Two-Dimensional Model of Mix of Disperse Materials

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***Abstract*— The numerical model of uniform mix of disperse materials which allows to predict her quality of dispersion of distribution of a key component depending on is offered: average concentration of a key component; size of his disperse particles; shares of the mix taken as test (the amount of test).**

***Keywords*— disperse material; mix; key component; quality of mixing; fractal dimension; dispersion of distribution of a key component; test volume; size of particles**

I. Introduction

Mixing of disperse materials makes a basis of production of the majority of modern materials and products on their basis. The mathematical analysis of process of preparation of mix is kept many decades, nevertheless, of still reliable technique of assessment of quality of mix and furthermore his forecasting [1–2].

For forecasting of quality of mix – calculation of uniformity of distribution of components in separate tests of material or in relation to products of the small size in the theoretical plan it is expedient to address methods of imitating modeling. Recently they with great success are used for the solution of tasks in various fields of science and technology.

II. Description of the mathematical model

There is a question in what the distinction of the mixes containing disperse particles of the different sizes and whether it is possible to measure this distinction consists. In this case only one dispersion isn't enough, it is necessary to use still some characteristic of mix.

The fractal dimension of a set of particles [10] can be such characteristic. Generally, if $N^{1/d}$ – a positive integer, then d – the measured rectangular parallelepiped can be spread out to number of parallelepipeds, each of which turns out from an initial N parallelepiped transformation of similarity with similarity coefficient [5–9] $r(N) = 1/N^{1/d}$. The dimension d (from the English capacity dimension – capacitor dimension) is characterized by a ratio

$$d = -\frac{\ln N}{\ln r(N)} = \frac{\ln N}{\ln \frac{1}{r(N)}} \tag{1}$$

We will consider uniform distribution N_o of points along some line, or one-dimensional variety in three-dimensional space ε. The set of points can be covered with small cubes $N(\varepsilon)$ with an edge length $(N(\varepsilon) < N_o)$. If the number N_o is large, the number of cubes that cover the line will change depending on ε how: $N(\varepsilon) \approx 1/\varepsilon^2$.

Similarly, if the points are evenly distributed over a two-dimensional surface in three-dimensional space, the minimum number of cubes covering the set will vary depending on ε how: $N(\varepsilon) \approx 1/\varepsilon^2$. The dimension in the General case is determined by the law of similarity

$$N(\varepsilon) \approx 1/\varepsilon^d, \tag{2}$$

from which the fractal dimension of the set of points follows:

$$d = \lim_{\varepsilon \to 0} \frac{\ln N(\varepsilon)}{\ln(1/\varepsilon)}. \tag{3}$$

From a multicomponent mixture of volume V, you can proceed to the analysis of a system that combines a plurality of coordinates of particles of its components. In General, the fractal dimension of such a set is determined by the expression (3), which, provided the finiteness of the particle sizes, will have the following form:

$d = \ln N / \ln(1/\varepsilon)$, где N – the number of elements of the set (the number of particles of the key component in the mixture); ε – the size of the unit cubes covering the points of the set (a measure of the set).

From a practical point of view, it is necessary to determine the possible deviation of the concentration of a given (key) component in an arbitrary sample from its average value in a mixture with a random distribution of components.

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The properties of the mixture are known: the volume of a single particle v_0; their volume average concentration c_0.

The external conditions are, the total volume V of the mixture, the volume of the sample $V^* = \alpha V$ ($0 \le \alpha \le 1$).

The development of this approach, based on the value of the fractal dimension of the mixture d and the sample d^*, allowed to obtain an expression for the calculation of the dispersion of the distribution of the key component in the volume of the mixture

$$\sigma = \frac{c_0}{\sqrt{2\pi e}} \Delta d \, \exp\{\Delta d\},$$

$$\Delta d = d - d^* = d_0 \frac{\ln(\alpha)\,\ln(c_0)}{\ln(V/v_0)\,\ln(\alpha V/v_0)} \quad (4)$$

In order to test this hypothesis, as well as the correctness of the expression (4), a numerical simulation of a mixture with a random uniform distribution of dispersed particles was performed.

A numerical model of the mixture can be obtained if these particles are randomly arranged in space. For ease of calculations, we construct a flat (two-dimensional) model of the mixture. Let's use the Monte Carlo method and place a certain number of particles in a square with a side equal to one.

In the case of a flat approximation of the expression to determine the coordinates of individual particles will have the following form: $x_i = \gamma$, $y_i = \beta$, where $-\gamma, \beta$ random numbers with uniform distribution from zero to one.

Since the particle sizes were not taken into account in the present case, it is not possible to use the expression (2) to calculate the fractal dimension. Here it is possible to use equation (1) and to construct dependence of number N of particles on the size of the considered area r.

The approximation by equation (1) yields a value $d = 1{,}981546$. At the same time, the size of the region varied from the smallest value of 0.000625 to one.

If the dispersed particles are absolutely evenly distributed over the surface of the unit square, the value of the fractal dimension must be equal to two.

The results of the simulation show d that it is not possible to obtain a value equal to two when performing calculations with finite accuracy.

This value changed with the change in the number of particles. When the number of particles to 10 000 consistently get a value d equal to two times with precision to the third sign (the calculations were carried out with eight significant digits). At lower particle numbers, the value d was less than two.

We can talk about the existence of heterogeneity of particle distribution (mathematical points) on the surface of a unit square, despite the fact that they are randomly distributed. At a certain ratio of the number of particles and the size of the mixture, the model exhibits fractal properties. No more information can be obtained from these views. Further development of the model involves taking into account the finite size of dispersed particles.

Within the framework of the plane problem we solve r_o, we assume that the key component is disks of size, which are randomly distributed over the plane of a square with a side equal to one. It is important that the disks do not overlap each other, i.e. it is necessary to maintain a distance of at least their diameter between any pair of disks. Since the position of the disk can be set by its two coordinates, the main limitation will be as follows:

$$\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2} - 2 \cdot r_0 > 0\,. \quad (5)$$

To calculate the coordinates of the individual disks included in this expression, use (5). The number of disks determines the volume content of the key component that must be obtained in the mixture. For calculation of dispersion of distribution of particles [3-4] it is necessary: to choose the size of sample; to divide the unit square into cells equal to the size of sample; to count how many disks (particles) got to each cell.

The calculation of dispersion is preceded by the determination of the average content of dispersed particles in a cell, or rather a fraction of the occupied surface of a unit square, which will be equal to the average content of the key component in the mixture $\langle c \rangle = \pi\, r^2 N_0$.

When calculating the variance, it is necessary to take into account the size of the cell, which was set as a part of the unit size of the square by dividing its size (unit) by an integer n. For example, if a single square was divided into one hundred parts, it was taken equal to ten. Then the expression for calculation of dispersion will have the following form:

$$\sigma = \sqrt{\frac{1}{n^2} \sum_i^n \sum_j^n (\pi\, r^2 n^2 K_{i,j} - \langle c_i \rangle)^2}, \qquad N_0 = \sum_i^n \sum_j^n K_{i,j}. \quad (6)$$

The expression (6) is written taking into account the specifics of the problem. It allows you to calculate the variance of the fraction of the surface occupied by particles in individual cells. Since the size of the analyzed area (the volume of the mixture) is one, the concentration of the target component in the sample is equal to the part of the surface occupied by particles in the cell.

At the same time $\pi r^2 n^2 K_{i,j}$ – the proportion of the surface occupied by the particles of the cell with coordinates i, j. The second expression reflects the fact that the total number of particles equals their sum in all cells.

When changing the number and size of disks, it is possible to change the volume content of the key component in the mixture, as well as to investigate the direct impact of the particle size on the quality of the mixture. The proposed model also allows for the analysis of the mixture using samples of different sizes. Dispersion (6) and fractal dimension (1) were calculated in all numerical experiments.

As the number of disks (dispersed particles) increases and their size increases, the distribution uniformity increases, as evidenced by the decrease of dispersion in relation to the average value of the content of the key component. The nature of the dispersion dependence on the sample size is in good agreement with the results of experiments, i.e. the proposed model correctly reflects the features of the dispersed particles distribution in the mixture volume.

For the first time on the basis of numerical experiments it is shown that the value of fractal dimension is directly related to the quality of mixing and, along with dispersion, can be its numerical characteristic. It can be argued that the mixture of dispersed particles exhibits the properties of fractal dimension only if the particles have a finite size. For a mixture with a lower relative dispersion of the best quality, the fractal dimension is calculated by expression:

$$d^* = 2\left(1 + \frac{\ln\langle c_0\rangle}{\ln(N)}\right)$$

III. Conclusion

The results of the calculations show that not every mixture with a random distribution of components is homogeneous. The proposed model of the mixture of dispersed materials, constructed using the Monte Carlo method, allows to predict the distribution of the key component in its volume depending on the size of dispersed particles and their volume content. Due to sufficient simplicity and transparency, the model can be successfully used in the development of compositions with the same distribution uniformity in the mixture of the original dispersed materials.

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