COMPUTER SIMULATIONS OF PARTICLE PACKING

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ABSTRACT

Computer code has been developed to rapidly simulate the random packing of disks and spheres in two and three dimensions. Any size distribution may be packed. The code simulates varying degrees of inter particle conditions ranging from sticky to free flowing. The code will also calculate the overall packing density, density distributions, and void size distributions (in two dimensions). An important aspect of the code is that it is written in C++ and incorporates a user-friendly graphical interface for standard Macintosh and Power PC platforms. Investigations as to how well the code simulates the realistic random packing have begun.

The code has been developed in consideration of the problem of filling a container (or die) with spray-dried granules of ceramic powder (represented by spheres). Although not presented here, the futuristic goal of this work is to give users the ability to predict homogeneity of filled dies prior to dry pressing. Additionally, this software has educational utility for studying relationships between particle size distributions and macrostuctures.

KEY WORDS: Particle Packing, Void Size Distributions, Computer Simulations

1. INTRODUCTION

The most common method of manufacturing ceramic parts from powders is to dry press spray-dried granules [1]. A major problem with dry pressing ceramic powders is that density gradients are often produced during the die filling and compaction operations.

Density gradients may result from problems with granule size distributions, non uniform die filling, interparticle forces, binder properties, compaction rates, die wall friction, etc. [1]. It is these density gradients that subsequently result in flaws and product failure. It is important to note that the absolute density of a powder compact is not of primary importance for predictability of a flaw free part. A part may have a high bulk density yet still possess density gradients on the order of ten percent [2]. The current industrial norm is to complete several empirical tests on die design, spray-dried powder properties, and compaction variables to achieve satisfactory fabrication methods. These experiments are time consuming and costly. If methods could be developed that would allow for quick computer based optimizations for fabrication processes that yield small density gradients, then industrial dry pressing operations could benefit significantly. It is the eventual goal of this work to develop a computer based method to predict packing and density gradients of filled dies of spray-dried granules.

To date, the computer code is based on the random packing of circles (or disks) in two dimensions and spheres in three dimensions. Each circle or sphere is intended to represent a single spray-dried granule. A self-imposed restriction of the executable software is that it must be usable on readily accessible personal computers. With this restriction, and in the interest of speed, the code uses assumptions about interactions between granules and the paths by which they pack that do not account for every classical interaction that may be occurring. Whether or not these simulations adequately represent the realistic conditions is still being investigated.

2. SOFTWARE DEVELOPMENT

The software developed for the random packing of disks (in two dimensions) and spheres (in three dimensions) is written in the C^{++} language for Macintosh and Power PC platforms. A graphics interface and animation capability makes the package user friendly.

The code is intended to simulate macroscopic particles (i.e., greater than 10 microns) which fill a container. Practically any particle size distribution may be simulated and packing density, density distributions, pore size distributions, and pore coordination numbers may be calculated. Particles are placed one at a time using three different packing routines to simulate interparticle conditions ranging from sticky to free flowing (see Figure 1). The "sticky" routine does not allow any rotation of particles around previously placed particles. That is, each particle is physically stuck to the first particle it hits, and locked in place. The next routine allows for a particle to rotate once around the particle that it first hits until it comes in contact with another. That is, once a particle is in contact with two other particles,

it is considered to be in a stable configuration. "Free flowing" or "multiple rotations" allows particles to continue to rotate around previously placed particles until the lowest configuration is determined. Conceptually, the packing routines are the same in three dimensions, although much more complicated. In less than 30 minutes, several hundred thousand disks can be packed and analyzed for density and void size distribution in two dimensions. In three dimensions, hundreds of thousands of spheres can be packed in several hours.

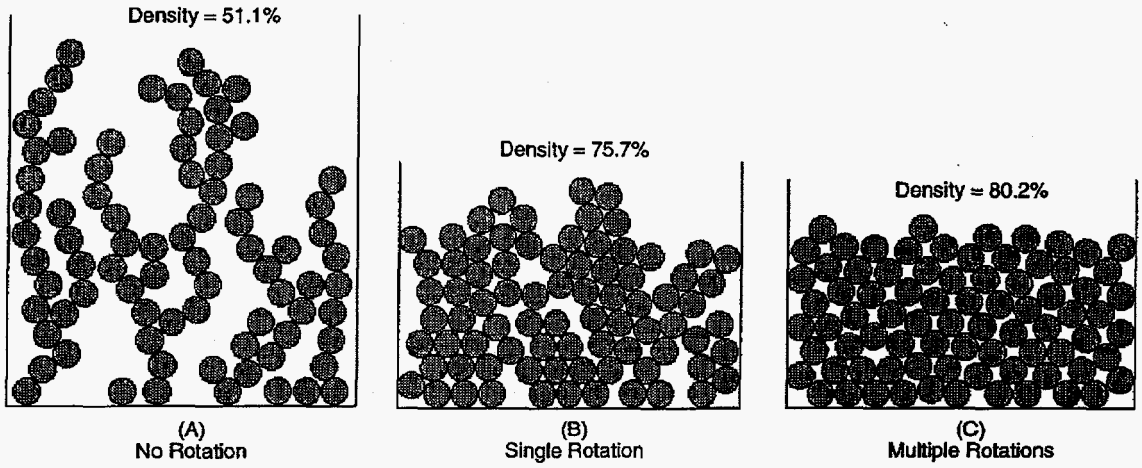

Figure 1 Packing simulations of two dimensional disks showing the effect of different packing routines on the percent of the area occupied by the disks: A) disks stick to each other upon contact; B) disks are allowed one rotation until a disk is in contact with at least two other disks; C) disks are allowed to rotate until the lowest position is reached.

In reality, particles that fill a die can impart momentum and movement to previously placed particles. The amount of movement depends on the size of the particles and the friction between the particles. The effect of this movement is to allow particles to fill space that would otherwise be inaccessible. This code attempts to simulate this space filling effect in a computationally fast way by assuming infinite friction between particles (unless a particle is rotating) and allowing the falling particle to rotate completely underneath a previously placed particle, if that space is available during rotation. In other words, even though particle motion as dictated by particle momentum and gravity is not adhered to, appreciable space filling is still allowed to occur.

3. RESULTS

Initially, simulations were completed in two dimensions to examine the effects of container width and bimodality on the packing of disks. Since packing in the vicinity of a wall can be very different from packing in the interior there is an effect on the packing of spheres due to

container width. The effect is seen not only on the overall packing density but also on the variability of packing from run to run. This effect is demonstrated in Figure 2 which shows that the standard deviation in packing density of disks is very appreciable until the container width is at least 500 disk diameters. These type of packing problems are also found in laboratory experiments when filling narrow dies.

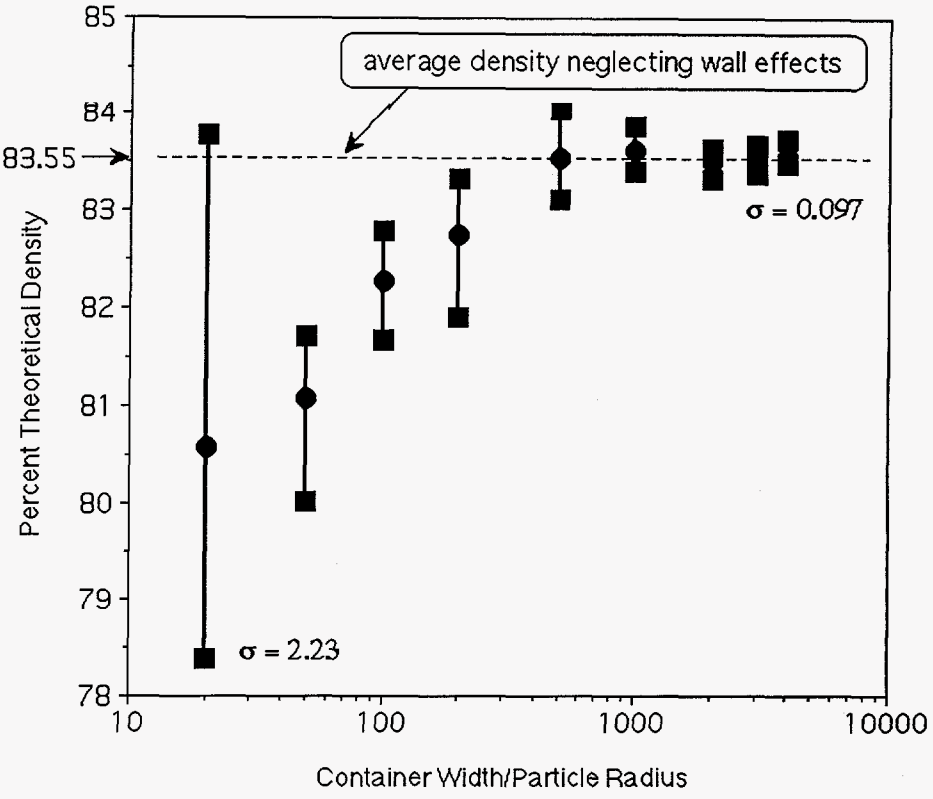

Figure 2 The effect of container width on simulated packing density for disks. As the container width is increased the variability between similar runs decreases.

In another set of simulations, the bimodal packing of disks was compared to the well known results of Furnas [3] shown in Figure 3. Simulations of 40,000 disks were packed using various fractions of radius = 10 and radius = 65. The results are shown in Figure 4. The results are in significant agreement with Furnas, showing that maximum packing density occurs when approximately 25 % (by area or volume) of the particles are of the smaller radius. The unexpected minimum in density that occurs at 88% fines in Fig. 4 is believed to be due to inefficient packing that occurs in the vicinity of large inclusions. Much like packing disruptions that occur in the vicinity of walls in two dimensions. This result has implications on the sintering of ceramic bodies which have inclusions; and will be further examined in three dimensions in future work. The minimum in density may not occur in three dimensions.

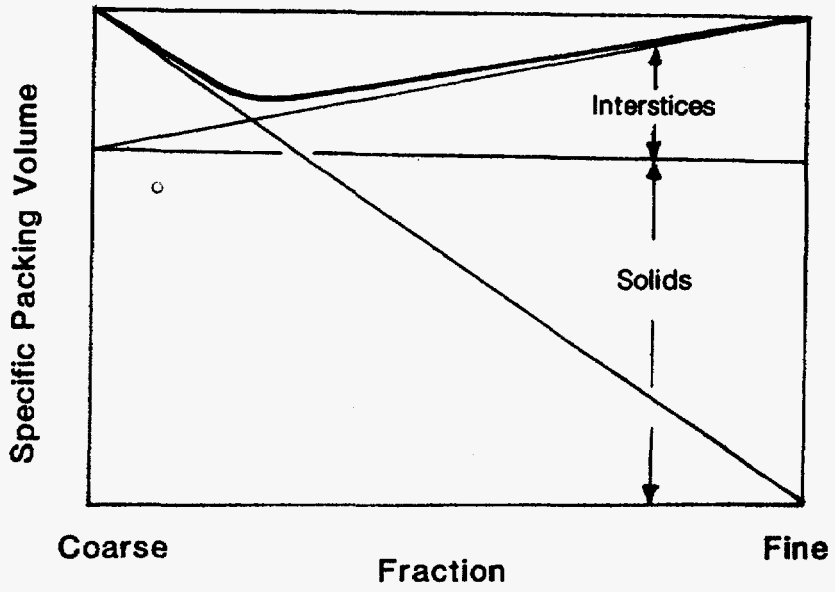

Figure 3 Theoretical variation of packing volume for the packing of smaller particles among coarser particles. The straight lines correspond to ideal packing when the size ratio is infinite, and the heavy line indicates typical behavior [3].

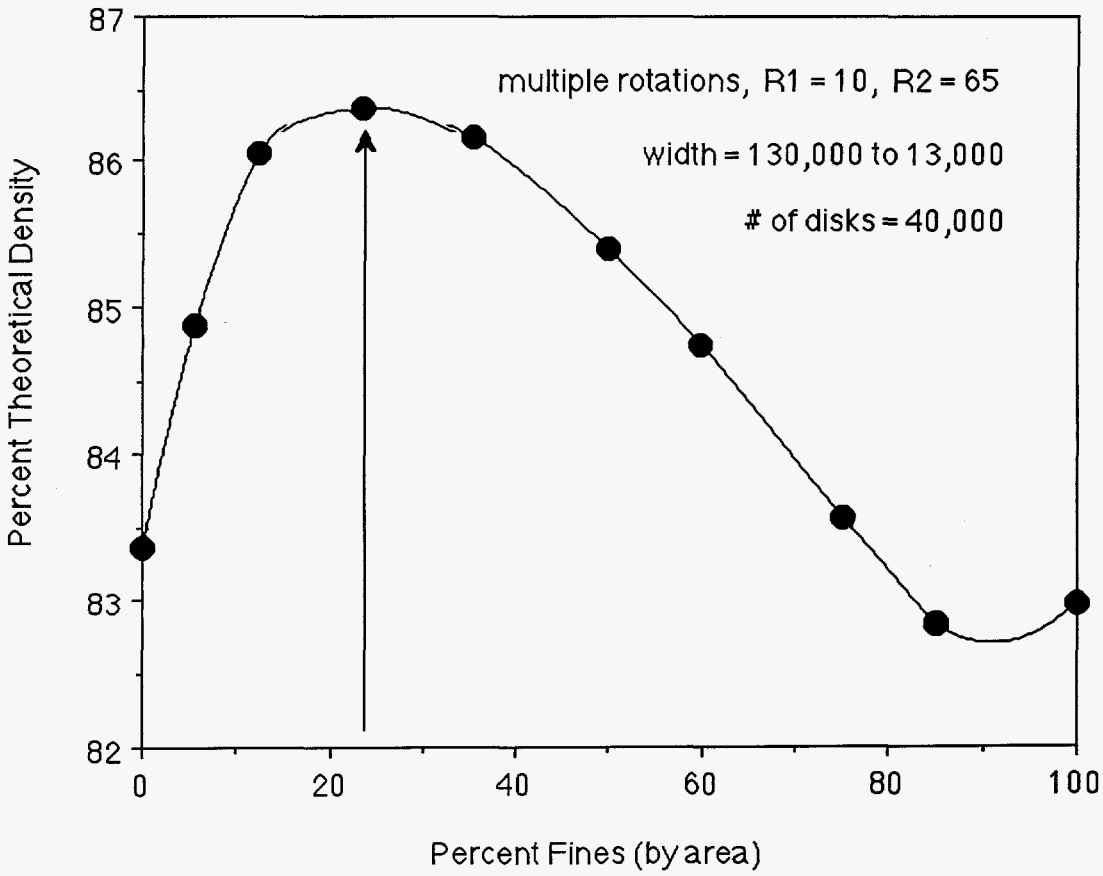

Figure 4 Simulations of bimodal packing of disks with radii equal to 10 and 65. Data points are averages from multiple simulations of 40,000 disks with multiple rotations.

The code also has the capability to calculate void size distributions and void coordination number. That is, the number of particles that border the void. This type of information is useful in determining the overall density uniformity throughout the compact, and if there are voids large enough to be considered critical flaws. Large voids with large coordination numbers can be color coded for easy identification as shown in Figure 5. The large void with coordination number of 13 could possibly result in the formation of a crack upon further processing. Three dimensional plots of coordination number versus void area versus frequency are also useful for determination of packing uniformity.

The software has also been developed to simulate the packing of spheres in three dimensions with an example shown in Figure 5. Using the "multiple rotations" packing routine, spheres randomly packed into cubic containers show packing densities of approximately 59 vol% when the container is large enough to ignore wall effects. This corresponds closely to the 60 vol% usually reported for the random packing of spheres [1].

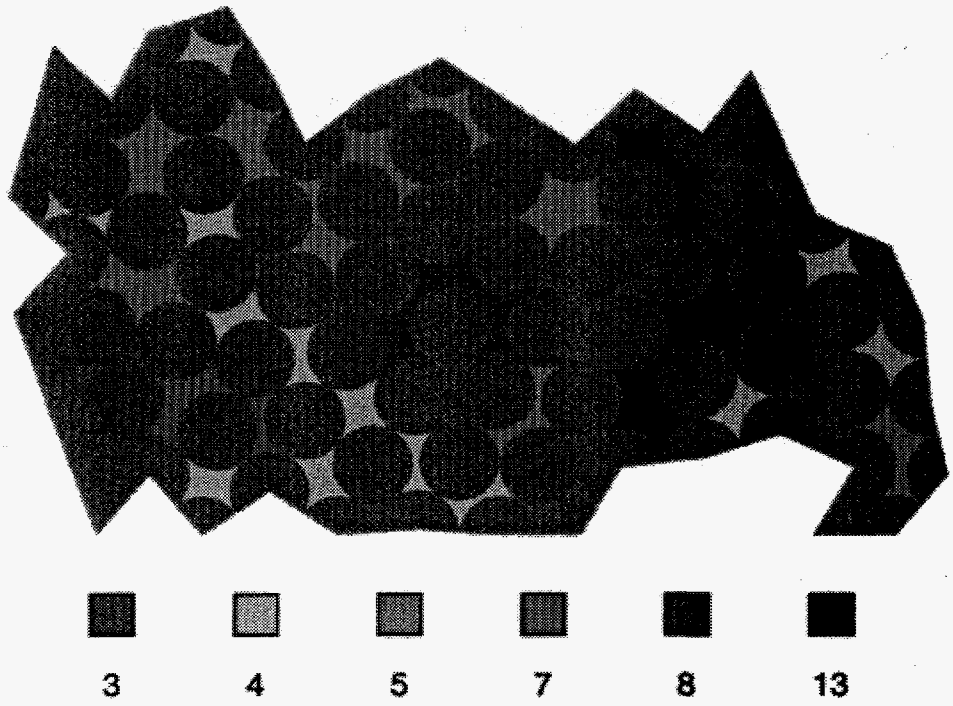

Figure 5 A color coded representation of void size and coordination number for a simulated packing of monosize disks using a single rotation packing routine.

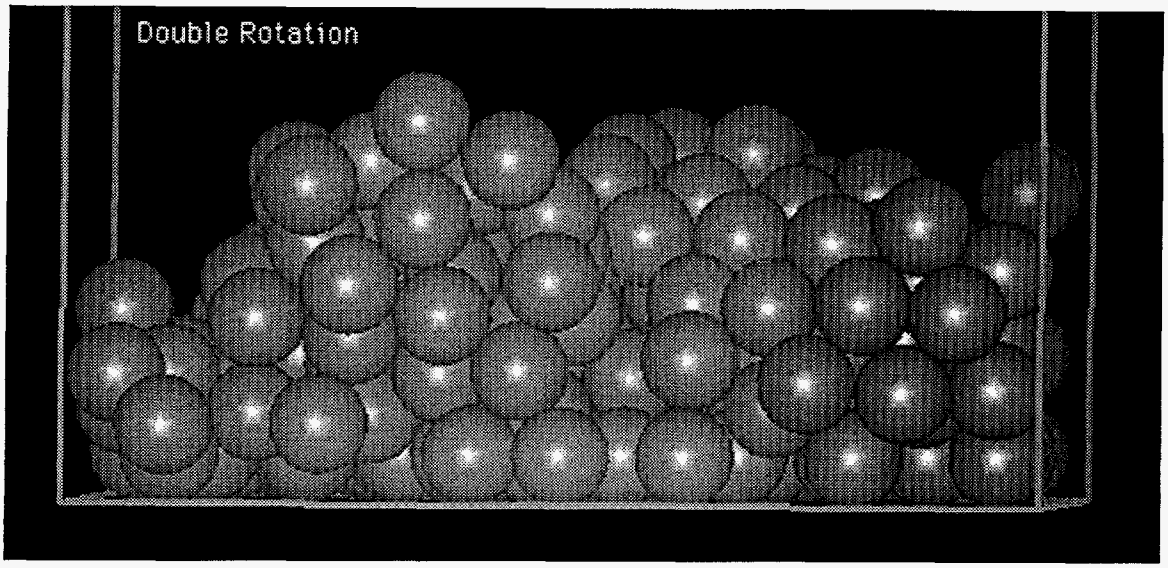

Figure 6 A graphical representation of simulated packing of spheres filling a cube.

4. SUMMARY

Computer software has been developed that simulates the random packing of disks (in two dimensions) and spheres (in three dimensions). Preliminary simulations of packing versus container width and packing of bimodal size distributions show that the software can accurately describe trends that are observed experimentally. Information regarding the coordination number and size of voids is also useful for determination of packing uniformity. Preliminary simulations of three dimensional packing of spheres appears to represent realistic random packing of spheres.

Future work will include more detailed investigations of how well the computer code simulates disks and spheres filling containers. Ultimately, the goal for this work to be able to accurately simulate the filling and compaction of spray-dried granules in dies of various shapes.

5. ACKNOWLEDGMENT

This work is supported by the Department of Energy contract #DE-AC04-94AL85000.

6. REFERENCES

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