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Computer Simulation Modeling of an Inhomogeneous Medium with Ellipse-Shaped Irregular Elements

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Abstract. The article substantiates the main possibilities of filling with irregular bodies, and provides a visual analysis of the parameters formed as a result of structures. It was found out that the form factor acts as the main indicator of the characteristic parameter of changes in the structure and all other parameters of an inhomogeneous medium. It was also found out that when filling a container with irregular ellipsoid elements, the conditions for non-opening (one-way contact) must be met. The obtained calculations of the form factor show the minimum value of the average coordination number of an inhomogeneous medium. This allows us to assert and predict reliable modelling results (± 2-3%). It is also important that the developed simulation model for modelling an inhomogeneous medium using an irregular (ellipsoid) shape of elements can significantly reduce the time spent on conducting field experiments, as well as simulate irregular elements with different shape factors.

1 Introduction

The modern period of human development is characterized by the rapid influence of computer and information technologies that penetrate into all spheres of activity, ensure the spread of information flows in society [1, 2, 3]. The use of the latest technologies makes it possible to make a transition from specific observation and statement of facts to forecasting various properties of a heterogeneous environment, products, materials, processes, etc. [4, 5, 6]. Due to their properties, modern heterogeneous media and ellipsoid-shaped elements find a variety of applications in many industries and require constant improvement at a high-quality and up-to-date level [7, 8]. Obtaining new materials with high-quality structural properties is possible using traditional methods [9, 10]. When developing such materials with the necessary set of qualitative properties, it is necessary to control the parameters of their structure during implementation at all its stages [11, 12, 13]. This applies primarily to the operation of simulating filling in ellipsoid elements [14]. It is known that real forms of structurally inhomogeneous materials have various shapes and sizes, as well as a wide range of parametric composition [15, 16, 17]. In the case of using elements of regular, spherical (spherical) shape, inhomogeneous materials with more or less uniform properties in volume are obtained [18, 19]. The situation becomes more complicated when using elements of an ellipsoid irregular shape [20, 21]. It is difficult to study the structures and physical and mechanical characteristics of such an inhomogeneous medium obtained using such elements (ellipsoid shape) in field experiments due to the wide variety of their parameters, the influence of shape and size [22]. Therefore, the study of the structure of an inhomogeneous medium taking into account elements of irregular (ellipsoid) shape by computer simulation modelling is an urgent task of our time.

2 Main Part

The analysis of structurally heterogeneous environments is carried out by scientific teams under the guidance of [23]. The peculiarity of these works is that the structural characteristics of materials made from elements of a regular shape are modelled. Variants of monodisperse and polydisperse backfilling are considered [24]. The results of computer simulation modelling of backfill of spherical particles of two standard sizes are presented in the activities of scientists [25]. The simulation results were tested on field experiments in the manufacture of some structurally inhomogeneous material, which proved the high efficiency of modelling. The obtained results qualitatively reproduce the process of simulating and filling in irregular elements in the works [26]. But with such a large volume of research, the authors have an unreliable deviation error, which appeared when correlating theoretical and practical experiments. The authors of scientific articles [27] performed modelling of spherical elements that interact with each other. Basically, attention was focused only on the nonlinear behaviour of spherical elements. The works [28, 29] provide a detailed description of computer modelling of a specific discrete element, including the degradation of elements (particles). It should be noted that the destruction of these elements is mainly represented in the form of clumps of spheres (i.e., large spots), which made it impossible to set parameters and control the process of simulating filling at the initial stage of the study. In scientific experiments [30, 31], a simulation simulation of the packaging of non-spherical elements (ellipsoids) is presented, which mainly have an irregular shape of elements and do not take into account the sphericity coefficient. The works [32] highlight the large-scale nature in the field of modelling. Spherical elements (balls) are mainly modelled for inhomogeneous media, which provides a narrow level of abstraction for numerical modelling using irregular and ellipsoid elements [33, 34]. From the material described above, it follows that the development of a computer simulation model for the study of an inhomogeneous environment, as well as the process of simulating elements of ellipsoid and irregular shapes is an urgent task.

Purpose of the work is to develop a computer simulation model for the study of a heterogeneous environment, as well as to simulate the packing of elements of an elliptical (irregular) shape. Based on the obtained results, conduct a visual analysis of the parameters of the resulting structures.

Materials. Some physical and structural characteristics of elliptical elements depend on the shape of their particles, therefore, when studying these characteristics on mathematical models, it is necessary to take into account the deviation of the shape of the elements (particles) from the spherical one. As a criterion for irregularity, the parameter - the elliptical shape of the elements was used. Figure 1 shows the window of the developed software for modelling a heterogeneous environment using an irregular shape of elements - ellipsoids.

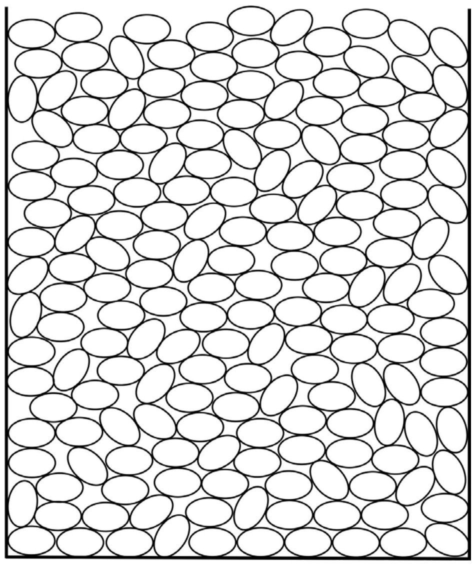

Fig. 1. Modelling of an inhomogeneous medium using an irregular shape of ellipsoid elements

When developing a computer simulation model, the following conditions were used: each element in the package is described by nine generalized center coordinates, the lengths of three semi-axes, and three Euler Nodes (guide axes of the ellipsoid). Spin ellipsoids are a special case of a three-axis ellipsoid in which two axes are equal. Hence, spin ellipsoids are fully described by eight generalized coordinates. The conditions for non-intersection of two ellipsoids are much more difficult to determine, since they are associated with finding the absence of the roots of a system of two elliptical equations. One of the ways to determine not their intersection is that from both equations of ellipsoids, one of the coordinates is expressed explicitly, for example, an applicator, and in the equation for an ellipsoid with a larger applicator of the center, a radical with a negative sign is taken, and in the second - with a positive one. After that, the second one from the first equation is subtracted and the minimum of this difference, for example, using the fast descent method is found. If this minimum is not negative, then the ellipsoids do not intersect. Similarly, the conditions for non-intersection of ellipsoids with the boundaries of a hypothetical container are determined. These conditions do not have an analytical record, and solutions are made only by numerical methods. The sequence of these operations is shown by denoting the elements of the transformation determinant using the following system of equations:

$$
\begin{aligned}
&l_1 = \cos\varphi \ cos\,\psi - cos\,\theta\ sin\,\psi \sin\varphi;\\
&m_1 = \ sin\,\psi\ cos\,\varphi - \ cos\,\theta\ cos\,\psi\ cos\,\varphi;\\
&n_1 = sin\,\theta\ sin\,\varphi;\\
&l_2 = \ - cos\,\psi\ sin\,\varphi - cos\,\theta\ sin\,\psi\ cos\,\varphi;\\
&m_2 = \ - sin\,\psi\ sin\,\varphi - cos\,\theta\ cos\,\psi\ cos\,\varphi;\\
&n_2 = sin\,\theta\ cos\,\varphi;\\
&l_3 = sin\,\theta\ sin\ \psi;\\
&m_3 = \ - sin\,\theta\ cos;\\
&n_3 = cos\,\theta.
\end{aligned}
\tag{1}
$$

where φ – angle of rotation around the new applicator axis (Fig. 2);

ψ – the angle between the abscissa axis and the direct intersection of the coordinate planes with a constant appliqué;

θ – angle between the applicator axes.

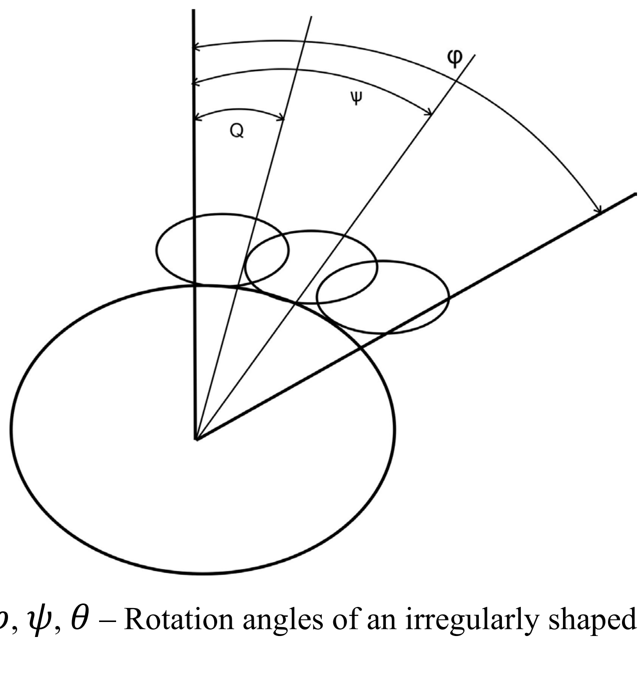

Fig. 2. φ, ψ, θ – Rotation angles of an irregularly shaped ellipsoid

It should be noted that the angles φ, ψ, θ are generalized coordinates of an ellipsoid in space. In turn, the form factor in modelling is determined by the random value of these angles, which reflect the individual structural properties of an inhomogeneous medium. The results of calculating the rotation angle relative to the coordinate axes, and even the form factor, are shown in Tables 1 and 2.

Tests. The conditions for non-intersection (one-way contact) of ellipsoids with the walls of a given container were determined by Formula (2). In addition, the packed spheres could not extend beyond the bunker either. For all packages analyzed, in particular packages with polydisperse elements of ellipsoid shape (i.e., when the container was filled with elements of irregular shape), the following conditions were met, such as:

$$\begin{aligned} X_1 \le x_i \pm a_i \le X_2 \\ Y_1 \le y_i \pm b_i \le Y_2 \\ Z_1 \le z_i \pm c_i \le Z_2 \\ i = 1, 2, \ldots, n, \end{aligned} \tag{2}$$

where (x_i, y_i, z_i) – center coordinates of the ellipsoid;

a_i, b_i, c_i – the lengths of its semi-axes;

X_1, X_2, Y_1, Y_2, Z_1, Z_2 – the boundaries of the bunker in the form of a rectangular parallelepiped according to the corresponding coordinates.

Table 1 presents the results of porosity by form factor. Table 2 presents the results of the angle from the form factor.

Table 1. Dependence of porosity on form factor

P, [%]	**FF**
0.3	90
0.35	80
0.4	70
0.5	60
0.55	50
0.6	40
0.65	30
0.7	20
0.75	10

Table 2. Dependence of the angle on form factor

α,°	**FF**
0.3	0,95
0.4	0,9
0.5	0,7
0.6	0,5
0.7	0,3
0.8	0,1

In Fig. 3 shows the experimental dependence of porosity on the form factor in the range from 0° to 9°. In Fig. 4 shows the experimental dependence of the angle on the form factor in the range from 0° to 9°.

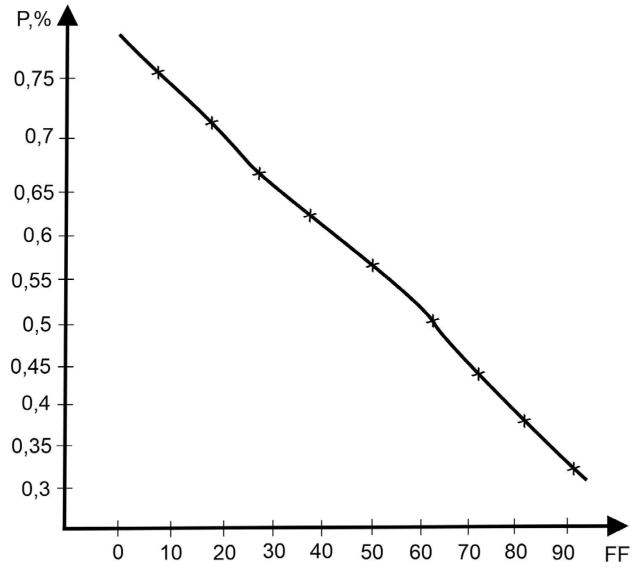

Fig. 3. Experimental dependence of porosity on the form factor in the range from 0° to 9°

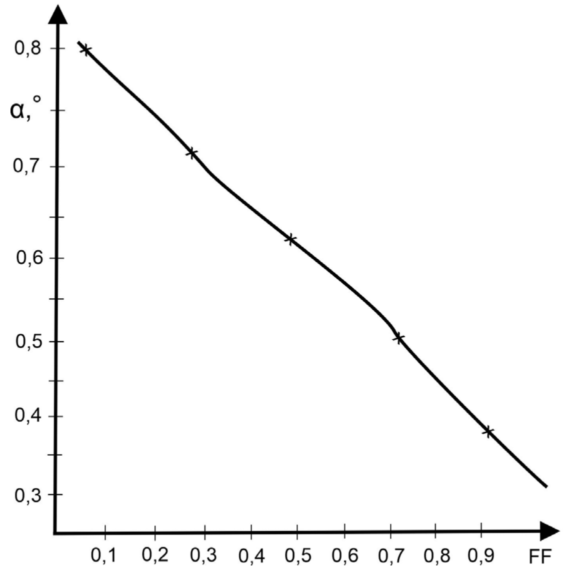

Fig. 4. Experimental dependence of the angle on FF in the range from 0° to 9°

Given Equation (1) of the *i*-th ellipsoid, the following equality will take the form:

$$\frac{(l_{1i}x+l_{2i}y+l_{3i}z+x_i)^2}{a_i^2}+\frac{(m_{1i}x+m_{2i}y+m_{3i}z+y_i)^2}{b_i^2}+\frac{(n_{1i}x+n_{2i}y+n_{3i}z+z_i)^2}{c_i^2}=1 \quad (3)$$

where $x_i,\ y_i,\ z_i$ – coordinates of the ellipsoid;

$a_i,\ b_i, c_i$ – lengths of semi-axes, generalized coordinates of the i-th ellipsoid.

From equation (3) *z* is defined as expression:

$$z = f_1(x,y) \pm \sqrt{g_i\,(x,y)} \quad (4)$$

where $f_1(x,y)$ and $g_i\,(x,y)$ polynomials of the second degree calculated by the transformation coefficients of equation (1) and other generalized coordinates. To determine the non-intersection of the i-th and j-th ellipsoids, the following expression is applied and get:

$$\varphi_{ij}\,(x,y) = f_i\,(x,y) - f_j\,(x,y) - \sqrt{g_i\,(x,y)} - \sqrt{g_j\,(x,y)} \quad (5)$$

which is the difference of the second part of the curve of equation (3) of the i-th ellipsoid, as well as the upper part of the j-th ellipsoid, if $z_i > z_j$. In the domain of definition $\varphi_{i,j}\,(x,y)$, this expression has a positive minimum, if the ellipsoids do not intersect, the following condition will be fulfilled and get:

$$\min \varphi_{i,j}\,(x,y) \geq 0 \quad (6)$$

where $i = 1, 2, \ldots n$; $j = 1, 2, \ldots\ldots n$; $i \neq j$, after which all n ellipsoids will form a packing of an irregular (ellipsoidal) shape, which is presented in (Fig. 5). In Fig. 6 shows the packing of elements of an elliptical (irregular) shape with a form factor of 0.4 and a porosity of 0.6%.

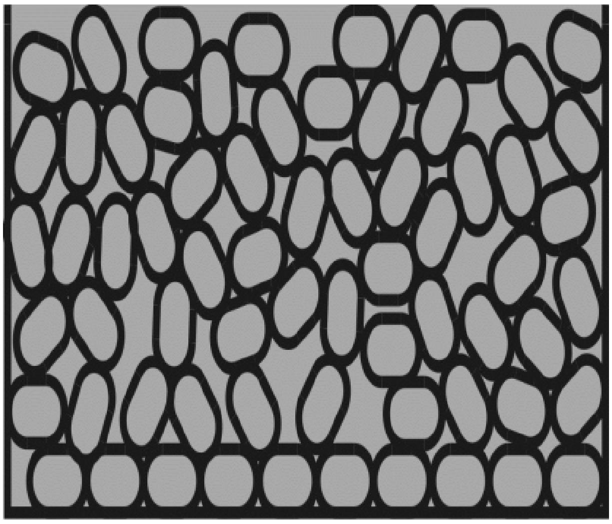

Fig. 5. Packing of elements of an elliptical (irregular) shape, where: FF = 0.3 and P = 0.7

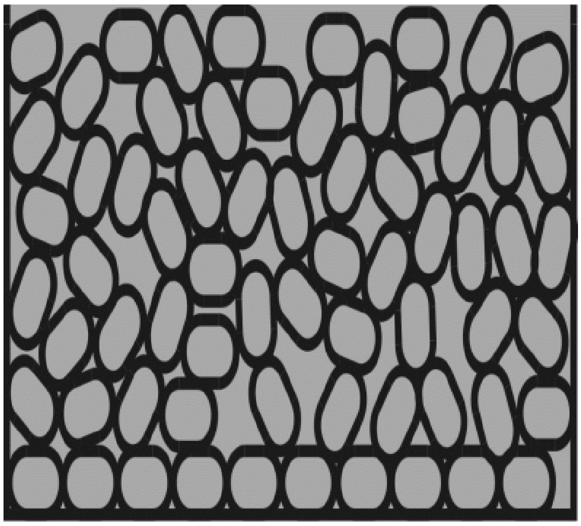

Fig. 6. Packing of ellipsoid (irregular) shaped elements, where: FF = 0.4 and P = 0.6

The results of calculations of the average coordination number depending on the form factor (FF) of the elliptical elements are shown in Fig. 7. In turn, the shape factor FF of elliptical elements was calculated according to the dependence $FF = 1 - (H/D)$, where H – is the height of the cylindrical section of the element (particle) of elliptical shape, and D – is its diameter.

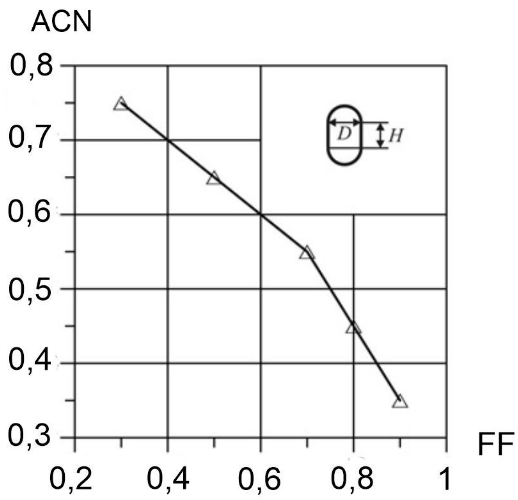

Fig. 7. Experimental and calculated dependence of the average coordination number on the shape factor (FF) of ellipsoid elements

From the one shown in Fig. 7 the experimental dependence of the average coordination number on the shape Factor shows that the lowest average coordination number value is achieved in the case of elements of ellipsoid (irregular) shape. It is known that minimizing the average coordination number is important when studying an inhomogeneous medium, while high or moderate porosity is important for elements of certain filter installations.

3 Conclusion

From the data of computer simulation modelling of packing ellipsoid-shaped elements in a container, it can be concluded that the form factor acts as the main indicator of the characteristic parameter of changes in the structure and all other parameters of an inhomogeneous medium. It was found out that when filling a container with irregular ellipsoid elements, the conditions for non-opening (one-way contact) must be met. It is also important that the average coordination number of an inhomogeneous medium, which should reach minimum values, also depends on the calculations of the form factor. Since minimizing the average coordination number is an important component in the study of an inhomogeneous medium. Thus, it can be argued that the developed simulation model for modelling an inhomogeneous medium using the irregular (ellipsoid) shape of elements allows:

1) model elements with different form factors;
2) investigate the main indicators of packaging and elements of irregular (ellipsoid) shape;
3) predict reliable simulation results (± 2-3%);
4) significantly reduce the time spent on conducting field experiments.

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