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Development of New Constructive and Heat-Insulating Materials

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Abstract**: *The question of the development of a new methodological approach to the creation of a heat-insulating constructional building material for external enclosing structures of buildings and structures of railway transport is considered. The results of numerical experimental studies of the cellular concrete macrostructure are presented. The dependence of the fractal dimension of the pore structure of cellular concrete on the magnitude of porosity for hexagonal and cubic types of laying particles of concrete was obtained.***

Keywords: railway buildings and structures, structurally-insulating material, cellular concrete, macrostructure, modeling, optimization, fractal dimension.

1. INTRODUCTION

Improving energy efficiency and energy saving of buildings and structures is a priority in the energy policy of Uzbekistan. In this regard, the production on an industrial scale of energy-efficient, inexpensive and environmentally friendly structurally-insulating building materials is one of the urgent problems of construction science [10-14].

Successful implementation of such tasks in the field of civil engineering urgently requires the development of a new methodological approach to the creation of building materials for external enclosing structures with specified sets of properties. To develop a technique for modeling properties, a material was chosen that has a developed porous structure - cellular concrete, represented by various types of pores: capillary, large, conditionally closed, and gel. When implementing this task, an assumption was introduced that cellular concrete is represented as a quasi-homogeneous medium, as a set of packed particles and with integral physical characteristics [15-18].

The defining elements of such a matrix are the parameters of the macrostructure of cellular concrete, which characterize the relationship of the macrostructure with their strength and heat engineering properties.

For the first time the theoretical substantiation of the connection between the macrostructure of cellular concrete and their strength was proposed by G. I. Loginov and A. P. Filin [1, 2]. The researchers, on the basis of mathematical models characterizing the occupancy of a unit of volume by spherical bodies, derived fairly strict regularities describing the “ideal” structure of cellular concrete.

It follows from the above that solving the problem of optimizing the macrostructure of cellular concrete to increase their technical and operational properties theoretically, on the one hand, is an extremely difficult task because of its multifunctionality. On the other hand, solving a problem of such a plan on the basis of an experiment by the “trial and error” method is very long and laborious. Moreover, an experiment based on some technological approach does not guarantee a positive result when processing even a large amount of a specific material taken in a fairly wide range. Therefore, to solve the problem, it is most expedient to use an approach based on mathematical modeling, which allows, based on the developed physical and mathematical model, subjected to algorithmization and implemented as a software product, through numerical calculations, to obtain the desired optimal material parameters.

2. ALGORITHM FOR CONSTRUCTING THE IMAGE OF CELLULAR CONCRETE OF A GIVEN STRUCTURE AND ITS FRACTAL DIMENSION

Let $m \times n$ be the given matrix (base) of a sample of cellular concrete, where m is the width, n is the height of the matrix, respectively. This area will be packed with spherical pores (a circle on a plane), using two types of packaging - hexagonal and cubic. These two types of packaging are chosen, generally speaking, from obvious prerequisites, since the greatest value of porosity with a spherical shape of pores is achieved in the conditions of their geometrically correct packing (packing), to which, cubic and hexagonal belong.

Further, we denote the matrix and the components of concrete with black color of the image, and the pores with white. Then, the description of the structure of cellular concrete in terms of the formation of its image will be expressed in the form of pixels (the minimum element of the raster image) of black and white color - a binary image. Thus, the minimum unit of the pore radius is a pixel uniquely determined by the metric system of units in fractions of a centimeter. As a result, specifying the type of styling by building a system of polygons of a given type, place the pores (white pixels) at the vertices of this polygon. Then, algorithmically recognizing the “material - pores” border on an image is reduced to a simple procedure for determining the

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brightness level: black (000) is material, white (255) is pores. This is the main goal of the image quantization method introduced in the work to the *i*-th number of levels, of which the last, binary level, in fact, automatically determines the border of porosity in the sample. Now it remains only to calculate the percentage occupied by white pixels of the total area of the image, and we obtain the degree of porosity of the sample. On the basis of the developed method, the reverse formulation of the problem is also possible: on the basis of a given percentage of material porosity, obtain the most optimal pore arrangement (type of packaging) that meets the specified parameters of strength and thermal conductivity of cellular concrete. Having a specific type of image of cellular concrete, obtained as a result of modeling, otherwise, a specific type of package of pores of certain dimensions that meets the required (specified) parameters, further, we can set the technological task of obtaining it. Here it is necessary to note the following: the method described in this article is focused on a flat image, that is, a volume projection of the sample onto the plane is considered. Since we, when building the optical model of the image of cellular concrete, we operate with circles with given radii displayed on the plane, distortions about its three-dimensional image when calculating the porosity of the model "flat" image, for obvious reasons, occur. However, the application of the method to real samples showed that the magnitude of the errors does not exceed 3%. Moreover, in our opinion, there are no principal difficulties in applying the proposed method to volume realization, for example, the consideration of stereographic or holographic images.

Further, using formula (1), we calculate *D* - the parameter of the fractal dimension of the structure of cellular concrete using the modified Peano algorithm - the “Box Counting” method [3]. According to this method of calculating the fractal dimension D is determined by the expression:

$$D = \frac{\ln N}{\ln\left(\frac{1}{\delta}\right)}, \qquad (1)$$

Where δ is a square grid cell with the size δ×δ covering the binary image, *N* is the number of square cells where the points (with coordinates x_i, y_j, i=1, m, j=1, k) are located on the image “material – pores”.

Next, the dependence of *D* on the number of squares covering the fractal is plotted in a double logarithmic scale. As will be shown below, this dependence is well approximated by a straight line (linear regression)

$$Y = kx + b \qquad (2)$$

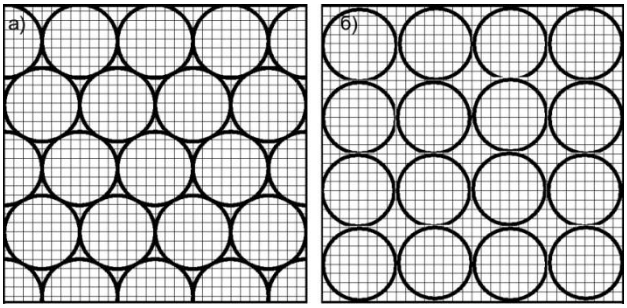
The slope *k* of the line determines the fractal dimension

$$D = -k \qquad (3)$$

The accuracy of this method was tested using the Koch curve [4], the theoretical fractal dimension of which is D = 1.262. For this curve in our test version, based on the method described above, the dimension of this curve was D = 1.250. Thus, the error of the “Box Counting” algorithm used does not exceed 1%.

3. NUMERICAL MODEL EXPERIMENTAL STUDIES AND RESULTS OF THE CELLULAR CONCRETE MACROSTRUCTURE

Numerical experiments were carried out aimed at identifying features of the connection of the fractal structure, as a function of the type of laying, cellular concrete with its porosity, and therefore with the strength and heat engineering properties. Pore sizes in modeling the structure of cellular concrete, in accordance with [5], were set in the range of pore radii from 0.2 to 2 mm with a step of 0.2 mm. Thus, the range of porosity ranging from 10 to 90% was considered. The variation of the percentage of porosity was carried out by changing the distance between the pores of a fixed radius, representing the nodes of the hexagonal and cubic lattice.



Pic. 1. Model representation of cellular concrete with an ideal maximum dense packing of hexagonal (a) and cubic (b) types with a square grid for the implementation of the algorithm for calculating the fractal dimension

Table 1 Calculation results of the fractal dimension of cellular concrete with different pore radii with hexagonal packaging

$S(R_п)$, %	$R_п$, мм	$\log\frac{1}{2R_п}$	$\log S(R_п)$	*D*
10	0,2	0.998	1.000	1,874
20	0,4	0.698	1.301	1,540
30	0,6	0.521	1.477	1,355
40	0,8	0.396	1.602	1,235
50	1,0	0.299	1.699	1,150
60	1,2	0.219	1.778	1,105
70	1,4	0.153	1.845	1,065
80	1,6	0.094	1.903	1,020
85	1,8	0.044	1.929	0,995
90	2,0	0.0060	1.954	0,965

Note: $R_п$ - pore radius; S ($R_п$) - area occupied by pores; *D* is the fractal dimension.

In pic. 1 shows a modeled (within the framework of the developed software complex) image of cellular concrete with perfect hexagonal and cubic packs with a grid with squares superimposed on the image, which were used to determine the fractal dimension of the model samples according to the algorithm. The results of the calculations are presented in Table. one.

The relationship of porosity of cellular concrete with various types of laying with its fractal dimension is presented in Table 2.

Table 2 Connection of porosity of cellular concrete with various types of laying with its fractal dimension

P, %	Type of laying		
	Hexagonal	Cubic	«Random»
	D	*D*	*D*
10	1,283	1,321	1,546
20	1,525	1,407	1,587
30	1,775	1,497	1,632
40	1,817	1,511	1,659
50	1,833	1,523	1,671
60	1,847	1,541	1,682
70	1,852	1,582	1,694
80	1,638	1,525	1,546
85	1,541	1,461	1,482
90	1,431	1,432	1,383

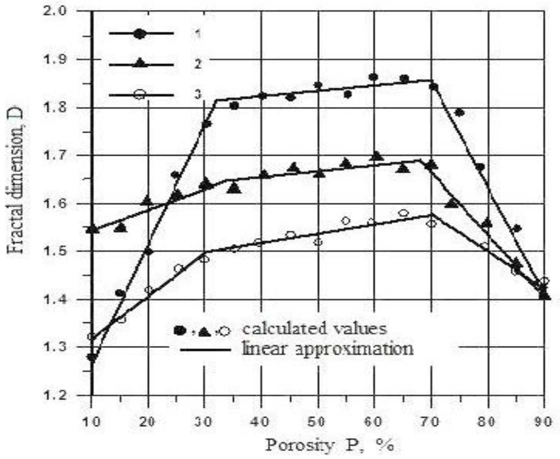
In pic. 2, which shows the dependence of the fractal dimension of the pore structure of cellular concrete on the magnitude of the porosity for the hexagonal and cubic types of laying. One can see the presence of three sections: with an increase in porosity in the range of ≈10 - 35%, the fractal dimension linearly increases; in the range of ≈30– 70%, the linear growth of the fractal dimension is insignificant; in the range of ≈ 68–90%, the fractal dimension linearly decreases. At the same time, the rates of growth and reduction of the fractal dimension of the structure of cellular concrete are different for the types of laying considered. So, for hexagonal type of laying:

- on the interval of 10-33%, a noticeable increase is approximated by a straight line
$$D = 0.02498 P + 1.0166;$$
- in the range of 33 - 70% slight growth – direct
$$D = 0.00114 P + 1.777;$$
- in the range of 70-90% linear reduction – direct
$$D = - 0.02236 P + 3.444.$$

For cubic styling we have:

- on the interval of 10-30%, a noticeable growth is approximated by a straight line
$$D = 0.0893 P + 1.2277;$$
- in the range of 30 - 70% slight growth – direct
$$D = 0.00195 P + 1.454;$$
- in the range of 70-90% linear reduction – direct
$$D = - 0.00786 P + 2{,}128.$$

As can be seen from the presented results, the changes in the fractal dimension described by a straight line at the corresponding intervals are unequal for the hexagonal and cubic packings: the slope *k* of the straight line, which characterizes the rate of increase (decrease) of the function, for the hexagonal pack has larger values than for the cubic one. These two types of ideal structure of cellular concrete can be considered as limiting types of packages from the point of view of the upper and lower limits of the rate of change of the fractal dimension of the structure of a porous material.



Pic. 2. The relationship between the fractal dimension *D* and the porosity P (%) in cellular concrete with hexagonal (1), cubic (3) and random (using a random number generator) types of laying (2) with a given percentage of porosity.

A rather nontrivial change in the fractal dimension of the structure of cellular concrete, associated with the nature of the change in the pore structure, directly indicates the features of the organization of the structure of cellular concrete itself, namely:

- the first interval (≈10 - 35%) - is the transition of the pore structure from isolated spherical pores to interconnected pore clusters, where the spherical pores merge and form pore clusters with branched boundaries, which causes an increase in fractal dimension;
- in the second interval (≈30 - 70%) with an increase in the pore space, where the fractal dimension changes (increases) slightly (slope coefficient - $k \approx 10^{-4}$), the geometrical configuration of the pore boundaries does not change, but only their length;
- in the third interval (≈70- 90%), in which the fractal dimension decreases, very large pores formed, as a result of which the boundaries are geometrically smooth, and their irregularity decreases, which determines the decrease in the fractal dimension.

It seems to us that this behavior of the fractal dimension is related to the percolation thresholds known in porous materials [6, 7].

Thus, on the basis of the developed method for analyzing the surface of the porous structure of cellular concrete, it was possible, in addition to its fractal nature itself, to obtain a correlation with known features in the behavior of porous materials. However, these results were obtained on simulated samples with an ideal structure, which cannot be obtained technologically in practical production work. Therefore, it is to be expected that, when applying the appropriate technologies, only to one degree or another can approach the model obtained in this article and possibly occupy an intermediate position in terms of their fractal characteristics. In this connection, a numerical experiment was performed in which the structure of cellular concrete was modeled to conditions close to real samples. To do this, using a random number generator for specified ranges of sizes of spherical pores and a given percentage of porosity, the structure of cellular concrete was modeled. The simulation results were analyzed on the basis of the constructed histograms for a given pore content in the entire considered range (from 10 to 90%). The results of model calculations were approximated by Gauss curves (the normal law of probability distribution) and Cauchy – Lorentz curves [8].

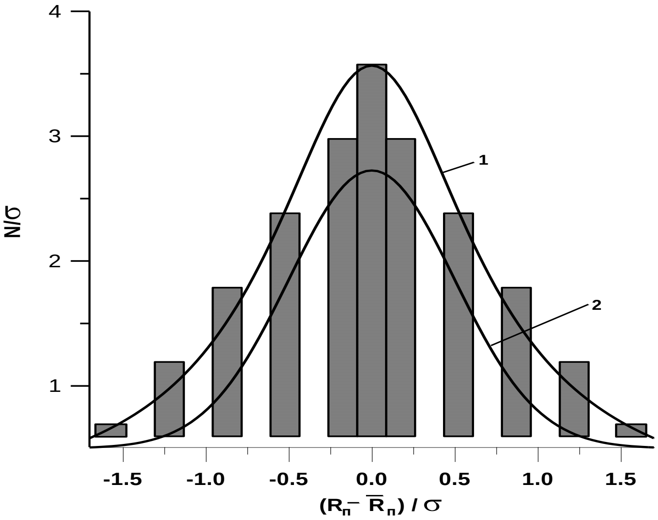
In pic. 4, as an example, a histogram of the model calculation of the structure of cellular concrete using a random number generator for a pore space of 50% in the range of pore sizes with a radius of 0.2 to 2 mm, approximated by the Gauss function:

$$G(\Delta R_{п},\sigma)\cong \exp([\Delta R_{п}]^2/\sigma^2) \qquad (4)$$

Where, σ is the standard deviation, and the Cauchy – Lorentz function:

$$P(\Delta R_{п},\overline{R}_{п},b)=\frac{1}{\pi}\cdot\frac{b}{(R_{п}-\overline{R}_{п})^2+b^2} \qquad (5)$$

Where $R_{ï}$ - is the radius of pores, is the average value from the specified range, b is the scale parameter of half-width at half-height. The Gaussian function modeled the distribution function describes very roughly, while the Cauchy-Lorentz function describes it with sufficient accuracy (Pic. 4) [9].



Pic. 3. A histogram of the probability density distribution of pores in size, normalized to the standard deviation and its approximation by the Cauchy – Lorentz functions (1) and Gauss (2).

Note*: N is the percentage number of pores of a given radius from the specified range, σ is the standard deviation.*

4. CONCLUSION

The results of calculations of the fractal dimension for the structure of cellular concrete modeled in a “random” manner are shown in Pic. 4 (curve 2). As was to be expected, the position of this fractal curve, or straight lines in three sections, occupies some intermediate position between the fractal curves with perfect hexagonal and cubic layouts. It is important that the ranges of variability practically coincide with those calculated by the model with ideal packaging. Therefore, the obtained conclusions based on the analysis of the fractal structure of cellular concrete with theoretically ideal packaging fully apply to the model, which in its structural organization approaches the real, that is, technologically secured.

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