

Predicting Packing Characteristics of Particles of Arbitrary Shapes[†]

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Abstract

A computer model for particle packing is of importance in both theories and applications. By taking a very different approach from existing packing algorithms, our digital packing algorithm – called DigiPac – is able to avoid many of the difficulties normally encountered by the conventional algorithms in dealing with non-spherical particles. Using the digital approach, it is easy to pack particles of arbitrary shapes and sizes into a container of any geometry. This paper briefly describes the digital packing algorithm, but the focus is on validation of the DigiPac model through several case studies involving mono-sized non-spherical particles and also powders with different size distributions. Packing densities from DigiPac simulations are compared with those measured experimentally by ourselves in some cases and in others with data published in the literature using other models. The results show a good agreement in all the cases, which enhances our confidence in DigiPac that despite being a geometrical packing algorithm with no explicit consideration of particle interactions, it is able to predict quite accurately the packing structure of particulates whose shapes are commonly encountered in both industry and everyday life.

1. Introduction

The packing of particles is of importance in both theoretical and practical terms. For example, the random packing of spheres has been used as a model to represent the structure of liquids and glassy materials; to study phenomena such as electrical conductivity, fluid flow, stress distributions and other mechanical properties in granular materials; and to investigate processes such as sedimentation, compaction and sintering [1]. Since the 1960s, computer simulation algorithms have been widely used to simulate the packing of granular materials mainly on the basis of either sequential addition or collective rearrangement. The computer-generated random packing of particles is obtained either by using a so-called packing algorithm or by adopting a dynamic simulation model. Packing algorithms usually neglect

the physical process of packing in order to provide a computationally efficient method to generate the structure. Particle dynamics models, on the other hand, are designed to simulate the process of a particulate system and, when used to simulate the packing process, produce the packing structure as a result.

It has been recognised for many years that both particle size and shape have a strong effect on the packing characteristics of granular materials. Most attempts at computer simulation assume a spherical shape, although some simulations of non-spherical particles have been reported [2-7]. The main reason for this is the inherent complexity of representing and handling geometries of asymmetric particles. The effects of particle size and size distribution on the packing of particles [1,8-13] have been extensively investigated based on the packing of spheres, and the literature is full of results in this field [11-13]. In contrast, the study of the effects of particle shapes is very limited and mostly focused on the identical particles with simple analytical geometries such as cylinders or discs [2,4], ellipsoids [3,4,14,15] and parallelepipeds [4].

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In reality, particles with irregular geometries constitute the majority of powders. In these cases, how to simulate the packing of particles with the real shape had been a challenge. Traditionally, the shape of a non-spherical particle may be represented by a sphere-composite. In principle, the 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 [16] and has also been used in particle packing simulations [17,18]. 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 [19] avoids many of 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 irregularly shaped particles. This is the focus of this paper.

Since the full details of DigiPac have been reported elsewhere [19,20], Section II only gives a brief description of the algorithm and emphasis will be on comparing and contrasting DigiPac with traditional approaches. Section III describes the case studies performed, including experimental and simulation set-ups, shape modelling and methods of calculation to obtain packing densities. Section IV presents results and comparison of DigiPac simulations with experiments and other simulation models.

2. Methodology of DigiPac

2.1 Particle representation

In DigiPac, shapes are digitised and represented by pixels (in 2D) or voxels (in 3D). A particle is just a coherent collection of pixels or voxels after the particle is digitised, as shown in **Figure 1**. These pixels (or voxels) can be stored and manipulated as integers or

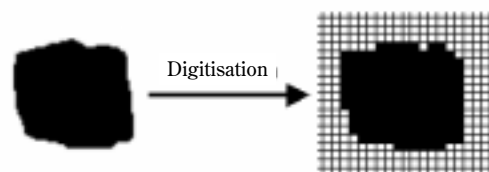


Fig. 1 Schematics in 2D showing digitisation of particle shape and the packing space.

as bits, making DigiPac quicker and potentially less storage-demanding than the traditional approaches for complex shapes. In addition, apart from the initial errors in digitisation, the digital algorithm does not suffer from rounding errors as traditional approaches do. The number of pixels or voxels to be used for a shape does not depend on the complexity of shape, which again translates to substantial savings in storage when dealing with complex shapes.

Using the pixel/voxel 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.

2.2 Digitisation of packing space and particle movements

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 DigiPac model, particles are allowed to move randomly, one grid cell at a time, on a square lattice. In 2D, there are 8 possible directions, 4 orthogonal and 4 diagonal, to choose from, all with equal probability. In 3D, the possible directions are 26, i.e. 6 orthogonal and 20 diagonal. 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.

2.3 Control parameters of simulation

In DigiPac, there are several ways to control how particles are added and how particles move in packing space. For example, during a packing process, particles are allowed to rotate in addition to translation. Rotation usually, but not always, results in a 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 affects the packing density. Generally, slow addition leads to denser packing structure, and a high addition rate leads to a less dense structure [21]. Laterally, the boundaries can be either solid walls or periodical.

3. Particle packing 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 objects of a non-spherical shape in each case. The objects used are tubes, polyhedrons, oblate spheroids (M&M candies), cylinders and spherocylinders. The packing properties for these simple case studies were obtained either from experiments carried out by ourselves or from published results by other researchers [4,6,7,22,23].

We then report packing results for nine industrial powders and compare them with measured packing densities in eight of the nine cases and with the prediction of an empirical model [25] in the last case. For reasons of confidentiality with industrial collaborators, the identities of the powders are withheld and they will simply be referred to as **PWD1** to **PWD9** in the following text.

3.1 Methods of digitising particles

There are many ways to digitise particles, of which we have used three in the present work. Particles with a regular and well-defined geometry (including sphere, tube, polyhedron, M&M candy, cylinder and spherocylinder) were generated directly in the digital format using DigiPac utility software. They are shown in **Figure 2a**.

The industrial powders PWD1 to PWD8 are used in the case studies. They are chemically pure. Therefore, given their measured bulk density by weight and their true particle density, the volume bulk packing density can easily be derived. Random samples were taken and imaged using X-ray Micro Tomography (XMT). Their shapes were obtained by stacking the XMT images. Two examples of digitised powder particles are shown in **Figure 2b**. The number of individual particles scanned and digitised using XMT ranged between 59 and 175. Size distribution was deemed to be adequately represented by the sample particles for each powder. These digital particles were multiplied to make up the population used for the packing simulations. Therefore, with the DigiPac approach, predetermined 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.

For practical reasons, particles from PWD9 were modelled rather than digitised directly. SEM images of PWD9 powder show that particles may be regarded as round in form and rough in texture. To model such particles, we used a so-called sphere-on-sphere (SOS) method. With the SOS method, a given number of small spheres are mounted and half buried on the surface of a large core sphere. An example is given in **Figure 2c**. The small spheres are primarily used to simulate surface roughness. To some extent, they also change the particle shape away from that of a perfect sphere. The use of small spheres has the effect of increasing the distance between the centres of adjacent particles as well as increasing inter-particle frictions. In essence, the SOS method is similar to the random sphere construction (RSC) method used by Smith and Midha [26] to model the iron powder particles produced by water atomization. Although both SOS and sphere-composite methods use small spheres to make up a non-spherical particle, a crucial difference is that in SOS, spheres can overlap whereas in the sphere-composites used for DEM simulations [5,27], they are not allowed to overlap.

Size distribution for PWD9 was extracted from SEM images. In addition, eight variations from the original distribution were used in the simulations in order to assess if and how the bulk density may be enhanced by varying the size distribution. These distributions are shown in **Figure 3**. Results from DigiPac simulations were compared with those from a so-called linear packing model (LPM) developed elsewhere [25].

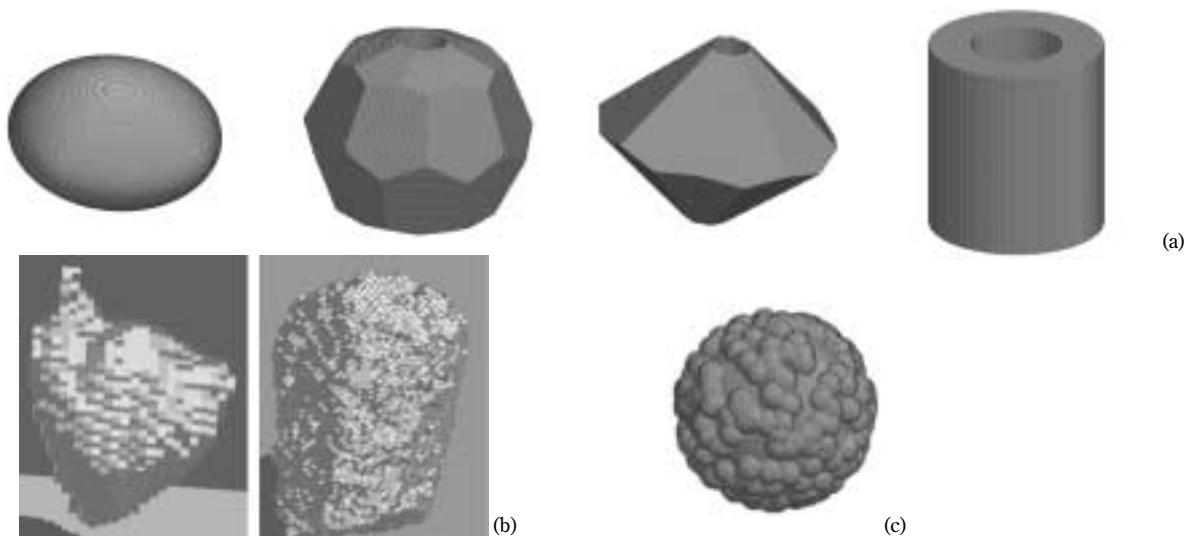


Fig. 2 Examples of digitised shapes used in the case studies. (a) Computer-generated replica of everyday objects. (b) XMT digitised shapes. (c) Shape generated using the SOS method.

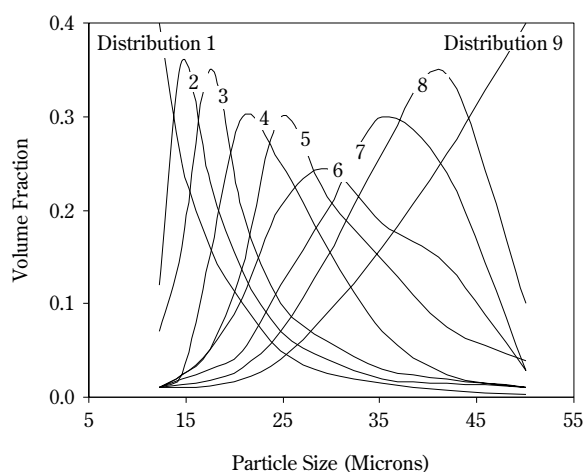


Fig. 3 Particle size distribution of PWD9 (No. 6) and its eight variations.

LPM is a semi-empirical model for estimating the packing density of multi-component mixtures, requiring only experimental data for the packing of mono-sized particles and binary mixtures to determine the model parameters used. To use LPM, the initial packing density of each component was set to 0.523. This was based on the mean value simulated in the packing of mono-sized surface-roughed spheres. The particle diameters are set equal to the equivalent volume diameters. It is noted that these equivalent volume diameters are conceptually different from the equiva-

lent packing diameters used in LPM, and they may differ in value as well.

3.3 Method of calculating bulk packing density in DigiPac

Volume packing density is one of the most important and commonly measured structural properties of a packing. It is defined and calculated as the ratio of the volume of the solids to the total volume of the packed space. Where bulk density is to be calculated, a cubic simulation box was used as the container with periodic boundary conditions in the lateral (X and Y) directions. The regions affected by solid walls and free surfaces are excluded, and the bulk density is estimated using the central part of the density distribution profile along the vertical (Z) direction, as shown in **Figure 4**.

3.4 Details of packing experiments and simulations

Seven simple but illustrative case studies were performed using the following shapes: tube, 16-face-polyhedron, 32-face-polyhedron and oblate spheroid (M&M candy). Except for the M&M candies, the particles are all made of plastics and obtained from toy shops. During each experiment, particles were poured into a container. Two short cylinders and a small baby food jar were used as containers. The two cylindrical containers had a flat bottom. The bottom of the baby food jar is domed. Dimensions of the particles and container are summarised in **Table 1**.

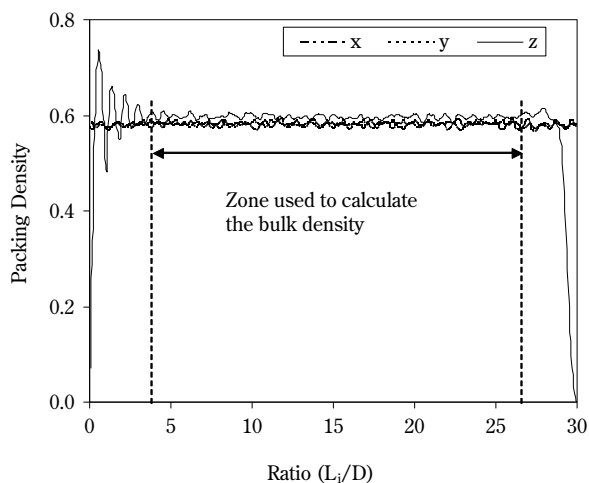


Fig. 4 Packing density profiles along X, Y and Z directions in a cubic simulation box with periodical boundary conditions in the lateral (X and Y) directions. The bulk density is calculated by taking the average over the central part in the profiles to avoid wall effect and the influence of free surface. L_i is the dimension of the simulation box along direction i and D the average particle diameter.

The simulation conditions were set to match the experimental set-up as much as possible. For instance, 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 dimension and shape. These differences were ignored in the simulations where each shape is replicated exactly to make up the required number.

To encourage particles to find a better fit, they were allowed to rotate randomly during the packing. The rebounding probability was set to a value between 0.2 and 0.5. The number of particles used ranged from 5000 to 15000. The length-to-diameter aspect ratio of the cylinders varied from 0.1 to 30, and covers the range considered by Coelho et al. [4]. The spherocylinder particles had the same volume in all the

cases but their aspect ratio changed between 0.125 and 3.5, which is in line with the work of Abreu et al. [7]. The geometry of these particles is given in **Table 2**. **Table 3** summarises the conditions used for DigiPac simulations.

Table 1 Geometric parameters of objects and containers and number of particles used

Particle	Particle size (mm)	Number of particles
Sphere	$d=6$	660 (in C4)
Short tube	$d_{out}=4.6, d_{in}=2.4, h=5.1$	534 (in C1)
		721 (in C4)
32-face polyhedron [†]	$d=8.2, d_{hole}=2.0$	176 (in C1)
16-face polyhedron [*]	$d=4.1, d_{hole}=1.5$	546 (in C2)
		1113 (in C4)
M&M candy	$d_1=d_2=9.3, d_3=4.8$	126 (in C3)
Cylindrical container 1 (C1)	$D=44.8, h=50.9$	
Cylindrical container 2 (C2)	$D=44.8, h=25.7$	
M&M candy container (C3)	$D=27.5, h=97.1$	
Baby food jar (C4)	$D_{in}=5.8, h=6.8$	

Table 2 Geometric parameters of the spherocylinders

Diameter (D)	Length (L)	Aspect Ratio (r)
19	2	0.125
18	4	0.250
17	8	0.500
16	12	0.750
14	16	1.100
14	20	1.500
12	30	2.500
11	38	3.500

NB: L is the length of the cylindrical part, i.e. excluding the hemispherical ends.

Table 3 Summary of simulation conditions for cylinders, spherocylinders and powders

Parameter	Study case			
	Cylinder	Spherocylinder	PWD1 - PWD8	PWD9
Simulation box size	500×500×600	400×400×400 to 700×700×700	200×200×200	600×600×600
Number of particles	5000-8000	5000-13000	5900-17500	10000-100000
Number of components	1	1	59-175	9
Rebounding probability	0.3-0.5	0.3-0.6	0.1	0.2
Particle rotation	Yes	Yes	Yes	No

4. Results and discussion

The packing densities of mono-sized non-spherical particles and of mixtures of polydisperse particles are reported in this section. The scale and other settings used for DigiPac simulations are selected to give very good reproducibility of the results. For example, under the same conditions but changing the random number sequences, 12 simulations were performed, and the standard deviation was 0.001 and the maximum difference in density was 0.004. When DigiPac is applied to sphere packing, the packing density of 0.615 is obtained. This value is consistent with the experimental observation ($\rho=0.61$) carried out by Oweberg et al. [29], but lower than 0.637 – an accepted value for random dense packing [30]. This difference may be attributed to different packing methods and material properties.

4.1 Packing of aspherical particles with defined geometries

Table 4 compares results for the simulated and physical packed beds used in the simple case studies involving spheres, short tubes, 16-face polyhedrons, 32-face polyhedrons and M&M candies. 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. The former is much easier to do than the latter, and, more importantly, it avoids more calculations which may introduce extra errors. Therefore, the packing height rather than density was used for comparisons. From **Table 4**, it is clear that the predictions are in good agreement with the measurements.

Table 4 Comparison of the measured and simulated packing heights of packed beds

Particles	Height of the packed bed (cm)			
	Cylinder container		Jar container	
	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&M candies	8.5	8.8		

4.2 Packing of cylinders

The packing of cylinders was investigated by many authors [2,4,22-24,32,33]. All studies showed that the packing density depends only upon the aspect ratio r (length-to-diameter). Although the mechanism of cylinder packing is not yet fully understood, some empirical equations have been formulated under certain conditions.

Zou and Yu [22] proposed an empirical equation (referred to as ZY model) to quantify the relationship between the porosity and sphericity of cylindrical particles in dense random packing, based on the experiments of wood cylinder packing. For cylinders ($r>1$), the equation of dense packing reads:

$$\ln \varepsilon_{0d,cyl} = \psi^{6.74} \exp[8.00(1-\psi)] \ln 0.36 \quad (1)$$

and for discs ($r<1$):

$$\ln \varepsilon_{0d,Disk} = \psi^{0.63} \exp[0.64(1-\psi)] \ln 0.36 \quad (2)$$

The sphericity ψ is defined as the ratio of the surface area of a sphere having the same volume as the particle to the actual surface area of the particle [34]. By this definition, the sphericity of a cylinder is related to the aspect ratio by:

$$\psi = 2.621 - \frac{r^{\frac{2}{3}}}{1+2r} \quad (3)$$

Rahli et al [23] also proposed an empirical equation (referred to as RTB model), based on the excluded volume model elaborated by Onsager [35], as:

$$\varepsilon = 1 - \frac{11}{2r+6+\frac{\pi}{2r}} \quad (4)$$

Parkhouse and Kelly [36], based on the statistical approach to the distribution of the pores in the stacks, gave the following equation about the relationship between the porosity and the aspect ratio ($r>7$) of a cylinder (called PK model here):

$$\varepsilon \approx 1 - 2 \frac{\ln(r)}{r} \quad (5)$$

Figure 5 shows the porosity as a function of the aspect ratio r simulated by DigiPac. The results of other investigations [4,22,23,36] are included for comparison. It is clear that the porosity increases with the increase of the aspect ratio r . The porosities simulated by DigiPac are lower than those obtained by using the sequential deposition algorithm (RSA) carried out by Coelho et al. [4], but higher than those obtained by the empirical equations (1) to (5). The differences

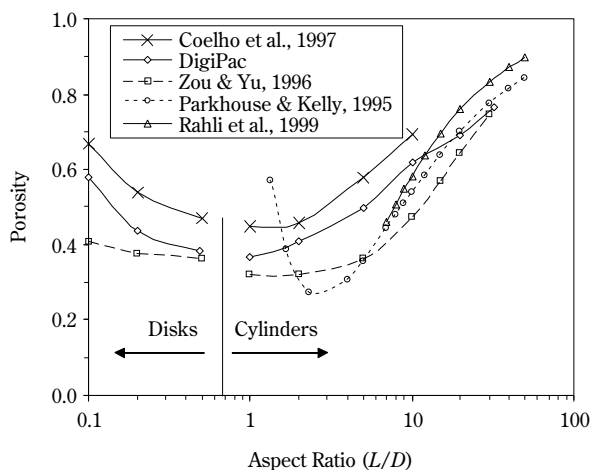


Fig. 5 Porosity versus aspect ratio for the packing of cylinders.

can also be observed in the ϵ - r curves investigated by different authors or methods, as can be seen in the curves from the work of Zou and Yu (ZY Model), Rahli et al. (RTB model), Parkhouse and Kelly (PK model) in Fig. 5. Especially, big differences can be observed when $r < 5$. This indicates that there is no universal model for a wider range of cylinders. The data also imply that particle packing is a complicated process and involves many factors such as packing methods and conditions and particle properties. For example, Evans and Ferrar [2] observed that a small degree of out-of-plane randomness enhances packing compared with both in-plane and 3D random orientation distribution.

One of the important factors in the simulation of particle packing is how quickly particles are introduced to the system, i.e., the particle addition rate. It is known [14,21] that the slower the rate, the higher the packing density. The particle addition rate could therefore be one of the reasons for the porosity differences in our Digipac simulations and the empirical estimations. In the present simulations, it has not been observed that the packing density of dense random packing of cylinders with a certain value of aspect ratio r is higher than that of spheres; but this feature has been reported in the literature [22,23]. This phenomenon needs further investigation to understand the mechanism. However, we observed it in the packing of spherocylinders described in the next section.

4.3 Packing of spherocylinders

Compared with cylinders, the packing of spherocylinders

is less investigated. Part of the reason for that is that spherocylinders are less common in reality. However, the study of spherocylinders can provide unique information for characterisation of the particle shape with packing density of the non-spherical particles [37-39].

Figure 6 plots the relationship between the porosity and aspect ratio of the spherocylinders. Again for the purpose of comparison, the simulated results, investigated by Abreu et al [7] and Williams and Philipse [6], are also given in Fig. 6. The porosity simulated by DigiPac is consistent with the results given by Abreu et al. [7] for a vibration amplitude of 2.0×10^{-3} m (twice the sphere diameter); but higher than the values given by Williams and Philipse [6]. Generally speaking, the porosity decreases and then increases with increasing aspect ratio. Similar trends have also been observed by Sherwood [3] and Donev et al [40] for ellipsoids, as well as by Aoki and Suzuki [32] and Zou and Yu [22] for cylinders. It shows that a small deviation in shape from that of a perfect sphere can lead to more efficient packing. Direct application of this result is in the field of powder storage and transportation. As noted by Donev et al [40], this has potential applications for a broad range of scientific disciplines such as ceramics, glass formation, etc.

When the aspect ratio $r=0.5$, the porosity is at its minimum. This aspect ratio is the same as that given by Abreu et al [7]. It is close to the value ($r=0.4$) given by Williams and Philipse [6]. For sphere packing, the porosity in Abreu's simulation is 0.425, higher than the 0.388 simulated by DigiPac. However, the differences in porosity among different approaches decrease with increasing r for $r > 2$. The reason is not

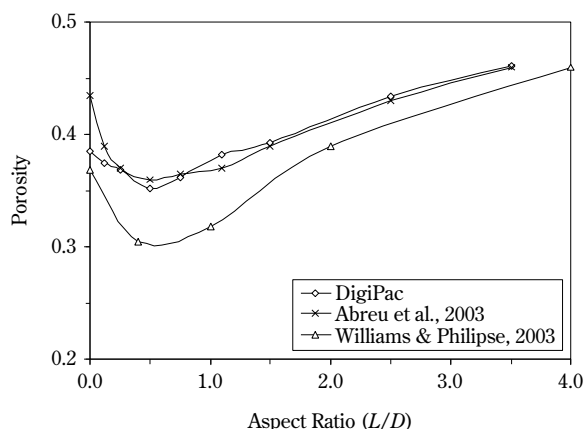


Fig. 6 Porosity versus aspect ratio for the packing of spherocylinders.

clear at the present and needs further investigation.

4.4 Packing of Powders

4.4.1 Experimental validation

Figure 7 compares the bulk packing densities of eight powders obtained by DigiPac simulations and measurements. It is clear that the simulated results are in good agreement with the measurements with an average error of less than 6%. When the eight powders were mixed and formed a composite powder, the packing density of the composite was 0.45 by simulation and 0.47 by measurement. These results directly demonstrate that DigiPac can predict very accurately the packing density of polydispersed non-spherical mixtures with real shapes encountered in industry.

As shown above, DigiPac is especially valuable for solving the packing problems of irregularly shaped particles. Conventionally, to investigate the packing of irregularly shaped particles, the characteristics of particle shape, angularity, etc. must be quantified first [41]. This is a tedious job and there is no universal method to quantify these parameters for real, complex-shaped particles. Obviously, one of the advantages of DigiPac over the conventional approaches is that no shape factors are required. This avoids the difficulty in the analysis of the complex shape of non-spherical particles. This is very useful for the particle systems in which particle shapes are difficult to quantify.

4.4.2 Validation by comparing with model predictions

As noted by Yu et al [25], their linear packing model (LPM) developed for spherical particles may

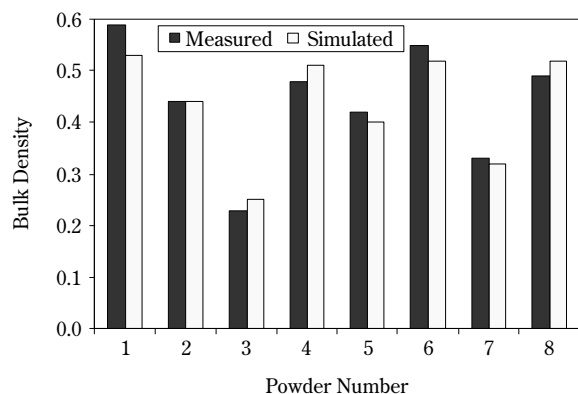


Fig. 7 Comparison of measured and simulated packing densities for PWD1 to PWD8.

be applied to mixtures of non-spherical particles if the particle shapes are not too different from spherical. The LPM was used to calculate the packing density of the powders, because it was successfully used to predict the packing density of irregular particles based on the concepts of equivalent packing size and initial porosity of mono-sized irregular particles [42]. Although there are a few packing models to predict the packing density of spheres [9,43,44], they cannot be used for the present system.

Figure 8 gives the packing densities of different distributions of the powder obtained by both DigiPac and LPM. Although simplifications were made to permit use of DigiPac and LPM, the bulk densities obtained by the two approaches are generally quite close. It was observed that the variation of packing density of the investigated size distributions is small, because of the narrow size range (10 to 50 microns). The results in Section 4.4.1 and this section clearly demonstrate that DigiPac can very accurately predict the packing density of powders with the real size distributions and shapes. This conclusion was also supported by the work of Gopinahan [45].

Whilst DigiPac can predict directly the packing density of a multi-component mixture, LPM needs as input the packing density of each individual component and of each binary mixture of the components under different compositions to determine the empirical constants used in the model before it can be used to predict the packing density of a multi-component mixture. On the other hand, since LPM is basically an analytical formula with empirical constants to be determined, once established, it can be used to quickly and easily predict the packing density for all

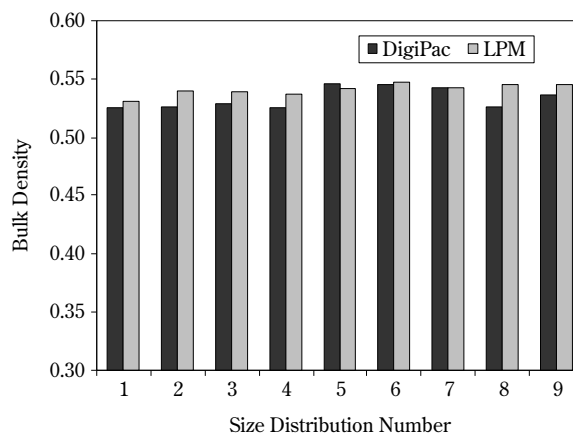


Fig. 8 Comparison of bulk packing densities obtained using DigiPac and LPM for PWD9 with nine different size distributions.

possible compositions involving the same components; whereas each run of DigiPac simulation only gives the packing density for a particular composition it is set up to simulate. Generally speaking, to use LPM for non-spherical particles, the equivalent packing size and initial packing density of each component [25,42] must be obtained first. These parameters are usually obtained from the experiments. It is tedious and time-consuming to determine these parameters experimentally. In DigiPac, the difficult part is digitisation of irregular shapes. Fortunately, with the help of a 3D optical scanner or X-ray tomography, 3D images of real particles are easily obtained. It is expected that DigiPac will become an attractive method for a number of applications [46].

Since the interactions of particles are limited to geometric constraints, the limitations of DigiPac are obvious in the present version. Therefore, further work should be carried out by integrating other interactions into the algorithm. However, as demonstrated above, DigiPac gives accurate predictions for the packing of not only mono-sized nonspherical particles but also of nonspherical mixtures with polydispersed sizes. The potential application of DigiPac may be found in ceramics, powder storage and transportation, multiphase flow, etc.

5. Conclusions

Through the case studies, DigiPac, a newly developed packing algorithm based on digitisation technology, has been validated by using non-spherical particles of uniform sizes and powders of different size distributions. Although the particles with well-defined geometries are used in simulations of mono-sized particle packing, the results are illustrative for the purpose of validation. The porosity obtained is consistent with the measurements and other model predictions.

Our simulation results indicate that the maximum packing density may also be obtained under the condition of minor particle shape deviations from that of a sphere, which is in line with the results reported recently by a number of investigators. The results have implications for a wide range of applications of scientific disciplines.

The DigiPac-simulated results of the packings of industrial powders with size distributions are in good agreement with the measurements; using DigiPac, the simulated packing density is also well comparable to the prediction from the accepted packing model – the linear packing model. These results give direct

evidence to confirm the validity of DigiPac in solving particle packing problems encountered in industry.

The case studies demonstrate that DigiPac is readily applicable in the packing of both mono-sized non-spherical particles and multi-component non-spherical mixtures. Such a successful packing algorithm provides a powerful means to solve various packing problems in a range of applications.

More work needs to be done to extend DigiPac to solve more complicated systems, such as particles where cohesive forces are involved.

Acknowledgement

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Nomenclature

D or d	Diameter of spherical particle	(m)
r	Ratio of length to the diameter in cylinder and spherocylinder	(–)
Ψ	Particle sphericity	(–)
Φ	Cylinder diameter	(m)
ϵ	Porosity of a packed bed	(–)
ρ	Packing density in a packed bed	(–)

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