Mathematical Modeling of Structural Organization of Constructive-Heat-Insulating Construction Materials

Shaumarov Said, Adilhodzhaev Anvar

Abstract—The article is devoted to the determination of the fractal dimension of the porous surface and further finding the relationship of the fractal dimension with the porosity of cellular concrete. A numerical experiment was carried out aimed at determining the fractal dimension of the structure of cellular concrete in order to clarify the relationship of the latter with its porous structure.

Keywords: fractal dimension, cellular concrete, structural simulation, porosity.

I. INTRODUCTION

One of the urgent tasks of modern building science is the implementation of directional structure formation of concrete, including cellular. Moreover, the effect on the structure of cellular concrete is of particular interest, since as a result of this, this building material can be obtained with characteristics that allow it to be used as structural, heat-insulating, and structural-heat-insulating [1-2].

The macrostructure of cellular concrete is represented by the predominant pore volume (50-92%) and inter-pore walls, which, in turn, consist of hydration products, an unhydrated binder and siliceous component, capillary, helium and contraction pores that characterize the concrete microstructure. The macrostructure of aerated concrete is formed as a result of technological methods, but in order to correctly develop the necessary operations that provide the required properties of the material (strength, thermal conductivity), you should know: what size pores should be and how they should be packed; what should be the density of the substance of the inter-pore septa and their thickness [3-5].

Theoretically, any set of particles can be quite fully described by the corresponding matrix, consisting of elements in the form of descriptions of all the individual properties of each of the particles, including their individual phase coordinates - physical state parameters. The defining elements of such a matrix are the parameters of the macrostructure of cellular concrete, characterizing the relationship of the macrostructure with their strength and thermal properties [6-7].

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 [8-11].

The properties of building materials, including heat insulating materials, are determined both by the state of the structure of substances from which they are produced and by the macrostructure formed as a result of technological conversion. According to [12-13], the optimal structure corresponds to the complex of the most favorable indicators of the building and operational properties of the conglomerate. On this basis, the optimal structures of cellular concrete include those that are characterized by maximum values of porosity with a uniform distribution of pores and aggregate by volume [14-15].

In the study of the properties of cellular concrete being developed, the main objects are a quasi-homogeneous medium, as an aggregate of a multitude of packed particles and its integral physical characteristics [16-17]. Theoretically, any set of particles can be quite fully described by the corresponding matrix consisting of elements in the form of descriptions of the individual properties of each of the particles, including their individual phase coordinates — the physical parameters of the state. The defining elements of such a matrix are the parameters of the macrostructure of cellular concrete, which characterize the connection with their strength and heat engineering properties.

II. A MATHEMATICAL MODEL OF THE STRUCTURE OF CELLULAR CONCRETE

To solve this problem, it is most expedient to use an approach based on mathematical modeling, which allows, based on the developed physical and mathematical model, algorithmized and implemented as a software product, by numerical calculations, to obtain the desired optimal material parameters.

As a result, to develop a mathematical model of the structure of cellular concrete, the following statement of the problem was adopted: for the required (given) value of the
thermal conductivity coefficient, obtain the macrostructure of cellular concrete (a certain porosity, pore size, pore packing, and size of partitions) corresponding to the required thermal conductivity. The correctness of the task, in addition to experimental studies, follows from the thermodynamic analysis of heat and moisture transfer in porous materials.

For a theoretical description of the process of heat and moisture transfer in porous media with sufficient accuracy, you can use the system of differential equations obtained by A. V. Lykov [18-19]:

\[ C_\varepsilon \frac{dT}{dt} - \varepsilon r \frac{dW_i}{dt} = \nabla(\kappa \nabla T) + (C_1 \frac{D}{\rho_l} \nabla W_i + C_1 \frac{D}{\rho_l} \nabla T), \]

\[ (1 - \varepsilon) \frac{dW_i}{dt} = \nabla(D_i \nabla W_i) + (D_n \nabla T). \]  
\( (1) \) \( (2) \)

In (1), (2): \( C_\varepsilon = C_s + W_i C_1 ; \) \( T, \) \( C_s \) respectively the temperature and thermal conductivity of a wet body; \( C_s \) – is the specific heat of a unit volume of the dry porous material \( W_i \), \( C_i \) is the concentration, specific heat, specific heat of evaporation, heat transfer coefficient of liquid moisture, coefficient of thermal diffusion of the liquid, respectively; \( \nabla \) phase transformation criterion, which is defined as the ratio of the change in moisture content through evaporation and condensation to the change in moisture content due to liquid transfer; \( \nabla = \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z} \) \( \nabla \) operator Nabla.

The system of differential equations of heat and moisture transfer in porous materials presented in form (1), (2) is undoubtedly simpler than its classical representation [19], but this simplicity, firstly, creates certain difficulties in their practical application, since the criterion phase transition is a “fictitious” physical parameter for which there is no fundamental possibility of measuring it. Secondly, from the point of view of the problem posed by us, it is extremely important that in equations (1), (2) in the explicit form there is no predominance for porous materials, in particular, for cellular concrete, the porosity parameter. Therefore, we transform equations (1), (2) to the form, eliminating the parameter \( \nabla \), from them, introducing the porosity parameter \( P \):

\[ C_\varepsilon \frac{dT}{dt} - r \frac{dW_i}{dt} = \nabla(\kappa \nabla T) + (C_1 \frac{D}{\rho_l} \nabla W_i + D_n \nabla T), \]

\[ R \frac{dT}{dt} + Q \frac{dW_i}{dt} = \nabla(D_i \nabla W_i) + \nabla[D_i \nabla W_i]. \]  
\( (3) \) \( (4) \)

\[ C_\varepsilon = C_s + W_i C_1 + W_v C_v; \]

\[ m = \frac{\partial \lambda}{\partial P} + C_1 \frac{D}{\rho_l} + C_1 \frac{D}{\rho_l} \]

\[ k = \frac{\partial \lambda}{\partial W_i} + C_i \frac{D}{\rho_l} + C_i \frac{D}{\rho_l}; \]

\[ W_v = \rho_v \left( P - \frac{W_i}{\rho_l} \right); \rho_v = \rho_v(T, W_i); \]

\[ R = \frac{\partial \rho_v}{\partial T} \left( P - \frac{W_i}{\rho_l} \right); \rho_v = \rho_v(T, W_i). \]

\[ Q = 1 - \frac{\rho_v}{\rho_l} + \frac{\partial \rho_v}{\partial W_i} \left( P - \frac{W_i}{\rho_l} \right). \]

Having got rid of the “fictitious” physical parameter \( \varepsilon \), having explicitly introduced the porosity parameter as a function of moisture and vapor

\[ P = \frac{W_i}{\rho_l} + \frac{W_v}{\rho_v}. \]

The presence of air is not reflected in equations (3), (4), so that when completely dried \( (W_i = W_v = 0) \) (3) - (5) lose their meaning. Therefore, it is necessary to perform the last step in transforming the original equations by introducing air into them. To do this, we transform (3) - (5) taking into account the air concentration \( W_{a} \), specific heat of air \( C_{a} \), air transfer coefficient \( D_{a} \), thermal diffusion coefficient of air \( D_{a} \) and air density \( \rho_{a} \):

\[ \frac{\partial W_{a}}{\partial t} = \nabla(D_{a} \nabla W_{a} + D_{a} \nabla T) + I, \]

\[ \frac{\partial W_i}{\partial t} = \nabla[D_i \nabla W_{a} + D_{i} \nabla T] - I, \]

\[ \frac{\partial W_v}{\partial t} = \nabla[D_{i} \nabla W_{a} + D_{i} \nabla T], \]

\[ \frac{\partial T}{\partial t} = \nabla(T \nabla T) - r \left[ (C_1 \frac{D}{\rho_l} + C_1 \frac{D}{\rho_l}) \nabla W_i + (C_i \frac{D}{\rho_l} + C_i \frac{D}{\rho_l}) \nabla T \right] \]

\[ P = \frac{W_i}{\rho_l} + \frac{W_v}{\rho_v} + \frac{W_{a}}{\rho_{a}}. \]  
\( (6) \) \( (7) \) \( (8) \) \( (9) \) \( (10) \)

Here, \( C_{\varepsilon} = C_s + W_i C_1 + W_v C_v + W_{a} C_{a} \),

\( W = W_i + W_v + W_{a} \), \( I \) – is the rate of change in the concentration of vapors resulting from the evaporation of liquid moisture.

III.RESULTS & DISCUSSIONS

Equations (6) - (8) describe the transfer of moisture and air, and equation (9) is the heat equation for a porous body (cellular concrete) taking into account the transfer of moisture, air and evaporation of liquid moisture. Equation (10), in contrast to (5), remains valid (does not degenerate) upon complete drying of the sample. Thus, in the absence of moisture, the entire pore volume will be occupied by air. In accordance with the task, this condition is considered in this paper, i.e. the connection of the thermal conductivity of cellular concrete \( (W_i = W_v = 0) \) with its macrostructure (porosity) in its pure form under conditions of complete drying in the absence of other conditions (moisture, liquid), distorting this connection, is considered.
Summing up equations (6), (7) and substituting I from (7) into (9), we obtain:

$$\frac{\partial W_i}{\partial t} + \frac{\partial W_a}{\partial t} = \nabla(D_i \nabla W + D_t \nabla T) + \nabla(D_a \nabla W + D_a \nabla T),$$

$$W = W_i + W_a = \rho_i a + \left(1 - \frac{\rho_a}{\rho_i}\right) W_i + \left(1 - \frac{\rho_a}{\rho_i}\right) W_a$$

And finally, assuming the above put forward condition - “absolute dryness”, $$W_i = W_a = 0$$ finally get the system

$$\frac{\partial T}{\partial t} = \frac{\rho_a}{\rho_i} \nabla \left(\frac{D_a \nabla W + D_a \nabla T}{\rho_i}\right),$$

$$C_T \frac{\partial T}{\partial t} = \nabla (\lambda \nabla T) + C_a D_a \nabla W \nabla T + C_a D_a (\nabla T)^2, \quad (17)$$

Where

$$R = \frac{\partial \rho_a}{\partial T} \frac{\rho_a W_a}{\rho_i} \left(1 + \frac{1}{\rho_a}\right)$$

$$Q = 1; W = W_a.$$

In the resulting system, there remained the parameter of the density of the liquid $$\rho_v$$, which (liquid) does not exist at the accepted “absolute dryness”, $$\rho_v = 0$$. However, it is easy to see that when substituting $$R$$ in (6), $$\frac{\rho_a}{\rho_i}$$ the relations in the left and right sides are reduced.

### IV. CONCLUSION

The resulting system of differential equations (1) and (2) describes the heat transfer process for a given coefficient of thermal conductivity, depending on the macrostructure of aerated concrete, characterized by the porosity parameter $$P$$.

Based on the obtained mathematical model, a software package was developed for calculating the macrostructure of cellular concrete for the required (given) thermal conductivity of the material. Numerical calculations were made. The results of modeling the macrostructure of aerated concrete for a thermal conductivity coefficient specified in the range of values from 0.085 to 0.334 W/m °C with a matrix density of 2000 kg/m³ and a “random” type of paving with a three-mode distribution density are presented in Table.

#### Table. The results of modeling the macrostructure of aerated concrete

| Coefficient thermal conductivity, W/m °C | Size since, mm | thickness partitions, mm | Average density, kg/m³ | Strength, MPa | Porosity, % |
|----------------------------------------|----------------|-------------------------|------------------------|----------------|------------|
| 0.085                                  | 2.426          | 2.086                   | 300                    | 1              | 85         |
|                                        | 1.618          |                         |                        |                |            |
|                                        | 3.466          |                         |                        |                |            |
| 0.095                                  | 2.473          | 2.251                   | 400                    | 2              | 81         |
|                                        | 1.649          |                         |                        |                |            |
|                                        | 3.534          |                         |                        |                |            |
| 0.123                                  | 2.403          | 2.187                   | 500                    | 3              | 74         |
|                                        | 1.602          |                         |                        |                |            |
|                                        | 3.434          |                         |                        |                |            |
| 0.143                                  | 2.220          | 2.020                   | 600                    | 4              | 71         |
|                                        | 1.480          |                         |                        |                |            |
|                                        | 3.171          |                         |                        |                |            |
# Mathematical Modeling of Structural Organization of Constructive-Heat-Insulating Construction Materials

| Reference | Description |
|-----------|-------------|
| 0.174     | $r_1=1.808$, $r_2=1.205$, $r_3=2.582$ | 700 | 5 | 66 |
| 0.199     | $r_1=1.429$, $r_2=0.952$, $r_3=2.041$ | 800 | 6 | 60 |
| 0.233     | $r_1=0.931$, $r_2=1.621$, $r_3=1.330$ | 0.847 | 900 | 8 | 55 |
| 0.262     | $r_1=0.575$, $r_2=0.384$, $r_3=0.822$ | 0.524 | 1000 | 10 | 52 |
| 0.314     | $r_1=0.161$, $r_2=0.107$, $r_3=0.230$ | 0.147 | 1100 | 12 | 45 |
| 0.334     | $r_1=0.073$, $r_2=0.049$, $r_3=0.105$ | 0.067 | 1200 | 16 | 40 |

## REFERENCES

1. Adilhodzayev A.I., Makhamataliev I.M., Shaumarov S.S. Theoretical aspects of the structural-imitation modeling of the macrostructure of composite building materials. *Scientific and Technical Bulletin of the Bryansk State University*, 2018, 3, 312-320.

2. Adilhodzayev A.I., Shaumarov S.S. The issue of improving the energy efficiency of buildings in railway transport. Modern problems of the transport complex of Russia. 2018, 1, 4-11.

3. Shaumarov S.S. Modeling the process of forming the temperature field of the external fencing of buildings on the railway transport. *Scientific and Technical Bulletin of the Bryansk State University*, 2018, 3, pp.338-346.

4. Shaumarov S.S., Shipacheva Y.A. An integrated approach to the problem of thermal renewal of the walls of panel buildings. «TRANS-MECH-ART-CHEM»: materials of the VII International scientific practical conference. Moscow, MIIT, 2010, pp.239-241.

5. Adilhodzayev A.I., Shaumarov S.S. The issue of thermal renovation of infrastructure of railway transport is evaluated. X International Scientific Conference “Transport Problems - 2018”, Wisla, Katowice, Poland. p. 13-18.

6. Shaumarov S.S. “On the issue of increasing energetic efficiency of buildings in railway transport”.: VIII International Scientific Conference “Transport Problems - 2016”, Katowice, Poland. 522-532 p.

7. S.S. Shaumarov, A.I. Adilhodzhayev, V.I. Kondrazhenko, Experimental research of structural organization of heat-insulating structural building materials for energy efficient buildings. XXII International Scientific Conference on Advanced in Civil Engineering «Construction the formation of living environment» p. 1-7 (2019).

8. A.I. Adilhodzhayev, S.S. Shaumarov, E.V. Shipacheva, U.Z. Shermuhamedov, S.I. Kandikhvor, Some Aspects of the Photo-Optical Method of Estimation Composition of Light Concrete. International Journal of Engineering and Advanced Technology (IJETT). ISSN: 2249 – 8958, Vol. 8 Issue-5, p. 1924-1927, (2019).

9. S.S. Shaumarov, A.I. Adilhodzhaz, E.V. Shipacheva, S.I. Kandikhvor, Development of New Constructive and Heat-Insulating Materials. International Journal of Recent Technology and Engineering (IJRTE). ISSN: 2277-3878, Vol.7. Issue-5S3, p. 577-580. (2019).

10. S.S. Shaumarov, A.I. Adilhodzhaz, E.V. Shipacheva, S.I. Kandikhvor, To the Question of the Influence of the Intensity of Active Centers on the Surface of Mineral Fillers on the Properties of Fine-Grained Concrete. International Journal of Innovative Technology and Exploring Engineering (IJITEE). ISSN: 2278-3075, Vol. 8, Issue- 9S2, P.219-222 (2019).

11. U.Z. Shermuxamedov, S.S. Shaumarov Impact of configuration errors on the dynamic International Scientific Conference on Advanced in Civil Engineering «Construction the formation of oscillation absorbers effectiveness of different masses on the seismic resistance of bridges. XXII living environment» p. 1-8 (2019)

12. A. Adilhodzhaz, S. Shaumarov, E. Shipacheva, U. Shermuhamedov, New Method for Diagnostic of Heat Engineering and Mechanical Properties of Cellular Concrete. International Journal of Engineering and Advanced Technology (IJETT). ISSN: 2249 – 8958, Vol. 9. Issue-1, p.6885-6887, (2019)

13. Rybyev I.A. Patterns in the structural-mechanical properties of asphalt concrete, VZBI materials, 1957, 1, 3-18. (in Russian)]

14. Andreja Abina, Uroš Puc, Anton Jeglič, Aleksander Zidanšek. Structural characterization of thermal insulation building materials using terahertz spectroscopy and terahertz pulsed imaging. Journal “NDT & E International” 2016, vol.77, 11-18.

15. Bouvard D., Chai J.M., Dendievel R., Fazekas A., Létang J.M., Peix G., Quenard D. Characterization and simulation of lightweight concrete. Journal "Cement and Concrete Research", 2007, vol.37, issue 12, pp.1666-1673.

16. She Wei, Chen Yiqiang, Zhang Yunsheng, Jones M.R. Characterization and fomed concrete. Journal "Construction and Building Materials" 2013, vol. 47, pp.1278-1291.

17. Kim H.K., Jeon J.H., Lee H.K Workability, and mechanical, acoustic and thermal properties of lightweight aggregate concrete with a high volume of entrained air. Journal of Construction and Building Materials, 2012, 29, pp.193-200

18. Lykov A. V. Phenomenon of transport in capillary - porous bodies. M.: GITTL, 1954 - 189 p.

19. Reshetin O. L., Orlov S. Yu. The theory of heat and moisture transfer in a capillary-porous body // Journal of Technical Physics, 1998, Volume 68, No. 2, P. 3-16. 

**Published By:**
Blue Eyes Intelligence Engineering & Sciences Publication