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TECHNICAL NOTE

Wall Effect in 3D Simulation of Same Sized Particles Packing

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ABSTRACT

In this paper, the effects of container size on the porosity of random loose packing of mono size particles have been investigated using an Event Dynamics (ED) based model. Simultaneous effects of square container walls on particles packing and their order are also investigated. Our simulation results indicate higher container size will increase the total packing factor and high density regions which can be attributed to decrease of low density regions near the walls and also the order imposed by them. By growing packing container size, reproducibility of packing factor values increases which is another indication of more packing randomness.

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1. INTRODUCTION

Generally, development of powder metallurgy techniques are based on understanding forming processes. These processes are the main stage of production, which control the density distribution of bodies. Density distribution and consequent size and spatial distribution of pores are of great importance in materials used for porous heat exchangers, implants, capillary porous powder metallurgy materials, etc. The size of pores in powder metallurgy products can be mainly controlled using initial particles sized from nano to millimeter [1-4].

Particle packing means putting together and configuration of particles in a confined space. Packing factor is the fraction of particles' volume to the volume occupied by them. Many parameters affect the particles' packing including particles size, size distribution, shape, interparticle friction, etc. [5-7]. Generally, there are two major types of packing: ordered packing and random packing [8, 9]. In ordered packing, particles are located in sites, which result in a long range order. In random packing, particles do not exhibit such an order.

Random packing of particles can be categorized into random close packing and random loose packing. Random close pack is the densest configuration of particles in random packing. Packing factor of this type is about 0.6366. Random loose packing is less defined in comparison with random close packing. This term is generally used for defining the loosest state of random packing which is mechanically stable [10]. Packing factor of random loose packing under gravity is about 0.6. Due to the fact that pouring powders is the first stage in production of powder metallurgy parts, simulation of particles random loose packing is of great importance. Random packing of mono-sized particles is widely used for modeling the atomic structures of amorphous solids, liquids and also for modeling phase transformation in colloidal systems [11-13].

Particles packing can be free or confined in a finite sized container. In random packing of particles in a confined space, wall effect will also affect the particles packing. Wall effect is the phenomenon of decrease in packing factor of particles in regions near the packing walls. Many researchers believe that the main reason of wall effect is large size of pores adjacent to walls and other parameters, e.g. decrease of packing randomness, are negligible [14]. The size of pores in regions near the walls became larger; because, particles adjacent to the walls cannot be packed like the ones located far from them. The fraction of pores is equal to one in the walls and has an oscillatory approach to a certain value by increasing the distance from the walls [15].

In this study, random loose packing of particles simulated using a parallel model based on Events Dynamics (ED) approach and wall effect on packing of mono-sized particles and reproducibility of packing factor values have been investigated.

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2. EXPERIMENTAL

2.1. Modelling Particles are assumed to be same sized rigid spheres. The walls of packing space assumed to be rigid and flat.

A conventional Cartesian coordination system is applied to all of the computations inside the simulation environment. Coordinates in the system are referred to as either X, Y and Z. The environment is oriented so that the Z-axis is in the direction of the gravitation field and the origin set in the corner of the container in the simulation process. The boundary region was a tetragonal confined container with a square floor. The bottom of the container which is assumed to be flat, is located on the X-Y plane.

2.2. Packing Algorithm We used a time independent model based on event dynamics approach for particles packing. In this model, particles are packed by sequential pouring into a box of defined shape.

In our model, we assumed particle collisions to be soft, which results in improvement of accuracy but prolongs the calculations. After impact, their next path is calculated from the impact plane tangent to the particles surface.

X and Y coordination of particles are generated randomly, in each step particles moved in gravity direction (-Z) for a certain amount, until they reach the box floor or impact with other particles. The falling of particles into the container was in random sequence.

The particle's height (Z) is found from the static stability of the particles on each other. The resulting state can be described as random loose packing.

The stability of particles is calculated based on the location of the particles existing in the container, and the next movement of the particles in each calculation step determined from particle's coordinate and its contact points with boundary walls or other particles.

If the falling particle contacts with the existing particles in the container, the dropping particle will roll around the standing particle towards the ground. If a second particle is encountered in the process, the dropping particle will roll around the first and second standing particles until a third or more contacts (the floor, another particle, or a wall) when the momenta about each contact point is computed, and if they satisfy each other, the particle is reached to its stable position. This deposition process is deterministic, after starting the location and particle size are randomly generated.

2.3. Parallel Algorithm and Implementation The present parallel algorithm for computing packing factors uses an implicit parallelism paradigm. In every stage of parallelism each task is the result of the partitioning algorithm invoked at the first iteration of the program that uses functional decomposition. This partitioning and using implicit parallelism leads this researcher to the point where it can send these tasks to each node in the cluster. Also, load balancing is achieved by sending the next tasks who definitely send their result. By checking algorithm finds that the data sent by the node is incomprehensive it sends again the task to another node. If the node gives the standard result the data will be accepted and the node which has given the wrong result will be given a negative point. If the node reaches a threshold it will be disbanded by the server and its tasks will be given to other nodes. The tasks which will be executed on the node have the same order of computation; that will be finished simultaneously. If otherwise, that has been given the task sends the wrong result again that will mean that the task has a problem so it will be registered on a file with initiation and will be checked manually on another system to find the problem. After discarding and registering the tasks the server will resume its work on other tasks. The parallel algorithm has been implemented using the MPI library and MPICH2 implementation. This implementation enabled the researcher to use Visual Studio. NET 2003 to produce more high quality codes that are optimized for systems with Microsoft Windows XP service pack 2 operating system. This MPI implementation has an advantage over other system, PVM, which does not completely support object orientation. Complete object orientation was tried in the use of the present code so as to utilizes the said code for future simulations.

The result was a higher compatibility with various utilities, and so the researcher was able to feed the wanted results to other simulation tools with adding a suitable formatting package to the said code and produce suitable result. The hardware used in the simulation consisted of six dual processor PCs with 512 MB RAM one of which was used for replication of data. These PCs were connected together in a star topology. Each simulation took almost 72 hours and the data was gathered in the server.

2.4. Packing Factor After finalizing the packing of particles in the container, to calculate the amount of packing factor, the normal height of box that has the average planar density of particles at the top height plane was found. The average particles planar density starting from bottom to half of the maximum particle's height was then calculated. The packing factor of the particles obtained from the division of total volume of particles involved in the normal box by its volume.

2.5. Calculation Parameters For investigation on the effects of relative size of packing box, all units are dimensionless. The accuracy of all calculations was 0.001. The friction between the particles was assumed to be infinite which is valid for small particles. This assumption has similar effect on all simulations and therefore, ignored in comparing results. The radius of particles was assumed to be 30. For reproducibility of packing factor, calculations carried out for 100 randomly generated particle sets. Regional packing densities were calculated using 1^3 cubic elements. Packing factor distribution contour lines were plotted with 0.2 intervals.

3. RESULTS AND DISCUSSION

Fig. 1 (a through c) illustrates the reproducibility of packing factor values for 500 mono-sized particles in 200×200, 300×300 and 400×400 containers, respectively. Statistical information of these results are listed in Table 1.

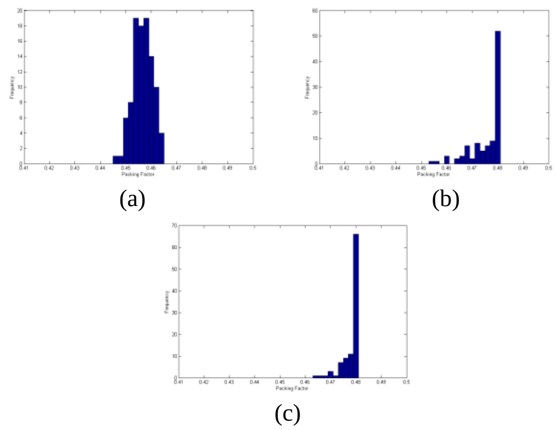

Figure 1. Packing factor values distribution for 100 simulations of 500 particles packed in a) 200×200, b) 300×300 and c) 400×400 containers.

TABLE 1. Statistical analysis of packing factor of 500 particles in 100 packing simulation.

Container size	Packing Factor			
	Minimum	Maximum	Average	Standard Deviation
200×200	0.4453	0.4641	0.4566	0.0039
300×300	0.4523	0.4938	0.4793	0.0099
400×400	0.4646	0.4955	0.4811	0.0058

Average packing factor resulting from this model is about 0.48; thus, the packing configuration can be classified as random loose packing. As it can be seen in this figure, by increasing container size with fixed particle numbers, the resulting packing factor values increase. This can be described as being due to less order imposed by regions of walls in particles' packing.
An increase in container size also results in an increase in reproducibility of packing factor values which can be an indication of increasing randomness by decreasing side wall area.
Regional packing factor can be calculated from the fraction of elements with the same X and Y coordination, occupied by particles, to the total number of elements.

Fig. 2 (a through c) illustrates the nonphotorealistic rendering of regional packing factor values of 500 same size particles in 200×200, 300×300 and 400×400 containers, respectively. As can be seen, small ratio of box to particles size induces good amount of order into particles packing. Packing factor in the distance of 60 from the container walls reaches its lowest value and then rises again. This distance corresponds to the diameter of the particles.

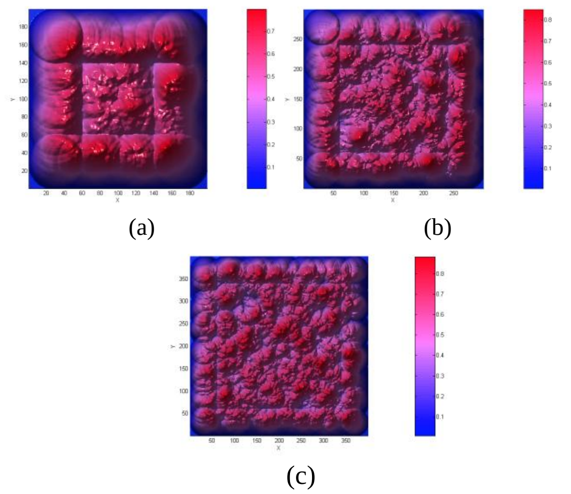

Figure 2. Regional packing factor of 500 particles packed in a) 200×200, b) 300×300 and c) 400×400 containers.

Fig. 3 shows the contours of regional packing factor values of Fig. 2. As can be seen, by increasing container size, the variation of packing factor values, and also the area of high packing factor regions will increase.

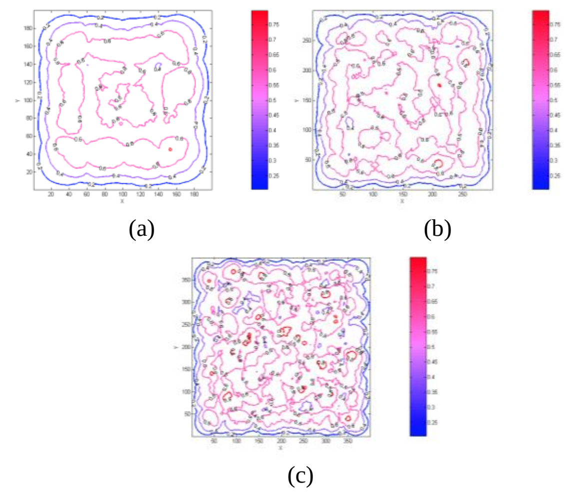

Figure 3. Contours plot of regional packing factor of 500 particles packed in a) 200×200, b) 300×300 and c) 400×400 containers.

Figs. 4-6 show the packing factor profile of 500 mono size particles, in various distances from the Y wall. Variations of packing factor in the distance of 10 to 40 from the container wall are shown in Fig. 4. As it is shown, by increasing distance from the walls, in the distance of 10 to 40, regional packing factor increases. Variations in the distance of 50 to 70 are shown in Figure 5 which indicates that there is a local minima value in the distance of around 60 from the wall.

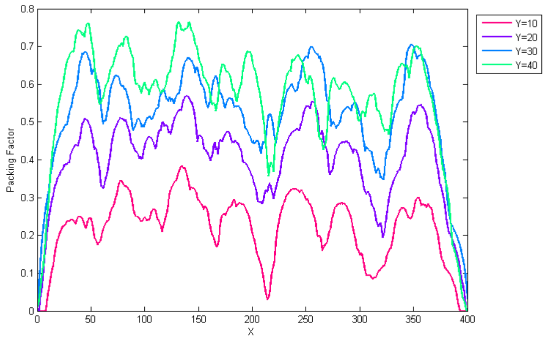

Figure 4. Variations of packing factor of 500 particles in the distance of 10-40 from the wall in a 400×400 container.

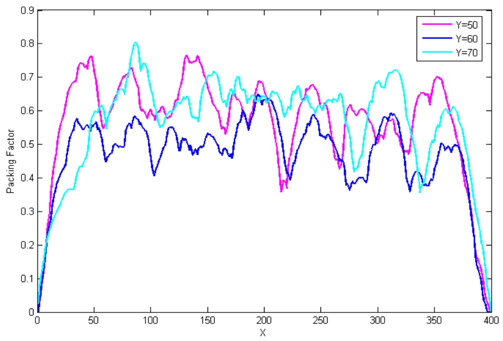

Figure 5. Variations of packing factor of 500 particles in the distance of 50-70 from the wall in a 400×400 container.

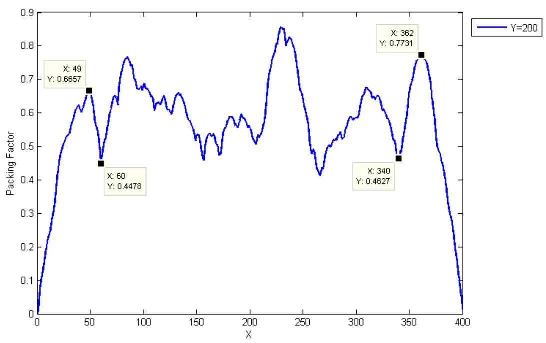

Figure 6. Variations of packing factor of 500 particles in the distance of 200 from the walls in a 400×400 container.

Figure 6 illustrates the packing factor variations in the middle of the box which should have the minimum normal wall effect. Randomness of particles packing proposes that the variation in X and Y directions must be symmetrical.

In this plot, as the distance from X walls increases packing factor will increase to a local maxima value in a distance of about 48-49 from the wall and there's a local minima in the distance of 60 which corresponds to the diameter of particles. This figure also agrees with the results of other studies about random close packing of particles which can be attributed to the order resulting from the wall effect [15].

4. CONCLUSION

In this paper, random loose packing of same size particles has been investigated using an event dynamics based algorithm. Results indicate that low ratio of container size to particles diameter will make the packing configuration of particles more orderly and will inhibit the random packing. By increasing container size, packing factor, the areas of high packing factor regions and also the reproducibility of results will increase. Results also show a local minimum of packing factor when the distance from the walls is correspondence with the particles' diameter.

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