Numerical Investigation of Materials Porosity Based on the 3D Computer Simulation Particle Packaging Model

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Abstract. This article presents the main components of Monte Carlo methods. An alternative to the basic processes of computer simulation of spherical elements in a stochastic medium is described. A 3D computer simulation model for packaging spherical cylinders (spherical elements) has been developed. The conditions for non-entanglement of two spheres (round particles) are presented mathematically. The motion pattern of spherical elements was modelled, in particular, the position of the lobes before movement and the position of spherical elements after movement. The authors of the paper found out that each sphere requires only three coordinates of the centre (*x, y, z*) in a certain enclosed space, the length of three semi-axes, three Euler angles, and the cross-sectional radius of the cylinder. The authors of the paper presented 3D modelling of round cylinders with a spherical base and described in detail the process of modelling spherical cylinders in a specific direction and point. The results obtained allowed us to study the close relationship between spherical components, as well as to find out how much the shape of non-spherical elements differs from spherical ones. Based on the developed 3D computer model for modelling spherical cylinders, the physical and mechanical properties of materials, in particular porosity, were studied. It was found that the experimental results of porosity increase with increasing diameter of spherical elements (i.e. particles). As a result, it made it possible to predict the porosity of the package. The authors of the paper have also investigated the influence of container parameters (width and height) on the properties (porosity) of materials. In this study, the phenomenon of edge effects was observed, which were caused mainly within the bunker width of 600…800 mm.

Keywords: Polydisperse Simulation, Monte Carlo Methods, Spherical Elements, Packaging, Software, No Intersection Condition, Center Coordinates, Bunker Parameters, Particle Size and Shape.

1 Introduction

Computer modelling of polydisperse simulation, which is carried out in a stochastic medium using randomly distributed spherical particles, is mainly used to study the primary structure of materials formed from various physical and mechanical properties. At the same time, it is very important to focus on modelling spherical cylinders (identical spherical elements), taking into account the main features of Monte Carlo methods. It should be noted that when applying this mathematical method, three main components must be observed: 1) repeated structure; 2) explicit method; 3) a method for selecting a certain chord length. It should also be noted that when modelling particles by Monte Carlo methods, such mathematical and computer modelling is laid down, which randomly selects the required chord length on the current and output track (stage) of neutrons during modelling. The advantage of this method is high computational efficiency, since bunker filling (particle simulation) can be performed using several geometries in a stochastic medium. As well as simulate non-stationary processes that occur when filling the bunker. However, due to the high volume of research and time-consuming experiments, a number of issues remain uncertain and unfounded in the field of modelling.

Therefore, the study of the main stages of modelling based on spherical cylinders or spherical elements in a stochastic environment by 3D computer and mathematical modelling methods is an urgent task.

2 Literature Review

The authors of the scientific work [1, 2] investigated the modelling of particles that interact mainly with dampers. Basically, attention was focused only on the nonlinear behaviour of particles [3]. Scientific works [4] are typical for modelling materials of a particular discrete element, including particle degradation. It should be noted that the destruction of particles is represented in the form of clumps of spheres, which made it impossible to set the parameters of the bunker [5]. In [6], modelling of packaging of non-spherical elements (ellipsoids) is presented, which mainly have an irregular shape and do not take into account the sphericity coefficient. Scientific works [7] are large-scale in the field of modelling. Spherical elements are mainly modelled for heterogeneous materials, which provides a narrow level of abstraction for numerical simulations using particles or grids. The teams of work [8] investigated the microstructure of inhomogeneous materials by computer modelling. It is important to note that the algorithm of the element filling process (spherical and non-spherical) is well described, but it is not fully clear how the authors achieved a correlation between theoretical and experimental results. In [9], a two-stage classifier based on a model for particles only in air is analysed. And also, with computerized scanning electron microscopy. It should be noted that the main attention is paid to the classification of particles based on the elemental composition, while Stochastic media are not taken into account, which is very important for modelling polydisperse modelling. Scientific works [10] investigate the boundary conditions of modelling in arbitrary three-dimensional

boundaries, as well as in models of hydrodynamics of parallel-smoothed particles. It should be noted that the proposed new formula for a solid medium uses the local influence of fictitious elements (particles) that surround each liquid particle and move with it, but do not take into account the accuracy coefficient. Which in turn does not allow you to set the diameter and shape factor of spherical and non-spherical elements. Scientific works [11] are based on Euler-Lagrange predictions based on modelling methods of solid spheres. The authors of the work tracked the motion of particles used to describe the dispersed phase, and also briefly justified the modelling of free bulk. Thus, this operating conditions Matrix does not cover the entire range of spherical cylinder simulations. In scientific articles [12], it is proposed to improve the processes of obtaining heterogeneous materials for manufacturing parts with structural elements by computer modelling methods. It should be noted that the recognition of individual areas in microstructural images by the Smart-eye software package made it possible to study in detail the process of packing spherocylinds. Also, the computer software package made it possible to predict the main structural characteristics of any components in size and shape. In particular, the authors failed to carry out more detailed control between the particles of the initial components (density, porosity, etc.). Experimental data materials [13] characterize the effect of particle sizes on laser absorption and scanning. A three-dimensional model of laser absorption, the absorption capacity of round particles to the laser, and the basic absorption behaviour are investigated. This does not take into account or does not cover the conditions of non-entanglement of the computer model, which is extremely important for any sphere and one-way contact. In [14, 15], it was proposed to use a combination of high-speed Schlieren methods. This simulation should only be combined with a laser beam, which makes it impossible to evaluate 3D modelling at a high-quality level. Since the intervention of laser scanning will give more results in terms of mechanical properties (indicators of heat, mass, pulse of processes), and not imitation of computer backfill. Scientific papers [16, 17] investigate a hybrid liquid-kinetic model for neutral particles. The authors compare two hybrid models based on Monte Carlo methods. It should be noted that the statistical error of the study is 40%, which makes it impossible to study the modelling of round (spherical) elements with maximum accuracy. Thus, a number of issues in the field of computer modelling remain open and require further development and research.

3 Research Methodology

3.1 Computer simulation of spherical elements in a stochastic environment

The aim of the article is to develop a 3D computer simulation model for packing spherical elements, as well as to study the effect of the main edge effects of bunker parameters on porosity and spherical cylinders.

An alternative to the Monte Carlo method (MCM) is the selection of such a geometric position of the center of a spherical ball, which is replaced by computer modelling of the process of random filling with geometric (spherical) elements with distributed sizes, shapes and orientation. Moreover, each spherical element or each group of

them is described by a physical parameter of the material bounded by the surfaces of these geometric shapes, and the modelling process is transferred in the form of corresponding algorithms to computer-information technologies.

Computer simulation of spherical elements in a stochastic medium is shown in Fig. 1.

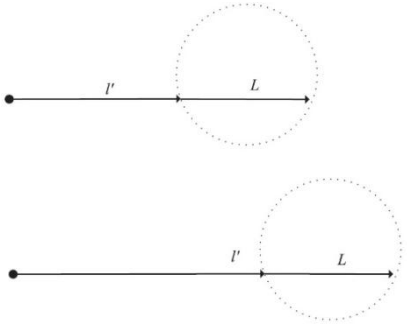


Fig. 1. Computer simulation of spherical elements in a stochastic environment

It should be noted that this study is based on choosing the correct chord length from the current track (position) to the surface of the sphere. Modelling of spherical elements by the traditional Monte Carlo method, which is shown in Fig. 1 makes it possible to estimate the drawing of coordinates of packed spherical elements with a uniform distribution over the volume of the packed container. For this purpose, a specialized software environment for generating pseudorandom numbers with a specific distribution law should be used.

Fig. 2 presents a simulation based on measuring the central position of an already selected element (spherical particle). Therefore, this gives us the opportunity to consider the limiting effect of a stochastic environment.

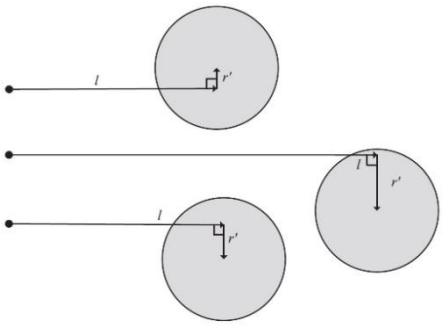
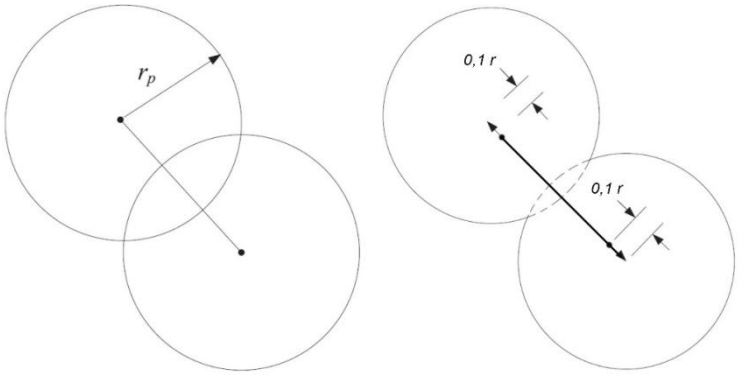


Fig. 2. Sampling the position (center position) of a spherical particle

If we denote by N the number of Poisson points with radius $R(l) + R(l_0)$ in a certain convex region of a unit volume, then the probability of hitting the center of the next packed sphere at one of these points will be equal to e^{-N}.

3.2 Basic motion diagram of spherical elements

The conditions for non-entanglement of two spheres (spherical elements or round particles) are much more complex, and are also associated with finding mandatory conditions for the absence of roots of a system of equations (two quadratic equations). One of these ways to determine their non-repetition is as follows: from both quadratic equations of spheres, only one of the coordinates is explicitly expressed, for example, an applicate, and in the equation for a sphere with a larger applicate, it is necessary to take the radical (center) with the sign (–), and in the second case it is necessary to apply with the sign (+). After that, it is necessary to subtract the second equation from the first equation and find the minimum of this difference, for example, using the fastest descent method. If this minimum or number is not signed (–), it means that the spheres do not intersect. In Fig. 3. the motion diagram of spherical elements is shown.



a) b)

Fig. 3. Diagram of the movement of spherical elements: a – position of the particles before movement; b – of the particles after movement

Such a model, first of all, requires the least number of generalized coordinates for mathematical and computer description of the structure. That is, each sphere requires only three center coordinates (x_{ki}, y_{ki}, z_{ki}) in some enclosed space, the lengths of three semi-axes and three Euler angles, and the cross-sectional radius of the cylinder (R_i). Secondly, it has the shortest, simplest, and fastest algorithms.

4 Results

4.1 Mathematical description of the computer simulation model

The basic condition for non-entanglement of a computer simulation model (i.e., one-way contact with the possibility of lagging) of spheres in the bases of various cylinders was described as follows. That is, we get:

$$\left(x_{ki}-x_{pj}\right)^2+\left(y_{ki}-y_{pj}\right)^2+\left(z_{ki}-z_{pj}\right)^2\geq\left(R_i-R_j\right)^2 \tag{1}$$

where x, y, z – basic coordinates of spherical elements;

i, j – indexes that indicate each individual item number in a packed container ($i = 1, 2,\ldots, n; j = 1, 2, \ldots, n; i \neq j$);

k, p– cylinder base number equal to: $k = 1, 2, 3$; $p = 1, 2, 3$;

R_i – radius of a fully filled container;

R_j – main cross-sectional radius of the cylinder.

It should be noted that to the basic conditions (1), it is necessary to add the conditions for non-entanglement of the spheres of the base of one cylinder with the surface of the spheres of another cylinder. To do this, do the following: alternately lower the perpendiculars from the center of the base of one cylinder to the axis of the other cylinder and then find the point of their intersection. Next, it is necessary to solve a system of equations of a straight axis and a plane perpendicular to it, which intersect through the center of the base of another cylinder. That is, we get the following:

$$\begin{gathered}\frac{x-x_{1i}}{x_{2i}-x_{1i}}=\frac{y-y_{1i}}{y_{2i}-y_{1i}}=\frac{z-z_{1i}}{z_{2i}-z_{1i}}\\ \left(x-x_{pj}\right)\left(x_{2i}-x_{1j}\right)+\left(y-y_{pj}\right)\left(y_{2i}-y_{1j}\right)+\left(z-z_{pj}\right)\left(z_{2i}-z_{1j}\right)=0\\ i=1,2,...,n;\ j=1,2,...,n;i\neq j;\ p=1,2.\end{gathered} \tag{2}$$

If we denote the system of equations (2) by $\left(x^0_{pi\,j}, y^0_{pi\,j}, z^0_{pi\,j}\right)$, and also that this point lies between the bases of the i-th cylinder, then it is necessary:

$$\begin{aligned}x_{ij}<x^0_{pi\,j}<x_{2i}\\ y_{ij}<y^0_{pi\,j}<y_{2i}\\ z_{ij}<z^0_{pi\,j}<z_{2i}\end{aligned} \tag{3}$$

Therefore, from the mathematical description proposed above, the condition must be met: the distance between the base point of a given perpendicular and the point from which this perpendicular is omitted must not be less than the sum of the radii of both cylinders. That is:

$$\left(x^0_{pi\,j}-x_{pi\,j}\right)^2+\left(y^0_{pi\,j}-y_{pi\,j}\right)^2+\left(z^0_{pi\,j}-z_{pi\,j}\right)^2\geq\left(R_i+R_j\right)^2 \tag{4}$$

It should be noted that to check the cross-section of cylinder sections of these spherical elements, it is sufficient to shift the center of the other base along the cylinder axis towards the first base when the center of one base is fixed. At the same time, it is necessary to continuously check the proposed conditions (2) and (3).

4.2 Packing of spherical cylinders (round cylinders with spherical base)

To model spherical elements (round cylindrical particles with a spherical base or spherical cylinders), each individual element was calculated using the form factor F_f. In turn, the form factor F_f was calculated by the dependence $F_f = 1 - H/D$, where H – is the height of the cylindrical section of the round particle (spherical cylinder), and D – is the diameter of round cylinders with a spherical base. It should be noted that as a quantitative indicator of the structural state of the container (package), the average coordination number (ACN) of the container of spherocylinders was used, as well as its relative density P, which is directly related to the porosity of the material under study, and is equal to: $P = 1 - Q$, where Q – is the porosity, which varies within the value from zero to one. It is also important to note that the sphericity coefficient was additionally introduced. Which generally showed how much the shape of non – spherical elements differs from spherical: $F_s = S_s/S$, where $S_s = 4\ \pi r^2$ – is the total surface area of the sphere around the spherical elements; S – is the surface area of the non – spherical ball. The obtained results of modelling round cylinders with a spherical base are shown in Fig. 4.

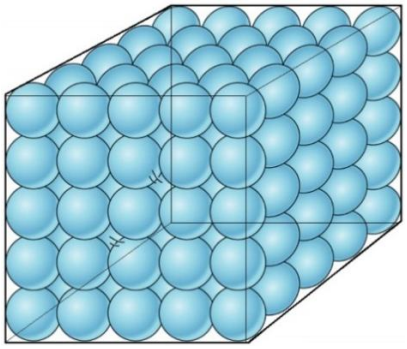


Fig. 4. Modelling of spherical cylinder packaging using the developed software, where: d = 0,5 mm; F_f = 0,5; Q = 10%

It should be noted that when we are dealing with structurally inhomogeneous materials that have a spherical shape, it becomes necessary to specify a specific direction or point in the unit cell. In order to determine the plane of atoms of particles, a fixed shape, a fixed volume, energy, etc. For this purpose, the authors of the paper have established some marking rules, in which three numbers (indexes) were used directly to indicate directions, points, and planes. It was based on a certain index value (i.e., a number), which was a unit cell in the coordinate system. In turn, the coordinate system of the model consisted of three axes (x, y, z). The coordinates of the points directly determined the location of the spherocylinders, as well as the position of their atoms in a container or individual unit cell. Fig. 5 shows modelling of spherical cylinders in a specific direction and point.

It is important that the particles (spherical elements) that are in a solid have a strong relationship and are mainly held together. The small spaces that arise between

the spherocylinders are very small due to the use of vibrational vibrations (i.e., the vibration process can be applied). The space for filling particles has a fixed shape and a fixed volume, because spherical balls can move slowly and at maximum speed if they have enough energy.

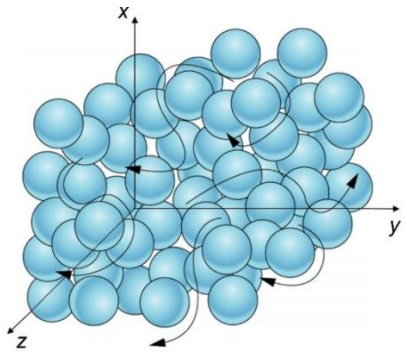


Fig. 5. Modelling of spherical cylinders by direction and point

Also, these elements slide relative to each other (i.e. forward-backward and further), but at the same time remain in their fixed positions.

4.3 Porosity studies based on modelling of spherical elements

A number of packages were made using the developed 3D computer simulation model. The simulation algorithm described above was used for spherical elements (lobules) with a diameter of 8, 10, 12, 14, 16 i 18 mm, packing them in a rectangular container measuring 800×800 mm. For each size of a rectangular container and the diameter of 3D spherical elements (particles), 7…10 variants of experimental backfills were analysed. Experimental data are presented in Table 1 below.

Table 1. Experimental results of porosity from the diameter of spherical elements (particles)

Diameter of spherical cylinders, D (mm)	Porosity, %
8	12.8
10	14.3
12	16.2
14	18.4
16	19.0
18	19.1

From the experimental results of porosity as a function of spherical elements diameter (Fig. 6) the following statement can be made: the obtained porosity results increase with increasing diameter of spherical elements (i.e. particles). Thus, the described 3D

modelling algorithm for spherical cylinders for this study fully reflects the porosity of the package.

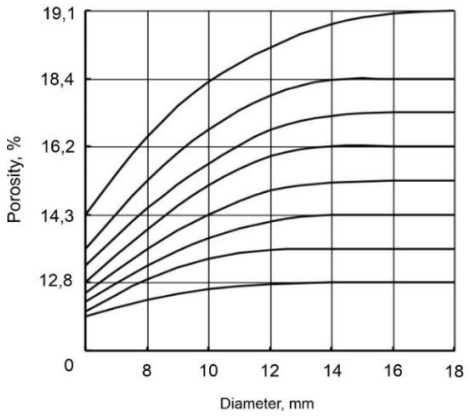


Fig. 6. Experimental dependence of porosity on the diameter of spherical elements

The authors of the paper have also investigated the influence of the specified container parameters (width and height) on the physical and mechanical properties of materials, in particular, porosity. Spherical particles (spherical cylinders) with a diameter of 10, 20 and 30 mm were studied. As a result, 7…10 packages were made for each value of the bunker width and the diameter of the spherical balls. It should be noted that the height of the packed bunker was constant and equal to 1000 mm. The results obtained are presented in Table 2.

Table 2. Porosity results from bunker parameters, particularly width and height

Container parameters, (mm)		**Porosity from the given diameter of spherocylinders, %**		
Width	**Height**	**10**	**20**	**30**
200	1000	16.8	21.0	25.1
400	1000	13.2	17.0	22.5
600	1000	12.1	15.0	20.0
800	1000	9.0	14.1	16.0
1000	1000	9.0	14.0	15.0

Fig. 7 presents experimental results of porosity from the main parameters of the bunker and modelling of spherical elements of different sizes.

It should be noted that from the conducted a number of experiments, which are presented in Fig. 7 there are some deviations in edge effects that are directly related to the main parameters (dimensions) of the bunker for modelling the three studied particle sizes (10 mm, 20 mm, 30 mm).

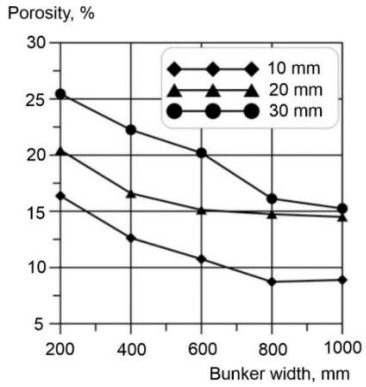


Fig. 7. Predicted porosity results from the main container parameters and modelling of spherical elements of different sizes

It was found that the porosity values change significantly within the bunker width of 600…800 mm and a constant height of 1000 mm. Due to further growth, the parameters of the bunker, in particular the width and height of the packed container, are levelled and do not affect the change in the porosity of the package.

5 Conclusions

The developed 3D model for modelling spherical elements (spherical cylinders) makes it possible to reduce the Ram of Information Systems. And also, to investigate two-dimensional and three-dimensional problems without setting up expensive and voluminous experiments. It should also be noted that the developed 3D software for modelling spherical cylinders allows you to:

1) optimize the porosity of any structural and non-uniform material;
2) model different shapes and sizes of spherical and non-spherical elements;
3) to investigate the relationships and patterns between packed elements, in particular, spherocylinders;
4) observe edge effects that are caused by the size of the bunker;
5) predict the results obtained with a reliable error (± 2%).

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