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Prediction of the Structural Properties of Powder Materials by 3D Modeling Methods

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Abstract. This article examines the main problems of modelling spherical (circular) particles. The main method of the initial process of filling lobules using the Cauchy and Reynolds problem is substantiated. An image of an object-oriented complex of free fall of a spherical particle and their many non-collision spheres is presented. Based on the obtained research results, the main parameters of the process of filling particles of heterogeneous materials. An example of visualization of the developed software product for filling material particles is given, taking into account a number of cross-sections of a cylindrical hopper in height. A histogram of the distribution of material particles from porosity over the volume of a cylindrical hopper is also constructed.

1 Introduction

Sustainable and modern trends in industrial development are the constant growth of standards and quality requirements for all types of new products [1, 2]. It is possible to obtain new materials, powder materials, and heterogeneous materials with stable characteristics using traditional manufacturing technology [3, 4] and powder metallurgy [5]. At the same time, it is necessary to control the main parameters of their structure during the manufacturing process [6, 7]. The most characteristic properties and characteristics that need to be controlled during the manufacturing process include [8]: the granulometric composition (starting material) of the charge, the shape and size of the grain, the density of the packed and molded billet, the quality of internal contacts, porosity, as well as its distribution over the volume of the entire mold [9, 10, 11]. However, traditional powder metallurgy manufacturing methods do not always provide parameters for the desired quality and uniformity of materials in the middle of their structure [12, 13]. And this leads to a big problem and to the fact that it is impossible to get the structural properties of materials at the desired (qualitative) level [14]. Therefore, in order to ensure the effectiveness of traditional methods and powder technologies [15], as well as to obtain better indicators and properties of products for a wide purpose [16, 17], while saving energy costs [18, 19] and reducing labour resources [20] in the process of manufacturing such materials, it is necessary to use modern technologies and capabilities [21, 22]. Namely, modern 3D modelling systems [23, 24, 25]. Thus, forecasting structural characteristics and properties by modern methods of computer modelling [26], forming their structure, as well as controlling parameters during their manufacture is an important task of materials science.

2 Main Part

In the works [27], mainly informational calculation methods and basic physical and chemical characteristics of powder materials are considered [28]. The peculiarity of these works is that the analysis of only the chemical composition of components or their aggregate state of the source material is studied [29, 30]. Reduction of oxides [31, 32, 33], electrolysis of inhomogeneous materials [34, 35], thermal and chemical dissociation of their compounds [36] are observed. However, the prediction of the main indicators and patterns of formation of the structure of

materials [37], as well as their internal properties [38, 39] depend on the geometric parameters of particles of any powder [40]. Therefore, an important question arises regarding the detailed study of this process and its computer modelling [41, 42], which will allow predicting the behaviour of initial and final particles of materials. In addition, the use and improvement of traditional technologies of powder materials is an economically feasible, relevant and modern issue of our time. Therefore, an important place here is occupied by model and computer experiments, namely: forecasting the basic properties of materials using analytical, complex, numerical and based methods and using modern 3D modelling systems.

The purpose of the work is to substantiate the methodology for predicting the initial powder packaging process using modern 3D modelling systems. And also, to conduct a reasonable analysis of the obtained structures with subsequent construction of a histogram of the particle distribution in the volume of a cylindrical hopper.

Materials. During technological operations of pressing and sintering powder and inhomogeneous materials, the particles of the starting material can have different degrees of internal bonds with neighbouring parts, which has a significant impact on the further properties of the composite material that is formed. It is known that the stable granulometric composition of the initial material makes it possible to predict with greater accuracy the main regularities of the formation of the structure and characteristics of heterogeneous materials, taking into account their size and shape, and establish correlations between the initial components, their structure and properties.

The current state of development of mathematical and discrete methods, together with the growing capabilities of 3D modelling computer systems, make it possible to create a new effective calculation methodology for studying any properties of powder materials, as well as to make forecasts within the framework of this study. To do this, it is necessary to solve a whole complex of differential equations with boundary conditions and initial data. It should be noted that a significant difference between these mathematical equations is the presence of a certain parameter h, when changing which it is possible to ensure the convergence of one of the proposed methods, as well as to adjust the specified parameters and properties of the initial and initial powder and inhomogeneous materials in advance.

Let us consider the proposed Cauchy problem (see equation 1):

$$\frac{d}{dx}u(x) - N\big(x, u(x)\big)\,u(x) = \varphi(x),\;\; u(x_0) = u_0, \qquad x \in (x_0 + \infty) \tag{1}$$

where: *N (x, u)* – a real function that is continuous for $x \in x_0 + \infty$ and an infinitely differentiable function for u on the real coordinate axis. That is $N(x,u)\,\epsilon\, C_{x,u}^{x_0,\infty}(x_0 + \infty) \cdot m\,\frac{du}{dt}$;

C – initial (output) parameter;

$\varphi\,(x)$ – continuously differentiable function on an interval $x_0 + \infty$.

Assume that for the proposed problem (1), some conditions for the existence and unity of the complete solution are met. The application of this method indicates that finding an approximate solution of a certain partial sum $u(x) = \sum_{i=0}^{\infty} u^{(i)}(x)$ will be carried out only for the conditions of a cylindrical hopper, when the movement of material particles is carried out according to the following proposed formula (see equation 2):

$$m\frac{du}{dt} = dm\left(1 - \frac{\rho}{\rho_s}\right) - \frac{1}{8}\,\pi D^2 \rho C_D u^2 - \frac{1}{12}\pi D^3 \rho \frac{du}{dt} \tag{2}$$

where: *d* – diameter of grains (particles) of materials;

m – grain (particle) density of materials;

ρ – packing density-hopper filling;

ρ_S – particle density of materials of the s-dimensional sphere;

D^2, D^3 – parameters responsible for the *x, y, z* coordinates of the cylindrical hopper;

C_D – initial particle concentration of materials under standard conditions;
u^2 – speed of movement of each part.

Tests. Since equation (2) is nonlinear, and usually has a differential character, which is solved using mathematical and numerical Reynolds methods, we can reproduce the basic conditions for reproducing the free-fall packing of a spherical particle ball. Also, based on the obtained equation (2), we have created an integrated environment in the form of a computer simulation model. The interface of this program is shown in Fig. 1. It should be noted that the computer simulation model is developed on the basis of the C++ programming language, which allows modelling material particles without setting up an expensive experiment, and is also an object-oriented complex through its accuracy classes and data types, which allows obtaining and predicting reliable particle modelling information.

In Figure 1 a schematic representation of an object-oriented complex of free fall of a spherical particle is presented based on the developed computer program for modelling material particles. And in Figure 2 shows a 3D collision of two or more multiphospheric particles of materials.

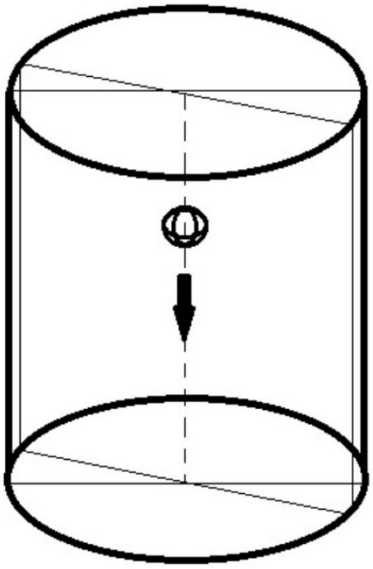

Figure 1. Schematic representation of the free fall of a spherical particle of materials

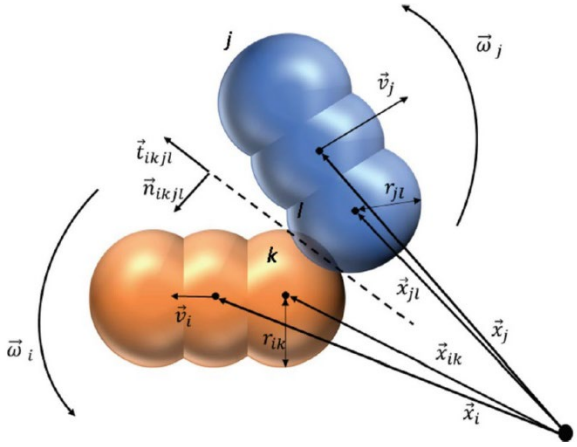

Figure 2. Collision of two or more multipharyngeal particles

Table 1 shows the main average results of computer modelling of packing globular particles of inhomogeneous materials in a cylindrical hopper with the size: H×D = 500×500 pixels.

Table 1. Basic parameters of the powder filling process

Hopper type	Hopper size H×D, [pixel)]	Angle, [α°]	Particle diameter, [pixel]	Porosity [%)]	Average coordination number *
Cylinder	500×500	10	18	21,1	0,34

*– average data from 10 ÷ 20 backfills.

In Figure 3 shows an example of visualization of the software for modelling the backfill of material particles according to the developed computer simulation model. It should be noted that for a reasonable analysis of the porosity distribution, a number of cross-sections of the cylindrical Hopper were performed in height, where: A-A cross-section; B-B cross-section and C-C cross-section, which is shown in Figure 4.

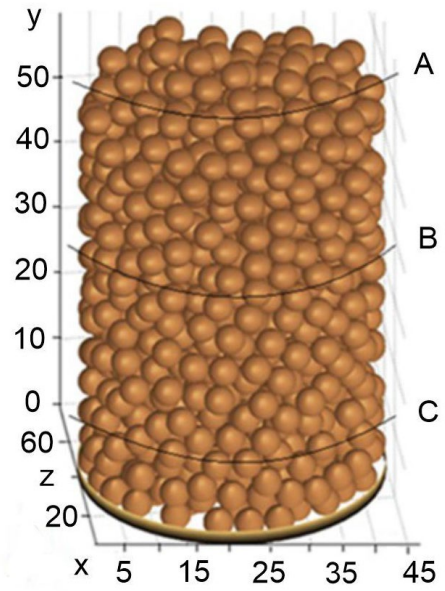

Figure 3. Filling a cylindrical Hopper with material particles using 3D modelling

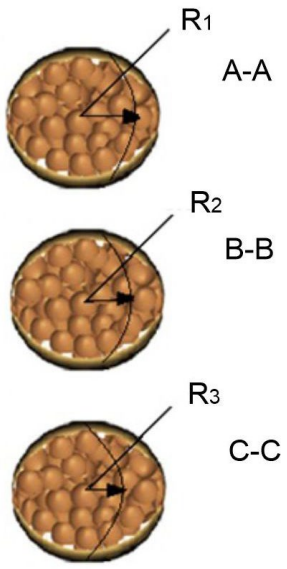

Figure 4. Location of individual particle regions by cross-section

It should be noted that a reasonable analysis of the porosity distribution was carried out using the application program. The application software allows you to determine all the necessary characteristics and parameters that are needed to obtain a qualitative and quantitative assessment of the structure of any structurally inhomogeneous material, including porous ones. The algorithm of operation of the application software package is as follows: Let us have $b_{i,j}$ – the original image, the value of $b_{i,j}$ – is equal to the brightness parameter at a certain focus point $i, j \in D$ where: $i = 1, 2 \ldots n$; $j = 1, 2, 3 \ldots m$. Then the image $b_{i,j}$ of real conditions, as well as the totality of all selected fragments on the image (individual selected objects) will be equal to the following mathematical relation (see equation 3):

$$b_{i,j} = H_1(i,j) + H_2(i,j) + \cdots + H_{s,k}(i,j) \tag{3}$$

where: H_S – total number of selected areas on real objects;

$H_k\,(i, j)$ – image of the k-th object, where: $k = 1, 2, 3, 4, 5 \ldots s$.

The proposed problem for recognizing a real image in this case will consist of finding all the selected (studied) objects, $H_S\,(i, j)$, $Hk\,(i, j)$, which are determined from the general criteria for the uniformity of the selected area (see equation 4):

$$\frac{max}{P \in R} |f\,(P) - m| \times T \tag{4}$$

where: T – initial-real value;

P – value in the selected area R;

m – the average value of any dimensional units (pixels, millimeters, micrometers, etc.) in a certain area of P;

$f\,(p)$ – component brightness distribution parameter function.

Based on the results obtained and the proposed mathematical and numerical methods, Reynolds calculated the average porosity value based on backfills, and also constructed a histogram of the porosity distribution from the radius of material particles. The obtained calculated data are presented in Table 2. The constructed histogram of the filling distribution of material particles is shown in Fig. 5.

Table 2. Dependence of porosity on the particle radius

R, pixel [pK]	Porosity (P), [%]
$R_1 = 250$	40
$R_2 = 150$	27
$R_3 = 50$	21

From the obtained results, it follows that the control and optimization of material particles during their manufacture makes it possible to obtain data on the average coordination number in the dispersed system. That is, to get data on the average number of contacts (connections) of particles with neighbouring components. It should be noted that this parameter allows us to generally assess the quality of the structure of inhomogeneous, powdered and dispersed materials, and also serves as a reference point for constructing any approximation dependences of the main physical characteristics on porosity. In Figure 5 a histogram of the distribution of filling particles of materials from porosity is presented.

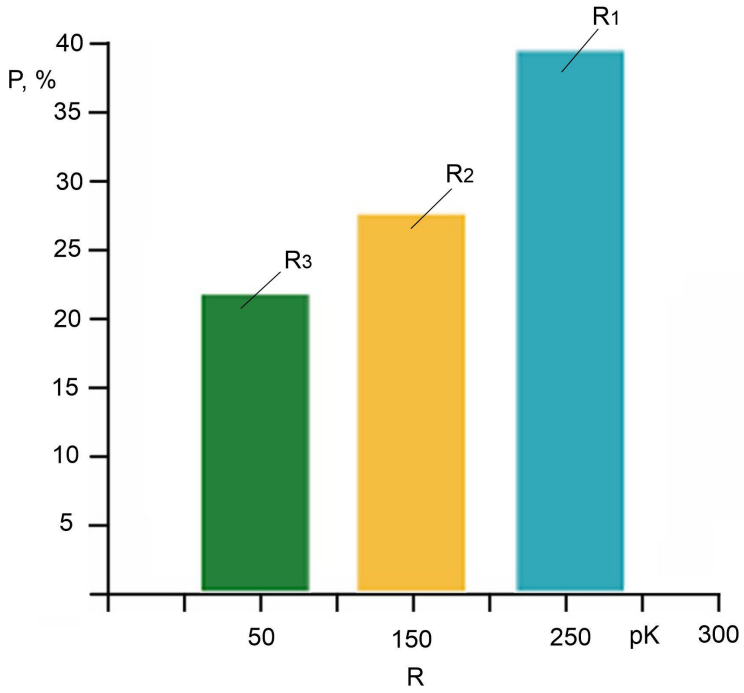

Figure 5. Histogram of the distribution of material particles over the volume of a cylindrical hopper, where: 1 – near the walls of the hopper $R_1 = 250$ pixel; 2 – on distance $R_2 = 150$ pixel; 3 – $R_3 = 50$ pixel

The resulting histogram provides a complete justification for the visual representation of the distribution of material particles by size and provided that the intervals of particle radii in the fractions are the same. In calculations, *n*-th is the number of particles in the range of radii equal r_i to r_j related to the average r_{is}, that is, it fully satisfies the following condition: $Q_n = h(r)$. This indicates that the results obtained fully characterize the differential distribution of material particles over the filling volume of a cylindrical hopper.

3 Conclusion

From the conducted research, it can be concluded that the proposed organization of modern 3D modelling systems, including the latest techniques, algorithmic software and software, can be successfully applied in scientific and technological research. In turn, the process of backfilling and packaging particles of powder materials can significantly improve the final indicators of the main

properties of heterogeneous materials and expand the possibilities of research in the field of modelling structurally inhomogeneous materials.

The implementation of this computer complex allows you to solve the following main problems:

1) investigate and predict the main properties when modelling particles of any materials;
2) 3D modelling of fracture processes on polyhedral structures with certain physical and mechanical properties of materials;
3) investigation of relationships between microscopic structural characteristics of compositions;
4) the ability to control the processes of forming the structure of structurally inhomogeneous materials.

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