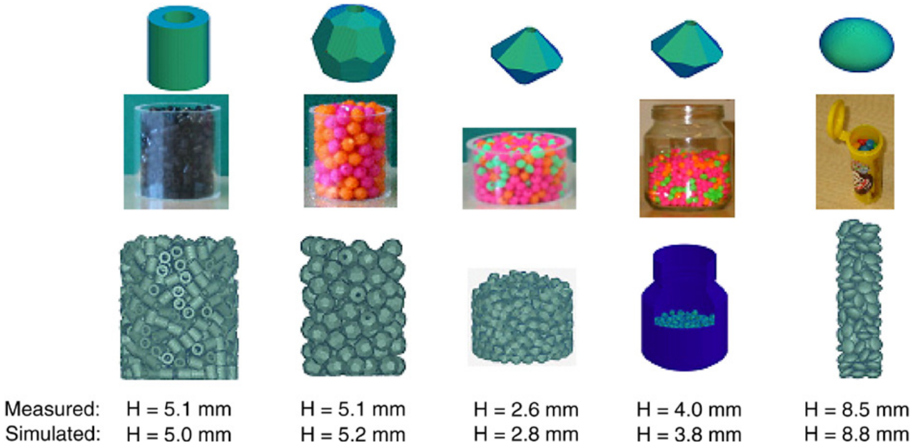

Fig. 2. Examples of actual and simulated packings of simple and mono-sized objects in containers.

density depends on the length-to-diameter aspect ratio. Fig. 3 shows the porosity as a function of the aspect ratio simulated by DigiPac. The results from other investigations are included for comparison. Predictions using different packing models are different, but the trend is essentially the same. DigiPac predictions lie well within the predicted range for all the cases investigated.

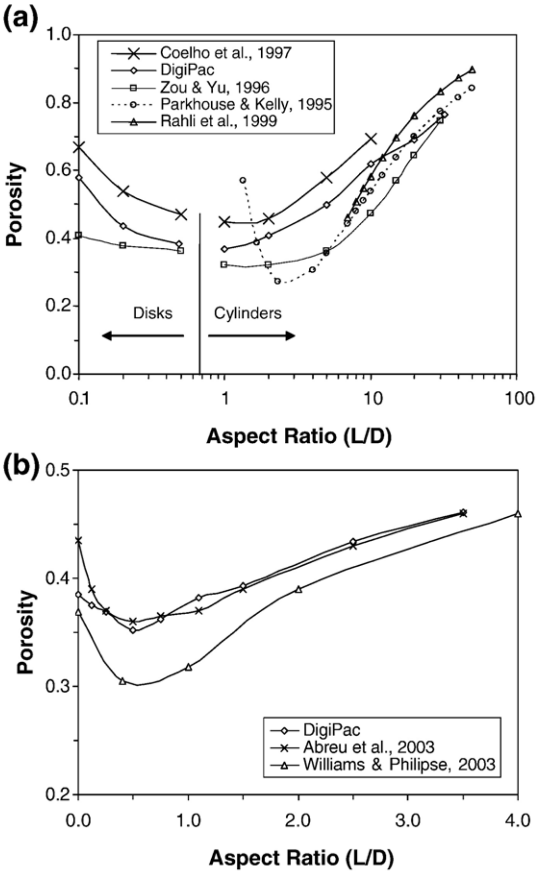

Fig. 3. Comparison of DigiPac predictions with published data for (a) cylinders and (b) spherocylinders.

3.4. Packing of powders

For the industrial powders, PWD1 to PWD8, random samples were taken and imaged using X-ray Micro Tomography (XMT). The number of individual particles sampled from each powder ranged between 59 and 175. Size distribution was deemed to be adequately represented by the sampled particles for each powder. These digital particles were replicated to make up the population used for the packing simulations. Therefore, with DigiPac approach, pre-determined size distributions and shape factors become redundant. Particles in some of these powders were porous — they were themselves agglomerates of smaller primary particles. The internal porosity of these particles was estimated by analysing XMT images of individual particles. Fig. 4 compares the bulk packing densities obtained by DigiPac simulations and measurements. It is clear that the simulated results are in good agreement with the measurements with an average error less than 6%. When the eight powders are mixed and formed a composite powder, the packing density of the mixture was 0.45 by simulation and 0.47 by measurement.

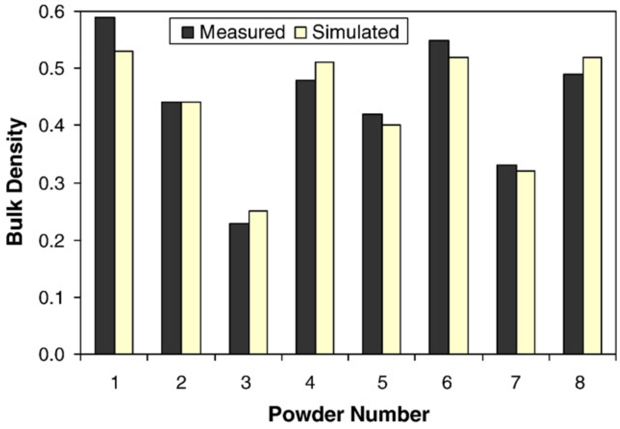

Fig. 4. Comparison of DigiPac predictions with experimental data for eight powders.

4. Conclusions

Through the case studies, it has been demonstrated that, although the present version of DigiPac is essentially a geometrical packing algorithm for non-spherical particles, it can predict the packing density of a wide range of materials from fine powders to large objects, in mono- or poly-disperse mixtures. More detailed validation is being carried out to compare, for example, particle orientation distribution, locations of particles of different sizes/shapes in a polydisperse mixture. DigiPac is also being extended to incorporate particle interactions.

Acknowledgements

M. Gan would like to acknowledge the financial support from the British Nuclear Fuels PLC.

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