An algorithm to generate a specimen for Discrete Element simulations with a predefined grain size distribution

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ABSTRACT
The discrete element method is a powerful numerical tool in simulating the behaviour of granular materials. It bridges the gap between continuum mechanics and physical modeling investigations. In spite of the significant achievements to date, some major problems still need to be solved including the development of realistic microscopic models and the lack of efficient algorithms to generate the initial conditions similar to those used in physical models. This paper introduces an effective computational method to generate the initial packing of particles with a pre-defined grain size distribution in 3D space. The method is implemented into the open-source code (YADE). Specimen properties obtained (i.e. porosity, coordinate number, radial distribution) are compared to other existing results in the literature.

RÉSUMÉ

1 INTRODUCTION

Since the first discrete element method code was first introduced (Cundall and Strack, 1979), it has been used extensively to investigate various engineering problems (Jensen *et al.*, 1999; Zeghal and Edil, 2002). One of the most important steps in a simulation using DEM is to generate a specimen (particle packing), consisting of entities, in a form that represents realistic conditions.

Particle packing has been long investigated by researchers and can be classified into two main types based on the spatial pattern of particle location: ordered packing and random packing. Ordered packing is performed by placing particles systematically in to periodic positions (O'Sullivan *et al.*, 2004). On the other hand random packing is done using a sequence of packing events that result in particles not correlated with one another with respect to their locations in the matrix (e.g. Feng *et al*,. 2003; Bagi, 2005).

In this study, the properties of the specimens generated using the dynamic packing method are intensively investigated. A new method to generate particles with a pre-defined grain size distribution is developed and implemented into a computer code. A parametric study is then conducted to examine the effects of dynamic variables and the total number of particles on the packing properties.

2 LITERATURE REVIEW

Several methods are currently available to generate particle packing. These methods can be divided into 3 main categories: geometric methods, sedimentation method and dynamic method. A brief review of these methods is given in the following section.

2.1 Geometric methods

In these methods, a specimen is generated using purely geometric calculation without simulating the dynamics of particle motion. Stoyan (1998) gave a summary of algorithms used to generate spheres starting from a set of randomly located points. The set of points is generated randomly employing the Poisson process (see Molchanov, 1993). Then a set of grains are shifted such that they coincide with the points as in Boolean model (Molchanov and Stoyan, 1994). As discussed in their paper, the points are allowed to grow until the corresponding sphere has first contact with one of the faces of the Voronoi cell corresponding to that point (Stienen model) or the growth process is stopped when it comes in contact with another sphere (lily-pond model). The sphere radii are dependent on the position of the points as located by the random generator. The particle size distribution cannot be directly prescribed in the above two methods.

An attempt to solve this shortcoming is introduced by Evans (1993) where a system called the Simple Sequential Inhibition model (SSI model) is developed. In the SSI model, spheres are placed sequentially and randomly in a given region. If a new sphere is placed so that it intersects a sphere already in place, then the new sphere is rejected. The placing process of spheres is usually stopped when it is impossible to place any new sphere. The method can be used with a user-defined grain size distribution. Improved versions of SSI model were proposed by Chib and Greenberg (1995); To and Zbigniew (2004). In these methods, an initial random arrangement of spheres is generated then the next stage is to insert, delete or relocate existing spheres with user defined probabilities for each action to succeed.

Another geometric method was suggested by Cui and O'Sullivan (2003) for 2D and 3D assemblies of circular/spherical grains based on the triangulation approach. The concept of this approach is to triangulate a

system of points within the domain of interest, creating a mesh of triangles/tetrahedrons. Then the particles are inserted as the incircles/inspheres of these triangles/tetrahedrons.

The above methods; however, generate a relatively loose packing specimen. An improved method to generate a dense random packing in 2D was proposed by Feng *et al.* (2003). In this method (advancing front approach), three initial disks which form an initial front are generated and placed at the center of the domain. With this initial front established, a new disk is generated to fill the space by incrementally advancing the front until it completely covers the original domain. While the method produces a relatively dense packing, large gaps may remain at the edge of the domain in the case of general grain size distribution. Consequently, the inward packing method (Bagi, 2005) was developed to generate a packing where the boundary grains exactly touch the walls. The initial front is created by placing the disk with maximum radius into the upper left corner, touching two walls then the next disk is attached to the left wall and to the previous particle. These methods; however, are only applicable to 2D problems, the extension to 3D encountered a lot of difficulties.

2.2 Sedimentation methods

In order to generate more dense arrangement than most of the geometric methods, several authors (Han *et al.*, 2005; Fu and Dekelbab, 2003; Tory *et al.*, 1968; Visscher and Bosterli, 1972) have been developed a so-called sedimentation techniques. The required domain is filled up by placing discs/spheres following the user-defined size distribution into the domain and translates it downwards, until it collides with an already existing disc/sphere in the system. Then the new disc/sphere is further moved just as if rolling down along the contacting sphere until it reaches a stable position by being supported by two discs (or three previous spheres).

Anisotropy in the loose packing generated using the sedimentation methods was observed by Jodrey and Tory (1985). The packing fraction (1-n) obtained was found to be approximately 0.582 which is close to the dense packing density.

It is worth noting that the translation of discs/spheres is determined based on purely geometric calculation, without analyzing the dynamics of the system. This leads to unrealistic packing structure in terms of radial distribution function (Jullien *et al.*, 1996) and mean coordination number (Liu *et al.*, 1999).

2.3 Dynamic methods

Dynamic packing process; however, involves various forces in addition to gravity (i.e. contact forces due to collision and friction among particles, inter-element forces such as the Van Der Waals or electrostatic forces). These forces can affect the packing structure either individually or simultaneously depending on the packing condition. These phenomena, which can only be simulated using the DEM itself, are not considered in the purely geometric packing algorithms.

A typical approach in dynamic packing method is to place a required number of particles into a large domain whose walls are slowly moved inwards until the required density is reached. Another possibility is to simulate gravitational deposition where particles fall down into the domain, and their equilibrium position is established under the effect of gravity (Kong and Lannutti, 2000).

Liu *et al.* (1999) proposed a method to generate packing by imposing an assumed centripetal force on particles randomly generated in a spherical space.

The above methods are considered to satisfactorily simulate the dynamics of forming a packing and produce more realistic structural information (Liu *et al.*, 1999). These methods; however, require a huge amount of calculation and therefore they are considered to be very time-consuming.

3 DISCRETE ELEMENT SIMULATION

3.1 Governing equation and force description

This simulation was carried out using the Open Source code YADE (Kozicki and Donze, 2008). The code is designed using dynamic libraries to facilitate the addition of user-defined models. The centered second order finite difference scheme is employed such that the position (orientation) of each particle remains unchanged during each time step and the forces are calculated from the force-displacement relationship. When all forces acting on a particle i, either from other particles or the boundaries, are known, the problem is reduced to the integration of Newton's equations of motion for the translation and the rotational degrees of freedom

$$m_i \frac{d^2}{dt^2}\vec{r}_i = \vec{f}_i \qquad (1)$$

and

$$I_i \frac{d^2}{dt^2}\vec{\Phi}_i = \vec{M}_i \qquad (2)$$

where m_i, , are the mass, the vector of position and the vector of orientation in space of particle i, respectively. I_i is the moment of inertia of particle I and is defined as:

$$I_i = q_i m_i (d_i/2)^2 \qquad (3)$$

where d_i is the diameter of particle i and q_i is the dimensionless shape factor.

Interactions are short range and active on contact only, so that the total force (torque) on particle i is $\vec{f}_i = \sum_c \vec{f}_i^c (\vec{M}_i = \sum_c \vec{j}$, where the sum runs over all contacts c of particle i. The torque $\vec{M}_i^c = \vec{l}^c \times \vec{f}^c$ is related to the force via the branch vector from the particle center to the contact point. The damping coefficients are applied to forces and moments for computational purposes. Hence the problems can be solved if all forces acting on the contact (see

Figure 1) are determined. The procedure to calculate the contact forces is discussed below.

3.1.1 Contact forces

The contact forces are calculated based on the penalty method which means that the contact forces are evaluated from the volume overlap of two interacting spheres.

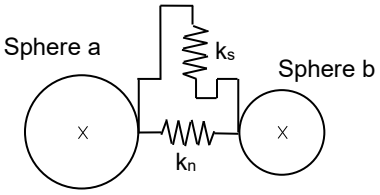

Figure 1. The force-displacement law

3.1.2 Normal forces

The normal forces are calculated as follow:

$$\overrightarrow{f_{nc}} = k_n \delta \vec{n} \quad (4)$$

where is the normal force at contact c of particle i, k_n is the normal stiffness at the contact, is the relative normal displacement between two particles and is the branch vector from the contact point to the particle center.

3.1.3 Shear force

The shear forces are calculated incrementally (Hart *et al.* 1988):

$$\Delta \overrightarrow{f_{sc}} = k_s \Delta \vec{u}_t \quad (5)$$

where is the incremental shear force, k_s is the tangential stiffness and , is the incremental tangential displacement.

The shear force is truncated if its absolute value is larger than the maximum value given by Mohr–Coulomb criterion:

$$|\vec{f}_{sc}| = |\vec{f}_{nc}| \times \tan\phi \quad (6)$$

where is the internal friction coefficient.

3.1.4 Macro-micro relationship

The strain energy stored in a given interaction cannot be assumed to be independent of the size of the interacting elements. Therefore interaction stiffnesses are not identical over the sample, but follow a certain distribution that depends on the shape and size of the pair of particles interacting. "'Macro-micro'' relations are then needed to derive the local stiffnesses from the macroscopic elastic properties and from the size of the interacting elements. The hypothesis of best fit (Liao *et al.*, 1997; Hentz *et al.*, 2004) is employed to fit the relationship between the Young's modulus E, Poisson's ratio and the dimensionless value of k_s/k_n:

$$E = \frac{D}{S_{int}} \frac{\beta + \gamma}{\alpha + \gamma} \quad (7)$$

$$\nu = \frac{1 - \gamma}{\alpha + \gamma} \quad (8)$$

where is the initial distance between two interacting elements a and b, coefficients are the fitted values and is an ''interaction surface'':

$$S_{int} = \pi(\min(R_a, R_b))^2 \quad (9)$$

These relations are simply inverted to obtain the local (micro) stiffnesses at contact level.

Material properties used in the simulation are provided in **Error! Reference source not found.**.

3.2 PACKING METHOD

3.2.1 Requirement of a specimen generation algorithm

It is important to clearly define the requirement of a specimen generation algorithm for granular problems. The specimens generated should be in equilibrium under gravitational loading and consequently will have realistic properties (porosity, grain size distribution, fabric tensor).

As the geometric and sedimentation algorithms become very complicated when dealing with particles of different shapes, the specimens generated by the above methods need to be compressed (or shaked) using a DEM simulator in order to acquire a dense packing. Moreover, since the specimens is generated once and then used various times in a specific application, the ability to reflect the real condition of the specimen is of more important than the performance in terms of the computational cost of the algorithm itself.

Motivated by the fact that dynamic methods can satisfactorily simulate the dynamics of forming a packing and produce more realistic structural information, an algorithm to generate a specimen with realistic properties (compared to samples generated experimentally) is developed. The packing method is described in the following section.

Table 1 Material properties

Parameter	Value
Particle density (kg/m^3)	2600
Young's modulus (Pa)	15000000
Poisson's ratio	0.5
Friction degree (degrees)	18

Box's Poisson's ratio	0.2
Box's friction degree	0
Force damping coefficient	0.2
Moment damping coefficient	0.2

3.2.2 The packing technique

A number of spheres are first generated without overlap in a predefined rectangular space (1 in width, 0.3 in depth). This step is similar to the SSI model. The positions and the space dimensions can be changed during the simulation by controlling the input parameters. The particles were then assigned a gravity force to settle down under gravity conditions, they would have interaction with neighbouring particles. Additional particles were generated after a predefined time interval. This process continued until a specific number of particles or a specimen height is reached.

The DEM computational process is kept running until a stable condition is obtained. The specimen is considered to be stable if the ratio of the unbalanced force to the total force is less than a predefine value. In this study, stability value was taken as 0.01

$$R = \frac{\sum |f_i|}{\sum |f_{nci}|} \leq 0.01 \quad (10)$$

where f_i is the resultant force on the body and f_{nci} is the force acting at the contact.

3.2.3 Generating spheres with a predefined grain size distribution

In the DEM simulation, sphere radii are generated randomly according to a given sieve analysis test results. The sieve analysis test generally provides the percentage of aggregates passing through a series of sieves. It is worth noting that in DEM, only the percentage of sphere numbers can be controlled, thus the percentage passing by weight should be converted to a percentage number of spheres (see **Table 2**). A random number generator is used to generate pseudo number distributed over the interval [0,1]. The radius of particle i is then calculated using the following equation in order to generate a population of aggregates consistent with the sieve analysis result:

$$r_i = [D_L + (RAN_i \times 100 - P_L) \times (D_s - D_L)/(P_s - P_L)]/2 \quad (11)$$

where is the radius of particle i, are the percentage number of total grain calculated from the percentage volume passing through sieves S1 and S2, respectively. D_1 and D_2 are the diameters of sieves S1 and S2, respectively. R is the ith random number generated for particle i. Sieves S1 and S2 are determined by comparing R with the sieve analysis percentage passing results. Note that $RAN_i \geq P_L$ and $RAN_i \times 100 <$. A representative set of parameters used to generate spheres based on sieve analysis results is provided in Table 2.

Table 2 Typical conversion from percentage by weight to percentage by number of spheres

Sieve ID	Sieve diameter (in)	Percent passing (weight)	Percent passing (number)
#200	0.0029	0	0
#100	0.0059	0	0
#50	0.0117	0	0
#30	0.0232	20	82.25
#16	0.049	50	98.07
#8	0.097	80	99.86
#4	0.185	100	100

An algorithm was implemented to generate arbitrary grain size distribution; however, only two different values of radii were considered in the present study in order to examine the effects of grain size ratio.

3.3 Variables considered

The variables examined in this study can be classified into two groups: the first group of variables are related to the particles size ratio whereas the second group of variables are related to the dynamic properties, i.e. the total number of spheres in the simulation, the number of spheres generated each time interval, the dimensions and position of the box (in which spheres are generated), mean sphere radius and sphere radius distribution. The ranges assigned to these variables are given in Table 3. Both groups were examined using 1000 to 20000 particles. Unless otherwise stated, the effect of each variable on the packing was examined while other variables were kept constant.

3.3.1 Porosity

Porosity is the most accessible parameter in defining macroscopically a packing and thus has been studied widely in engineering practice. It describes the fraction of void space in the material and is defined by the ratio:

$$n = \frac{V_v}{V_T} \quad (12)$$

where is the volume occupied by void and is the total volume of material including soil and void components

Table 3 Simulation parameters

Parameter	Base value	Varying range
Total number of particles	5000	[1000,20000]
Particle mean radius	0.0153	[0.009-0.026]
Dropping height	4	[1,4]
Number of particles	2	[1-20]

generated each time (percent)		
Sphere generation rate (time step)	5000	[200-5000]

3.3.2 Coordination number

Coordination number is the number of spheres in contact with a considered sphere. It varies with the definition of contact, i.e. the minimal or cut off distance between two spheres by which they are regarded to be in contact. In the present work, the critical distance was set to 1d.

3.3.3 Radial distribution function (RDF)

Radial distribution function RDF is the probability of finding one particle center at a given distance r from the center of a given particle and is defined by

$$g(r)=\frac{N(r)}{4\pi r^2 \Delta r} \quad (13)$$

where N(r) is the number of sphere centers situated at a distance between r and r+Δr from the center of a given sphere. In this study, RDF was averaged for spheres within the specimen and Δr is set to 0.001.

3.3.4 Fabric tensor F_{ij}

In soil mechanics, the term fabric is used to refer to the arrangement of particles, particle groups and pore spaces. Typically, quantitative measures of fabric are considered; however, fabric can be quantified using the fabric tensor (e.g, Cambou, 1998). The contact fabric (second rank) can be expressed as:

$$F_{ij}=\frac{1}{N_c}\sum_{N_c} n_i n_j \quad (14)$$

where N_c is a number of contacts, and n_i and n_j are contact normals in the I and j directions, respectively.

4 RESULTS AND DISCUSSION

A set of parameters (see Table 3) have been prepared for evaluation. Results in terms of represented volume were also investigated. Only a limited number of results; however, are presented due to space limitation. The first series is the results from the packing of mono-sized spheres and the second is the result from the packing of spheres of two different radius values.

4.1 Overall porosity

The overall porosity is determined using the calculated average volume of the specimen as:

$$V = h_{ave} \times A \quad (15)$$

where h_{ave} is the average height of the specimen and A is the surface area of the specimen.

To study the effect of the number of spheres generated each time increment (N_{ot}), five packing of 5000 spheres were generated with five different number of particle generated each time increment, i.e. 1, 2, 5, 10 and 20 percents of total number of spheres. The results shown in **Figure 2** are consistent with the simulation results of Zhang (2001). Generally, porosity increased as the number of spheres generated each time increased. For example, with 1 percent of spheres generated, the porosity is 0.418 while a value of 0.443 was obtained when the 20 percents of spheres are generated each time increment. This indicates that a denser packing can be achieved by generating a small percentage of spheres each time. When N_{ot} increased from 1 to 5 percent, a significant increase in the porosity was calculated; however, when N_{ot} is larger than 5 percents, the rate of increase is less significant. This can be explained by the arching or bridge phenomenon that results from the simultaneous dropping of spheres at a relatively close distance.

Figure 3 show the dependence of the overall porosity on the total number of particles. Obviously, the overall porosity decreases with increasing the number of particles. When the numbers of particles increased from 1000 particles to 5000 particles, the porosities decrease from 0.457 to 0.425; however, further increasing the total number of particles to 20000 particles results only in a porosity value of 0.421. As discussed by Jodrey and Tory (1985), homogeneous packing is possible when the packing size is large enough. As seen in **Figure 3**, a reasonably homogeneous packing can be obtained if the number of particles is larger than 20000 particles.

Effect of drop height on the overall porosity is shown in **Figure 4**. The overall porosity decreases as the drop height increased. Increasing the drop height implies that more energy is applied to the particles to rearrange leading to breaking of the bridge or arching among particles. Consequently, a denser packing is achieved. For the range of drop height of 40 to 164 sphere diameters, the threshold of drop height at which packing density does not change much as reported by Zhang (2001) was not found to clearly exist in the present analysis.

To study the effect of the particle size ratio on the overall porosity, fifteen packing with particles size ratio of 4:5, 3:5 and 2:4 were generated. As shown in **Figure 5**, the overall porosity increases with increasing particle size ratio. As the number of particles increase to 10 000, the changed rate in overall porosity significantly decreased. Note that similar behaviour was observed in the case of mono-sized sphere packings.

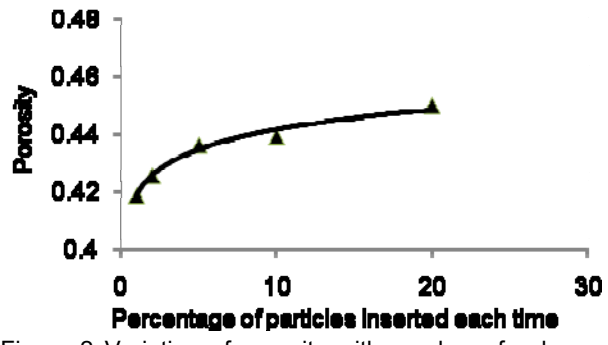

Figure 2 Variation of porosity with number of spheres generated each time

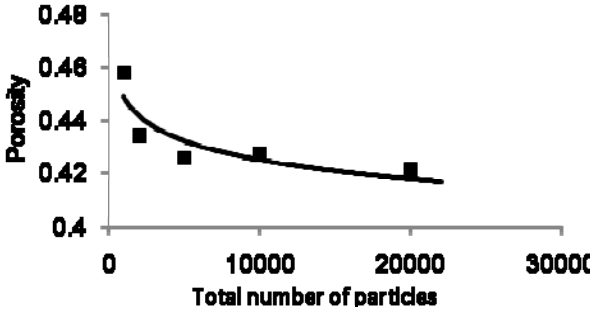

Figure 3 Variation of porosity with number of total spheres used in the simulation

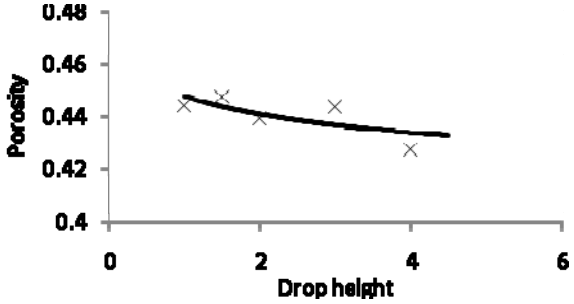

Figure 4 Variation of porosity with sphere drop height

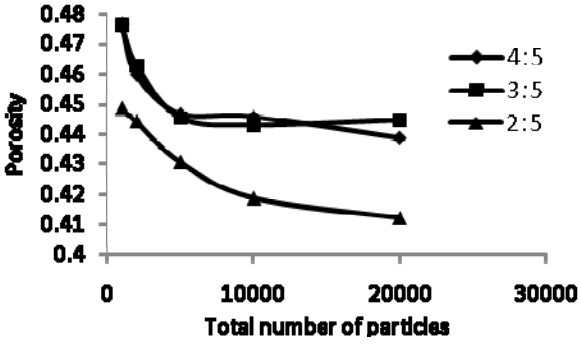

Figure 5 Variation of porosity with sphere size ratio and total number of particles

4.2 Coordination numbers

Figure 6 shows the mean coordination number for packings constructed using different N_{ot}. It can be seen that increasing N_{ot} results in decreasing mean coordination number. Variation of the coordination numbers with different value of total number of particles is shown in **Figure 7**. It is observed that as the number of particles increase from 1000 to 5000, the coordination number increases from 5.07 to 5.14; however, the coordination change only a small value as the number of particles increases from 5000 to 2000. It again confirms that homogenous packing can be obtained if the number of particles larges is large enough.

From **Figure 2**, **Figure 3**, **Figure 6** and **Figure 7**, it can be seen that decreasing porosity results in an increase in mean coordination number which is in well agreement with those observed by Pinson *et al.* (1998).

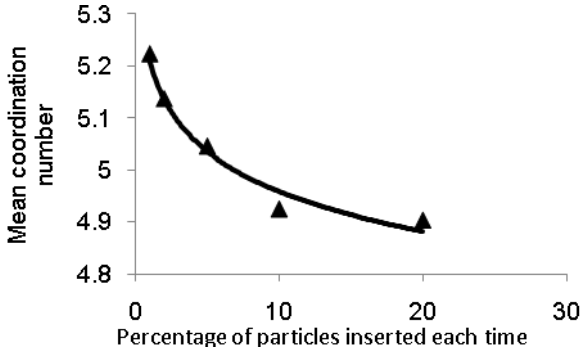

Figure 6 Variation of mean coordination number with number of total spheres used in the simulation

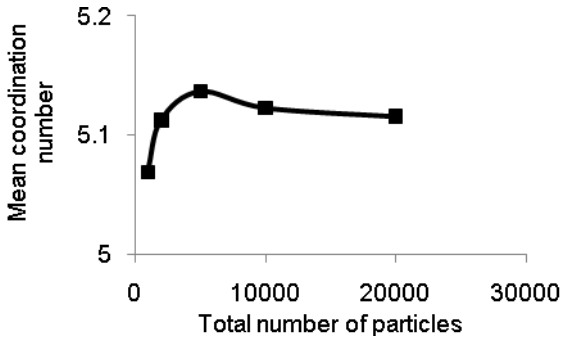

Figure 7 Variation of mean coordination number with total number of spheres used in the simulation

4.3 Radial distribution function

Figure 8 shows four radial distribution functions corresponding to the packings of 1000, 5000, 10 000 and 20 000 mono-sized spheres obtained by averaging the RDFs for all the particles. It can be seen that the four packings demonstrate a common feature of a split second peak, followed by other peaks. The four radial distribution; however, do not expose any clear difference in all four cases.

The positions of the second peaks are in consistent with the results of Finney (1970). It has been well established (Zhang et al., 2001 and Liu et al., 1999) that for a dense random packing, there is a split second peak in the RDF with its first component at $\sqrt{3}d$ and the second component at $2d$. The split peak phenomenon can be obtained by a collective but not one-by-one simulation algorithm.

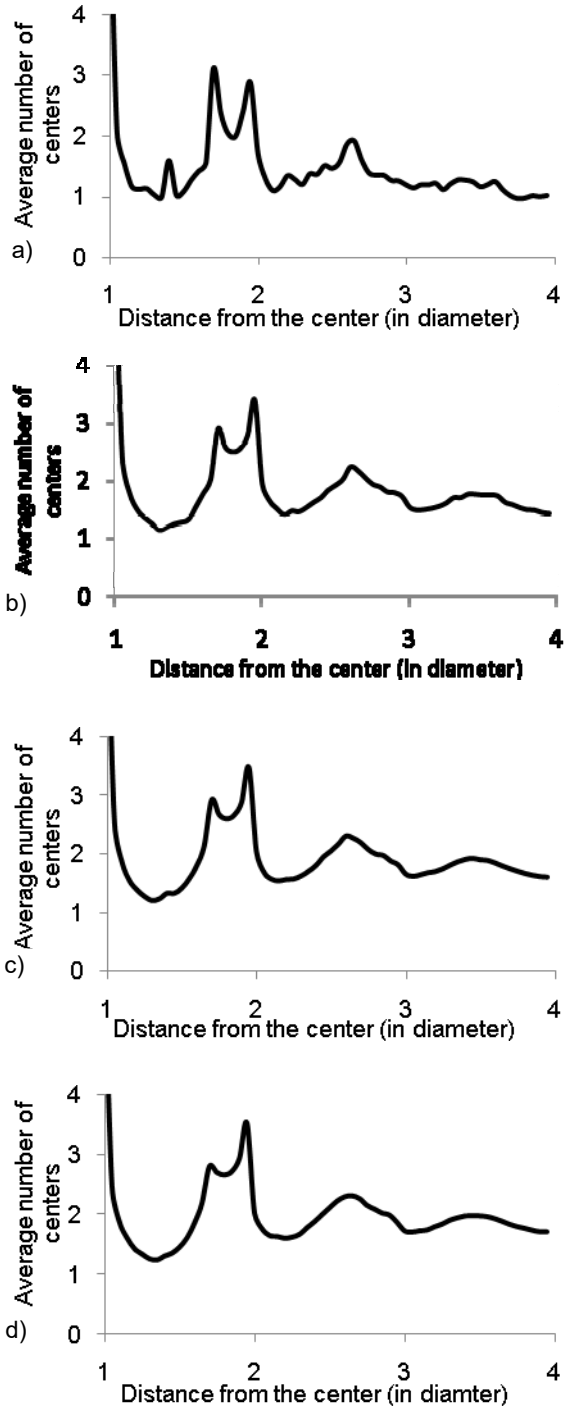

Figure 8 Radial distribution functions: (a)1000 particles; (b)5000 particles; (c)10000 particles; and (d)20000 particles

4.4 Fabric tensor

As the spheres settle down under gravity, the specimens exhibit a strong anisotropy in the direction of gravity. The anisotropy in the horizontal plane; however, is relatively small (see **Figure 9**). As the number of particles increase from 1000 to 10 000, the difference decrease to half of the magnitude (from 0.02 to 0.009). Further increasing number of particles to 20 000 results in a very small change (0.009 to 0.00894).

Figure 10 shows the effects of different particle size ratios on the packing anisotropy. Obviously, packing become more isotropic when the size ratios decrease and the numbers of particles increase. The packing is almost isotropy when the number of particles is 20 000 for all three particle size ratios.

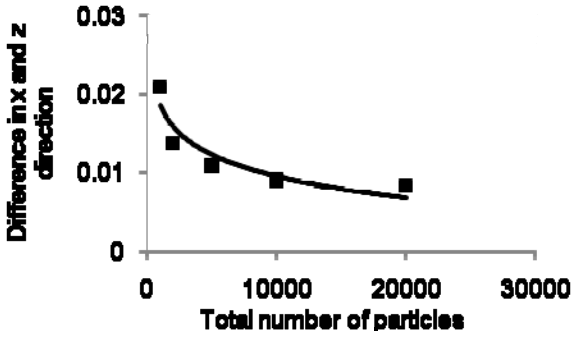

Figure 9 Change in second fabric tensors for monosized sphere packing

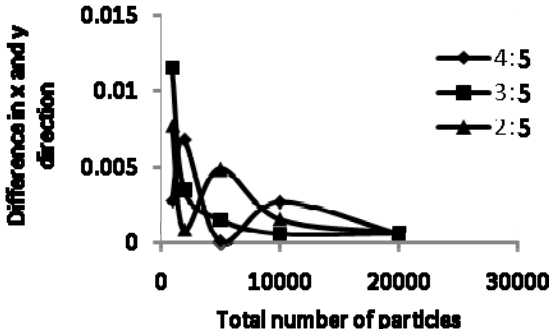

Figure 10 Change in second fabric tensors for different-size ratio packing

5 CONCLUSIONS AND IMPLICATION

A dynamic method of packing to a specified grain size distribution was proposed and used to investigate the properties of mono-sized sphere packings and packings with different-size ratios. The results obtained are in good agreement with those reported in the literature.

The packing of uniform spheres is strongly affected by the dynamic variables, i.e. drop height, number of particles generated each time.

The particle size ratio has a significant influence on the packing porosity and packing fabric tensor.

As the number of particles reached a certain value, the packing exhibited a very small change in all of the examined properties.

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