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SIMULATION OF RANDOM PACKING OF SPHERICAL PARTICLES WITH DIFFERENT SIZE DISTRIBUTIONS

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ABSTRACT

A numerical model for a loose packing process of spherical particles is presented. The simulation model starts with randomly choosing a sphere according to a pre-generated continuous particle-size distribution, and then dropping the sphere into a dimension-specified box, and obtaining its final position by using dropping and rolling rules which are derived from similar physical process of spheres dropping in the gravitational field to minimize its gravity potential. Effects of three different particle-size distributions on the packing structure were investigated. Analysis on the physical background of the powder-based manufacturing process is additionally applied to produce optimal packing parameters of bimodal and Gaussian distributions to improve the quality of the fabricated parts. The results showed that higher packing density can be obtained using bimodal size distribution with particle-size ratio from 1.5 to 2.0 and the mixture composition around n_2:n_1=6:4. For particle size with a Gaussian distribution, the particle radii should be limited in a narrow range around 0.67 to 1.5.

INTRODUCTION

Random packing of spheres is very useful for many applications in physical, chemical and engineering areas. The problem may be stated as follows: given spheres with radii distributed according to a prescribed probability density, and given that they are packed together by some rules to be specified, what is the nature of the resultant heap [1]? In the studies of concentrated colloids, amorphous solids and glasses, simple liquids and granular matter, it is used to investigate the microstructure of these physical systems [2-5]. A common technique in the chemical industry for obtaining extended solid-fluid interfacial areas or good fluid mixing is to pass the fluid through a bed of solid particles, such systems as catalytic reactors, packed filters [6], and the designs of these units are based upon the characteristics of those spheres packing systems. In addition, knowledge on random packing of spheres will help on further understanding heat transfer phenomena and fluid flow in powder-based manufacturing processes, such as the Selective Laser Sintering (SLS).

SLS is an emerging technology that can fabricate structurally-sound parts from powdered material using a directed laser beam [7]. It is a very useful rapid manufacturing technique because it allows for the manufacture of complex parts often unobtainable by more common manufacturing processes [8, 9]. One obstacle of SLS process is the balling phenomenon, in which melted powder grains stick to each other via surface tension forces, thereby forming a series of spheres with diameters approximately equal to the diameter of the laser beam [8, 10]. One way to overcome the balling phenomenon in SLS is to use a powder bed consisting of two different types of metal powders, one with a significantly higher melting point than the other as suggested by Bunnell [11] and Manzur et al. [12]. In addition to the physical properties of two types of metal powders, the structure of the powder bed which is composed by mixtures of two different particles is also crucial to the SLS process. Thus, it is necessary to study more details by using a packing model with binary size distribution, and this would help on improvements of the quality of the SLS products. As described in Ref [13], particles with uniform size distribution are impossible to be manufactured based on the current technologies, and Gaussian-like particle size distribution is suggested to the modeling works with commercial powders. Therefore, this paper also studies the structure of packing by using Gaussian particle size distribution. As a benchmark, the equal size sphere packing is investigated to verify the present model and determine the geometrical dimensions of the packing vessel.

Experimental investigations [14-15] and numerical simulations [1, 16-19] on random spheres packing have been intensively carried out by previous researches. Experimental work has identified some important variables, and it is well known that the mean packing density depends strongly the methods of packing, and the maximum for truly random experimental packing appears to be 0.6366 [14, 15]. However, the experimental results could not offer much insight into the details of the packing process, and thus it is necessary to use numerical simulation to assist these studies. There are various sphere packing algorithms, and two primary ideas are employed in these methods. For the first kind, the algorithm starts with a very dense configuration of large spheres which can even overlap [16-18]. It then moves the spheres in order to reduce the degree of overlapping. Dense packing structures were obtained by this method, which can result in packing density approach to or even be greater than the experimental results. The second algorithm simulates the successive packing of a container with spheres dropping in the gravitational field [1, 19, 20]. A sphere with three contacts with other packed spheres is considered to be in its final position if it is stable. This method describes the actual process of packing generation in experiments without considering interacted forces among particles and vibration as well; it yields loose packing with the density around 0.58 in the case of equal spheres.

With systems of hard spheres of equal or different sizes, there have been many theoretical studies of random spheres packing as mentioned above. Most studies have been concerned with maximizing the packing density. Jodrey and Tory [17] successfully simulated the equal spheres packing with density of 0.6366 which is the maximum value of experimental result. They then improved the algorithm and obtained packing density between 0.642 and 0.649 [18]. By using Force-Biased algorithm, Moscinski *et al.* [16] obtained the density up to 0.67. Recently, high packing density of binary spheres mixtures has been obtained by Kristiansen *et al.* [21] with mechanical contraction.

In this paper, three different particle-size distributions are employed to study their influence on the packing structure. Based on the authors' research interests, the study on packing structure focuses on its effects on the powder-based manufacturing process. Optimal packing parameters of bimodal and Gaussian distributions will be recommended to improve the quality of the fabricated parts.

COMPUTATIONAL METHOD

Before getting into discussions on packing structures with different particle-size distributions, the packing density and the coordination number, which determine the packing structures macroscopically and microscopically, should be defined. The packing density is defined as the volume of solids divided by the total volume of the arrangement (solids and voids), which means that total volume of spheres divides the volume of box taken by these spheres for our cases [22]. The coordination number is the number of spheres in contact with any given spheres. The average coordination number, which is defined as the summation of the coordination number of each sphere divides the number of spheres, is usually used to investigate the packing structures. Obviously, for higher sintering quality, higher packing density and larger average coordination number are desirable. Mechanical vibration is used to increase the packing density in experiments, but the coordination number is hard to obtain since it is not easy to record the contacting points for each sphere in such experiments. For numerical models, it is difficult to simulate the similar vibration process, but it is simple to make statistics to get the coordination number of each packing structure.

The computer simulation starts with randomly choosing a sphere according to a pre-generated continuous particle-size distribution, and then dropping the sphere into a dimension-specified box, and obtaining its final position by using dropping and rolling rules which are derived from similar physical process of spheres dropping in the gravitational field to minimize its gravity potential. Initially, the sphere is given a coordinate of (x, y, z), where (x, y) is chosen randomly and z is well above the top of the defined box. Each sphere moves along a linear trajectory (constant (x, y), decreasing z) until its surface contacts the floor of the box or another deposited sphere. If it contacts with the floor, its final position will be determined. If not, the rolling rules will be employed, and it then rolls down in a vertical plane on its contacting sphere until it is in contact with another sphere. So far, the generated sphere has already hit two deposited spheres, but it is in an unstable position, where its gravity potential can be reduced further. Thus, the generated sphere will roll downwards in contact with the hit two spheres until it hits the third one. In this case, a stable status will be examined to ensure that the generated sphere is in its stable position (with possible minimum gravity potential). If the sphere is stable, the final position of the sphere is determined and the model will turn to generate a new sphere. Otherwise, it rolls on the double contact that goes down most steeply or a sphere on which there is a most unstable position. During the above mentioned procedure, anytime the sphere contacts the floor, it stops. The program flow chart is shown by Fig. 1. In addition, an appropriate boundary of the box should be considered to eliminate the wall effects (smooth walls induce partial ordering [20]) during packing. Tory *et al.* [19] used rough constraining surfaces to eliminate the wall effects; however, they also suggested a better method which used periodic boundaries in their later research [20]. In the present paper, periodic boundaries are used to solve the problem of wall effects. By using these boundaries, any sphere that leaves the box through one of its four surrounding vertical walls or corners will immediately reenters the opposite wall or corner.

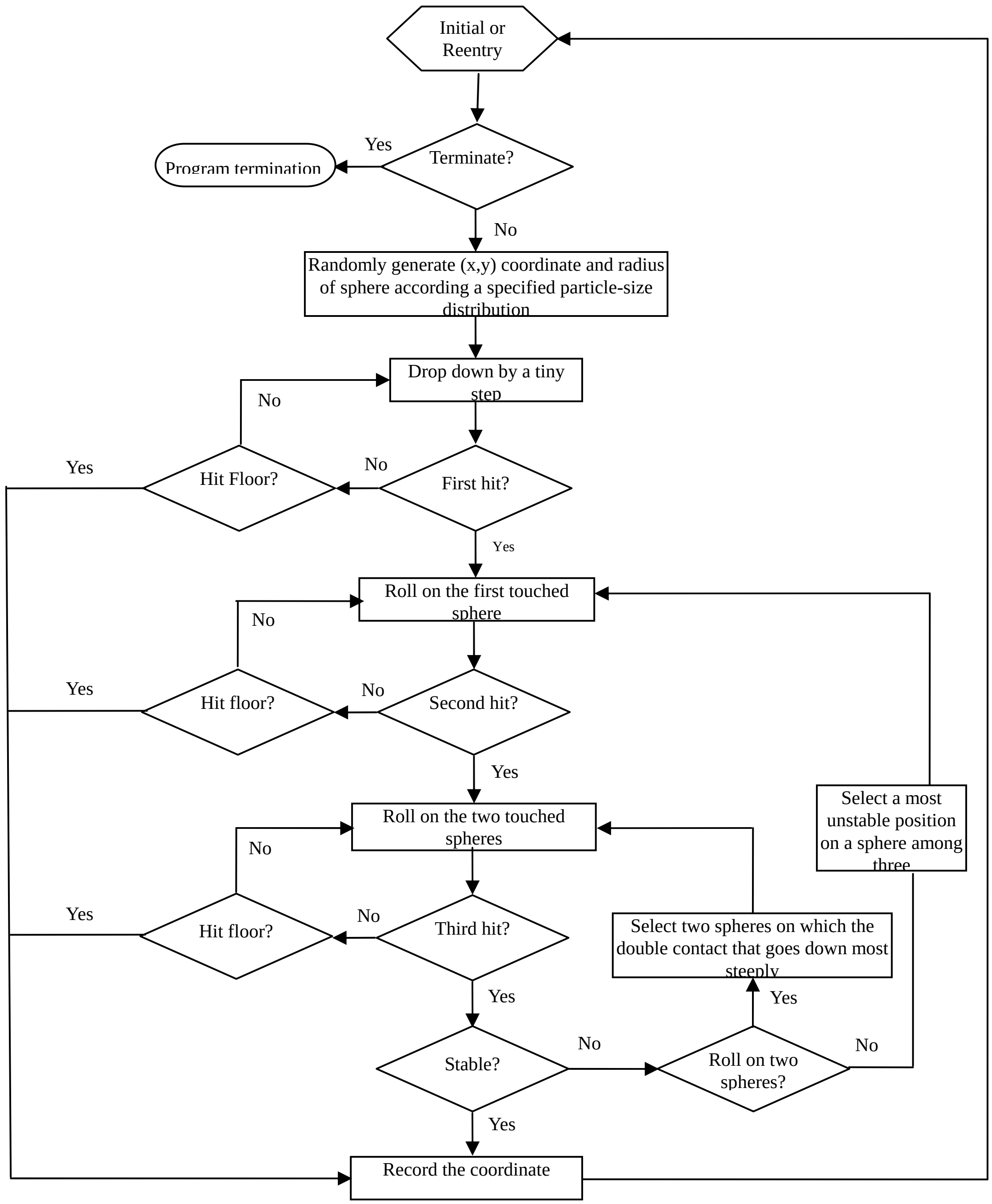

Figure 1 Program flow chart

RESULTS AND DISCUSSIONS

Equal Size distribution

For selective laser sintering, even though the equal size metal powders are impossible in a manufacturing process, it is still interesting to study the packing problem with monosize particles because it is helpful to verify the present model. It can also be used to determine the dimensions of packing volume, which can eliminate the effect of packing volume on packing structure in simulation. The radius of particle is set as the unit of the dimension, and thus all radii discussed in the present paper are dimensionless parameters, which are referred by the dimension size of the packing vessel. Five different size packing volumes are studied for monosize packing, and the packing density and coordination number are shown by Table 1 and 2, respectively.

Table 1 Packing density for monosize packing

Length Width / Height	20×20	25×25	30×30	35×35	40×40
10	0.565	0.570	0.569	0.570	0.567
15	0.569	0.574	0.571	0.573	0.572
20	0.573	0.575	0.574	0.576	0.575
25	0.574	0.576	0.575	0.576	0.576
30	0.576	0.578	0.575	0.578	0.577
35	0.576	0.578	0.577(0.0007)	0.578	0.578
40	0.576	0.578	0.577	0.578	0.579

Table 2 Coordination number for monosize packing

Length Width / Height	20×20	25×25	30×30	35×35	40×40
10	5.90	5.92	5.92	5.89	5.89
15	5.92	5.94	5.95	5.92	5.93
20	5.94	5.96	5.96	5.94	5.94
25	5.95	5.97	5.96	5.95	5.96
30	5.96	5.97	5.97	5.96	5.96
35	5.97	5.98	5.97(0.01)	5.97	5.97
40	5.97	5.98	5.98	5.97	5.97

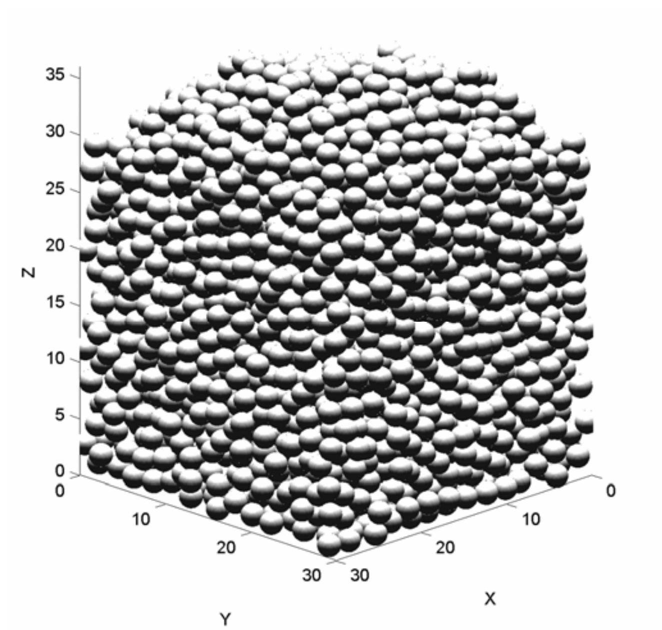

Figure 2 Packing with equal size distribution

As can be seen from these two tables, the packing density and coordination number increase with the increasing height at a given volume. When the height reaches to 30 or higher, these two parameters become independent from the height. At the same height, with the increasing bottom area of the packing volume, denser packing and larger coordination number are obtained before the packing volume reaches the value of 30×30×35. After this, these two parameters also turn to relatively stable. The stable packing density is 0.578, and the coordination number is 5.97, which are close to the reported value of 0.58 and 6.0 in Ref. [19]. In order to see the effects of random functions on the results, the program is run five times to obtain packing structures under the same volume of 30×30×35. It can be seen that the deviations are 0.0007 and 0.01 for the packing density and the coordination number; this means that randomicity of the program has little effect on the final results as long as the packing volume is large enough. The volume of 30×30×35 is utilized for the rest cases of the bimodal distribution and Gaussian distribution. The three dimensional packing structure for monosize packing is shown by Fig. 2.

Bimodal distribution

The balling phenomenon in SLS is a serious obstacle that results in low quality parts. One way to overcome the balling phenomenon in SLS is to use a powder bed consisting of two different types of metal powders. Besides physical properties of two types of metal powders, the structure of the powder bed that is composed by mixtures of two different types of particles is crucial to the SLS process. For a certain kind of metal powders, if their radii are within a very narrow range, it is reasonable to assume equal size distribution for these powders. Therefore, for a mixture of two kinds of metal powders, one can assume bimodal distribution for their packing, which means that there are two radius values for packing particles. Obviously, the ratio of two different radius values and the mixture compositions are significant to the packing structure with bimodal distribution. Fig. 3 shows the three dimensional packing structure with bimodal distribution. Tables 3 and 4 show the results of spheres packing with bimodal distributions under different particle-size ratios and different mixture compositions.

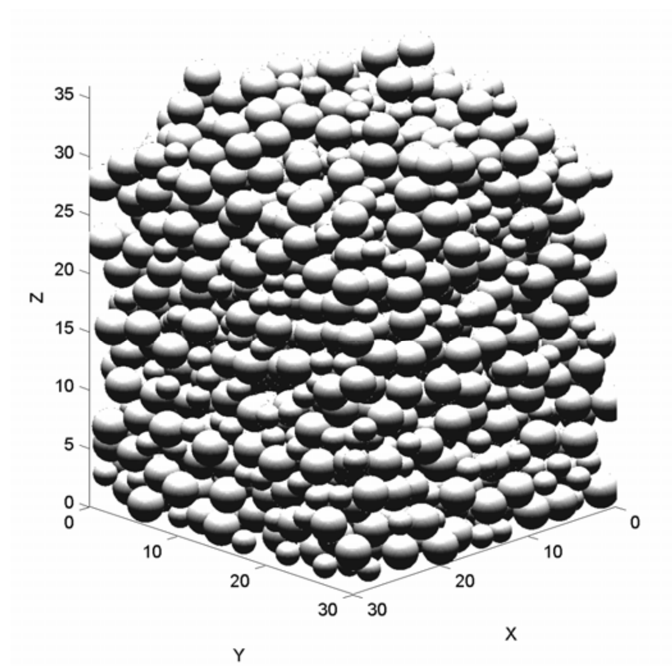

Figure 3 Packing with bimodal distribution

Table 3 Packing density of packing with bimodal distribution

	n_2/n_1=2:8	4:6	5:5	6:4	8:2
d_2/d_1=1.1	0.578	0.579	0.578	0.579	0.578
1.5	0.585	0.584	0.586	0.582	0.577
2.0	0.600	0.595	0.594	0.587	0.581
3.0	0.625	0.597	0.596	0.585	0.578

Table 4 Coordination number of packing with bimodal distribution

	n_2/n_1=2:8	4:6	5:5	6:4	8:2
d_2/d_1=1.1	5.947	5.934	5.940	5.948	5.940
1.5	5.925	5.890	5.911	5.923	5.903
2.0	5.904	5.846	5.824	5.872	5.830
3.0	5.781	5.626	5.611	5.683	5.579

It can be seen from Table 3 that with larger particle-size ratio, the packing density is higher. It can reach 0.625 in the case of that the big particle is three times larger than the small one since that small particles can fill with the voids among big ones. However, the coordination number of packing at this ratio is reduced significantly as shown in Table 4. Even though the large particles have higher coordination numbers considering many small particles around them, they also prevent adjacent small particles from contacting with more particles, and thus the coordination numbers of small particles are small, which results in a small average coordination number. For SLS process, higher packing density is desirable, but low coordination number will lead to loose contacts of particles during sintering, which causes lower strength of the fabricated parts. The effects of the mixture compositions on packing structures can also be observed from Table 3 and Table 4. For the cases of large particle-size ratios (2.0 and 3.0), more small particles in the mixture result in larger packing density and coordination number. For small particle-size ratios (1.1 and 1.5), the effects of the mixture compositions on packing density are not obvious. But the coordination numbers at the cases of n_2:n_1=6:4 are relative large, which can benefit the SLS process. Considering the trade-off between the effects of the particle-size ratio and mixture composition on the packing density and coordination number, particle-size ratio ranged from 1.5 to 2.0 with mixture composition around n_2:n_1=6:4 are recommended for the SLS process.

Gaussian distribution

In reality, the powders for SLS generally consist of particles of different sizes distributed over a certain range because of limitations of the process that powders are made. The particle size measurement technique will sort the particles into a small number *n* of size categories, where *n* is much smaller than the total number of particles *N*, and the technique may also produce a count of the number of particles within each category. For Gaussian distribution, the particles size distribution equation is expressed as follow [22]:

$$f_N(R) = \frac{1}{S\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{R-\bar{R}}{S} \right)^2 \right] \quad (1)$$

where $\bar{R}$ is the mean radius, and S is its standard deviation. A serious problem with the normal distribution is that it predicts a finite fraction of particles of sizes less than zero. Furthermore, the largest particle size does not have a limit and is infinite. Hence, it is necessary to make a range for the Gaussian distribution in this paper. The deviation of Gaussian distribution is obviously a key factor that affects the packing structure, and also the limited range will have its influence on the structure, and the results are shown by Tables 5 and 6 with mean radius of 1. The three dimensional structure is shown by Fig. 4 for the Gaussian distribution case.

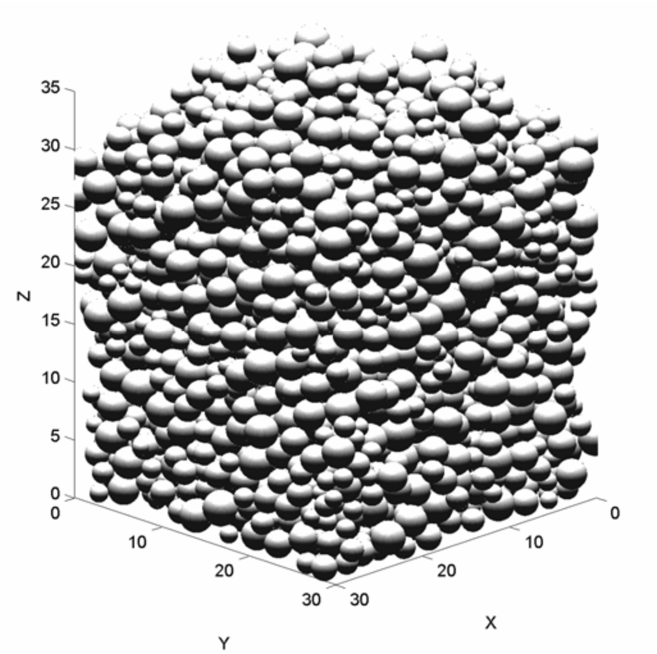

Figure 4 Three dimensional view of packing with Gaussian distribution

Table 5 Packing density of packing with Gaussian distribution

Radius range	Deviation: 1	2	3	4	5
0.34-3.0	0.600	0.594	0.593	0.592	0.591
0.5-2.0	0.592	0.592	0.591	0.591	0.593
0.67-1.5	0.585	0.586	0.586	0.587	0.584

Table 6 Coordination number of packing with Gaussian distribution

Radius range	Deviation:1	2	3	4	5
0.34-3.0	5.71	5.66	5.62	5.57	5.64
0.5-2.0	5.80	5.83	5.84	5.83	5.81
0.67-1.5	5.89	5.88	5.89	5.89	5.89

As can be seen from Tables 5 and 6, with broader radius range of particles, higher packing density is obtained, but the average coordination number is decreased, which can be explained by the same reason as the bimodal packing. For narrow radius ranges, the packing density slightly increases, while the coordination number is just reduced a little comparing to the results of equal size distribution, and there is little effect of deviation on packing structure. Therefore, in order to get high quality parts during the SLS process, powders with Gaussian distribution should be limited in a narrow radius range.

CONCLUSIONS

A numerical model for a loose packing process of spherical particles with different size distributions, including monosize particles, bimodal and Gaussian distributions, is presented. Packing of monosize particles was studied first to verify the validity of the current packing algorithm, and also to obtain a dimension size of the packing volume in order to eliminate its effect on final results. It is found a dimensionless size of 30 × 30 × 35 (x × y × z) is adequate. In order to obtain high quality SLS parts, a bimodal distribution with particle-size ratio from 1.5 to 2.0 and the mixture composition around $n_2:n_1=6:4$, and a Gaussian distribution whose particle radii are limited in a narrow range around 0.67 to 1.5, are recommended; both of them have high packing density and relative high coordination numbers.

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