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COMPUTER MODELING OF PROPERTIES OF A COMPOSITE MATERIAL WITH POROUS FILLERS

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The article is devoted to forecasting of heat-shielding and mechanical properties of composite materials based on porous fillers. Analytical dependencies for determining the thermal conductivity coefficient of materials of homogeneous and heterogeneous structure are given. Based on the finite element method, there has been developed a method for numerical determination of the thermal conductivity coefficient of composite materials with a variotropic structure. The results of computer studies are in line with the dependences obtained on analytical models. The expediency of using multilayer composite materials based on porous fillers in load-bearing and enclosing structures of shell and plate types has been shown.

Keywords: composite material, porous filler, thermal conductivity, finite element method, multilayer shell.

Introduction

Concrete retains its leading position in the modern construction due to its vast raw material base, the ability to control composition and structure, the variety of products, high technical characteristics and durability. Lightweight concrete is an effective type of composite material that combines mechanical strength with heat-shielding properties. Development of lightweight concrete technology is associated with the creation of highly porous fillers of form stability and development of rational structures of the composite material. Variety of shapes and heterogeneity of the surface of filler's particles, chemical instability of the binder stone, defectiveness of the contact zone set the concrete up as one of the complex artificial composite materials. The structure of concrete, as a composite material, consists of two main components as follows: a matrix (a binder stone) and a discrete component (filler particles). Regulation of lightweight concrete properties is achieved by changing filler's porosity, the content and structure of composite material's matrix.

To increase the efficiency of lightweight concrete, it is important that structure's indicators (the size and nature of filler's particles distribution, the content of the matrix) provide high heat-shielding properties, the maximum value of elastic modulus of the composite material without loss of system connectivity [1–3].

The criterion for heat-shielding properties of materials is the coefficient of thermal conductivity, the values of which are determined instrumentally using devices of various modifications and calculation methods [4–7]. For many natural and artificial materials, the values of thermal conductivity coefficient were determined and given in the reference literature. To develop technology and improve the efficiency of composite materials of a combined structure with balanced mechanical and thermal insulation properties, it is necessary to predict thermal conductivity at the stage of composite development [8–10]. Therefore, analytical and numerical methods for determining this characteristic for a composite material are very relevant. Formulas for calculating the thermal conductivity coefficient of porous concrete are known [11–15]. The use of newly developed porous granular filler and matrix requires refinement of methodology for determining the thermal conductivity coefficient of lightweight concrete.

The aim of the work is to study the nature of the change in thermal conductivity and mechanical properties of a composite material based on granular porous filler by numerical methods.

Previously, authors had carried out numerical studies of the influence of porous filler's characteristics on composite material's strength properties. The paper [4] represents the results obtained using the Lira Sapr program, which makes it possible to study stress-strain state of systems taking into account the plastic and brittle deformation mechanisms. The studies made it possible to determine boundary values of filler's packing density, to identify critical situations leading to grains flattening. This work is continuation of research on composite materials.

1. Object and methods of research

The object of the study was a cementless composite material of a multilayer variotropic structure, made from molding sands containing various amounts of porous granular filler. Variotropic concrete is characterized by variable values of density and strength over the section of the moulded product, smooth transition of layers with structural properties into heat-insulating layers. Instrumental determination of the thermal conductivity of composite materials of this structure is difficult.

Here are some well-known analytical dependencies for determining the thermal conductivity coefficient, which are used both for homogeneous porous media and for heterogeneous systems, for example, concrete with porous granular filler. To calculate thermal conductivity of binary mixtures (λ_{mix}), consisting of continuous matrix (stone binder concrete) with a thermal conductivity coefficient of λ_{mat} and discrete inclusions (concrete filler) with a thermal conductivity coefficient λ_{fil}, it is possible to use the formula of V.I. Odelevsky [4, 6, 8]. However, for calculation of concrete with high content of filler (for example,a large-pore structure), this formula is unacceptable.

Calculations by the method of Landau P.F. [4, 8, 16] for mixtures with the number of phases i, which occupy volumes Vi, provide an error of no more than 14% compared to the experimental data:

$$\lambda^{\frac{1}{3}}{}_{mix} = \sum_i V_i \lambda_i^{\frac{1}{3}}. \qquad (1)$$

To determine thermal conductivity coefficient of a binary mixture with a matrix volume content V_{mat} and filler volume content V_{fil}, the Burger formula is used [4, 8, 16], in which C is an empirical coefficient depending on distribution of phases in the system:

$$\lambda_{mix} = \frac{V_{mat}\lambda_{mat} + cV_{fil}\lambda_{fil}}{V_{mat} + cV_{fil}}. \qquad (2)$$

The need to select the value of the coefficient C for each composition reduces universality of the formula (2). The value of empirical coefficient can be calculated by comparing the formula (2) with other mathematical models, for example, with the well-known Maxwell formula [17]:

$$\lambda_{mix} = \lambda_{mat}\left(\frac{\lambda_{fil} + 2\lambda_{mat} - 2V_{fil}(\lambda_{mat} - \lambda_{fil})}{\lambda_{fil} + 2\lambda_{mat} + V_{fil}(\lambda_{mat} - \lambda_{fil})}\right). \qquad (3)$$

The solution of the system of equations (2) and (3) makes it possible to determine the value of the coefficient C:

$$C = V_{mat}\frac{V_{mix}\lambda_{mat}}{V_{fil}(\lambda_{mat} - \lambda_{mix})}. \qquad (4)$$

Using the dependences according to formulas (1), (2) the coefficients of thermal conductivity are calculated for arbitrary concrete compositions that differ in the content and properties of the components (Table 1). The values of the coefficient C (Table 1) are determined using equation (4). Analysis of the calculation results indicates sensitivity of analytical methods to changes in the composition of concrete. However, the use of calculation methods has limitations. For example, for concretes with a matrix, the thermal conductivity of which is equal to or less than the thermal conductivity of the filler, the coefficient C takes values close to zero. This is not typical for real concrete structures.

Wide opportunities for modeling and predicting the properties of composite materials are provided by computer programs [18-21]. The finite element method implements the solution of stationary and non-stationary problems of thermal conductivity and thermoelasticity [22, 23]. For a flat system, it is efficient to use the Agros2D program (University of West Bohemia, Pilsen, Czech Republic), developed for calculating physical fields of various nature.

Numerical modeling of thermal conductivity was performed on the example of a composite material with porous granular filler. Two options for the structure of lightweight concrete were considered. The first option is a regular packing of filler particles of the same diameter, equal to 0.7 cm (Figure 1a). The second option is filler particles with diameters of 0.7 and 1.0 cm are distributed according to the law of an equilateral triangle (Figure 2a).

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The method developed for numerical determination of thermal conductivity coefficient for the models under study is based on the well-known dependence relating the heat flux (q), the temperature of the outer surface of the layer (tc_1), the temperature of the inner surface of the layer (tc_2), the layer thickness (δ) and the thermal conductivity of the layer (λ) [4, 6]:

$$q = \frac{\lambda\left(tc_1 - tc_2\right)}{\delta}. \quad (5)$$

Based on equation (5), the thermal conductivity of the layer is equal to:

$$\lambda = \frac{q \cdot \delta}{(tc_1 - tc_2)}. \quad (6)$$

Calculation results using the numerical method are shown in Table 1.

Calculations of composite material's mechanical characteristics were made for the structures of roof and ceiling under the distributed load P = 10 kN/m^2. The accepted value of load corresponds to the normative indicator of permanent and temporary load for standard prefabricated and monolithic reinforced concrete structures.

To assess the level of stresses in the model under study, the method recommended by the Construction Norms and Rules 2.03.01.84 «Concrete and reinforced concrete structures» was used. The bending moment, M, in the design section can be expressed in terms of the height of the concrete compression zone, determined by the parameter, α_R, and the normal bending stresses in the concrete, R_b, and reinforcement, R_{SC}, by the formula:

$$M \le \alpha_R R_b b \delta_0^2 + R_{SC} A'_S \left(\delta_0 - a'\right), \quad (7)$$

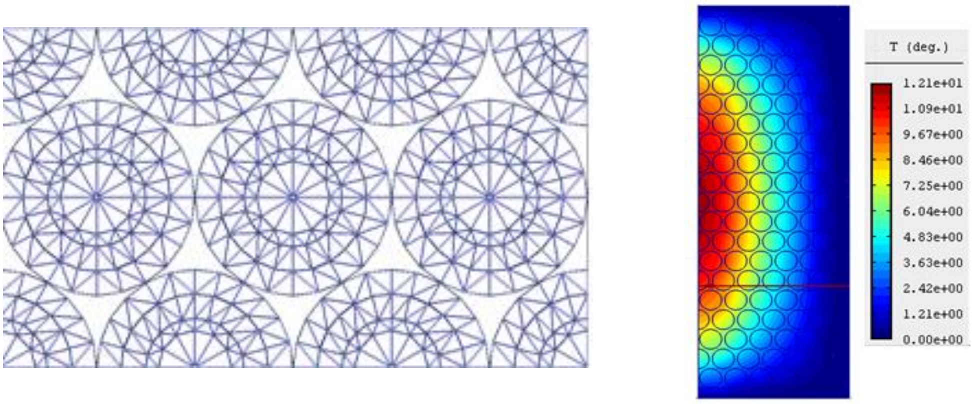
where, α_R is a coefficient equal to 0.4 for lightweight concrete; R_b is design resistance of concrete; b is design width of the wall section, equal to 1 m; δ_0 is the wall thickness of the coffered ceiling; R_{SC} is design resistance of the reinforcement, equal to 355 MPa; A'_S is cross-sectional area of reinforcement of the compressed belt; a' is thickness of concrete cover.

For the model under study, the case is accepted when the effect of reinforcement in the compressed zone is not taken into account. In such a situation, from formula (7) for normal stresses, σ, the dependence is obtained:

$$\sigma = \frac{M_{max}}{\alpha_R b \delta_0^2} \le R_b. \quad (8)$$

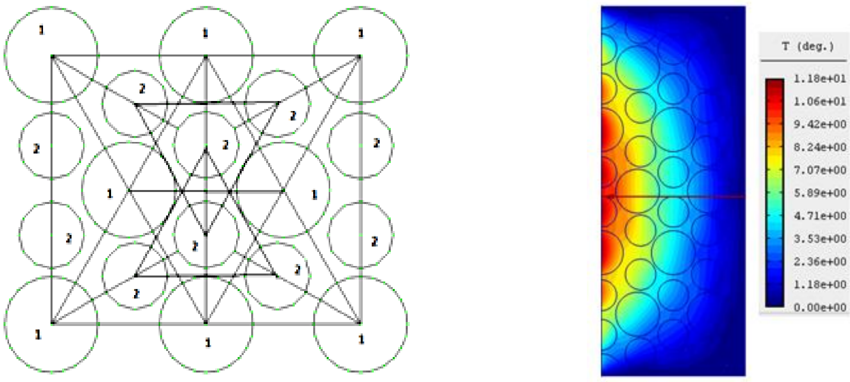
Table 1. Calculated values of thermal conductivity for concrete of various compositions.

Number	Content of concrete components		Thermal conductivity of concrete components, W/(m·ºc)		Thermal conductivity of concrete, calculated according to the formulas λmix, W/(m·ºC),			Coefficient C
	matrix, V_{mat}	filler, V_{fil}	matrix, λ_{mat}	filler, λ_{fil}	Landau	Burger	Numerical method	
1	0.300	0.700	1.90	0.08	0.305	0.491	0.269	1.469
2	0.300	0.700	0.80	0.10	0.220	0.263	0.396	1.412
3	0.300	0.700	0.50	0.08	0.157	0.179	0.189	1.389
4	0.300	0.700	0.20	0.20	0.200	0.200	0.240	0.000
5	0.337	0.673	0.10	0.04	0,058	0.057	0.081	1.288
6	0.500	0.500	0.70	0.07	0.275	0.329	0.329	1.429
7	0.510	0.490	0.80	0.10	0.344	0.397	0.396	1.412
8	0.673	0.337	0.10	0,80	0,200	0.193	0.210	0.305



a) b)

Fig.1. Model of a composite material with regular packing of granules of the same diameter: a) layout of filler's particles; b) temperature fields obtained in the Agros2D program.



a) b)

Fig.2. Composite material model with the packing of filler particles of different diameters according to the law of an equilateral triangle: a) arrangement of filler particles; b) temperature fields obtained in the Agros2D program.

2. Results and discussion

In accordance with the method developed, a flat layer was isolated in the form of a strip of length L with an aspect ratio L/δ>2. A heat flux with intensity of q = 100 W/m^2 is set on one of the faces of the computational domain. The temperature T= 0 is set for the other three faces. As a result of the calculation, the values of the temperature distribution inside the layer and on the active surface of the layer, along which the heat flux is set, are obtained. Taking into account the given boundary conditions in formula (6), it is assumed that tc_2 =T=0.

Numerical calculations showed approximate correspondence between the obtained values of the thermal conductivity coefficient for both cases at equal values of V_{mat}, V_{fil} and the corresponding thermal conductivity coefficients of the matrix and filler. Thermal protection layers with a thickness of 0.03 and 0.05 m were considered. The packing densities of the granules were controlled by assigning characteristics of the binder to some part of the filler. This made it possible to regulate the volume ratio of filler and matrix in the composite material. Figures 1b and 2b show the temperature fields obtained using the Agros2D program.

In the calculations, the ratio of the filler and matrix in the composite material was controlled by imparting the properties of the matrix material to some granules. In this way, the volume of the matrix was increased. It should be noted that the thermal conductivity coefficient of concrete with porous granules is almost three times lower than for the matrix material.

Numerical methods make it possible to compare the thermal efficiency of using multilayer shells made of different materials. Multilayer objects of traditional structure and those objects developed using composite materials with porous granular filler were used as a comparison [3, 24, 25].

The traditional object is represented by a three-layer shell with two outer layers of heavy concrete, thickness is $\delta_2 = \delta_3 = 0.04$ m, thermal conductivity is $\lambda_2 = \lambda_3 = 1.7$ W/(m·^{0}C); the central layer with a thickness of δ_1 = 0.05 – 0.20 m made of mineral wool with λ1 = 0.07 W/(m·^{0}C). The object developed is a 20 cm thick five-layer shell made of a composite material with porous granular filler. Separate layers are made of composite materials with porous granular filler, which have a similar composition and differ in structure (Figure 3). The outer layers of the object developed have the following fixed parameters: thickness is δ_2*= δ_3* = 0.04 m, thermal conductivity of the layers is λ_2*= 0.11 W/(m·^{0}C) and λ_3*= 0.13 W/(m·^{0}C). The calculated thickness of the central layer (δ_1*, m) with thermal conductivity of λ_1*= 0.08 W/(m·^{0}C) ensures that the thermal resistance of three-layer and five-layer shells is the same (Table 2). Assuming that the values of thermal resistance on the boundary surfaces of both compared shells are the same, we obtain:

$$r = \sum_{i=1}^{5} \frac{\delta^*_i}{\lambda^*_i} = \sum_{i=1}^{3} \frac{\delta_i}{\lambda_i}. \qquad (9)$$

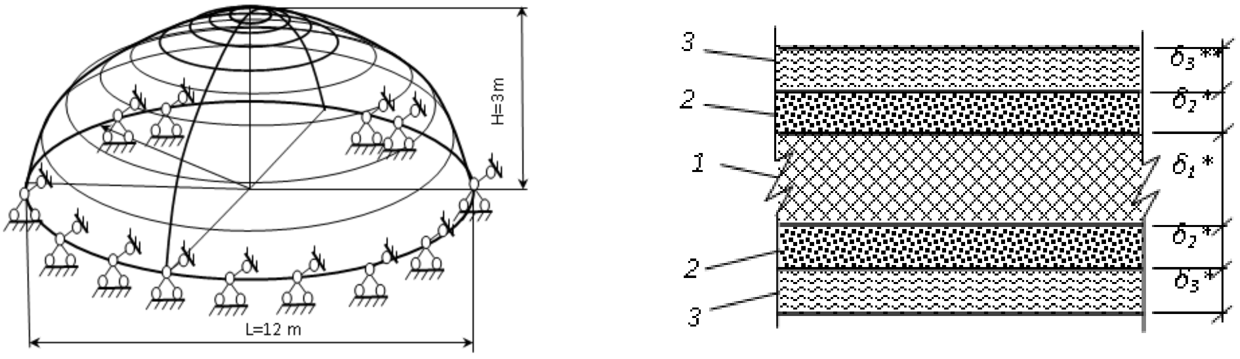
Table 2. Parameters of models of multilayer shells made of materials of various compositions and structures.

Number	Five-layer shell made of composite material with variotropic structure							Three-layer shell made of heavy concrete and mineral wool					
	λ_1^*, W/(m·^{0}C)	δ_1^*, m	λ_2^*, W/(m·^{0}C	δ_2^*, m	λ_3^*, W/(m·^{0}C)	δ_3^*, m	$\sum \delta_i^*$, m	λ_1, W/(m·^{0}C)	δ_1, m	λ_2, W/(m·^{0}C)	δ_2, m	$\sum \delta_i$, m
1	0.08	0.000	0.11	0.04	0.13	0.04	0.160	0.07	0.05	1.7	0.04	0.130
2	0.08	0.000	0.11	0.04	0.13	0.04	0.160	0.07	0.08	1.7	0.04	0.160
3	0.08	0.020	0.11	0.04	0.13	0.04	0.180	0.07	0.10	1.7	0.04	0.180
4	0.08	0.050	0.11	0.04	0.13	0.04	0.210	0.07	0.12	1.7	0.04	0.200
5	0.08	0.085	0.11	0.04	0.13	0.04	0.245	0.07	0.15	1.7	0.04	0.230
6	0.08	0.146	0.11	0.04	0.13	0.04	0.306	0.07	0.20	1.7	0.04	0.280
7	0.08	0.000	0.11	0.04	0.13	0.04	0.160	0.07	0.05	1.7	0.04	0.130
8	0.08	0.056	0.11	0.04	0.13	0.04	0.216	0.07	0.08	1.7	0.04	0.160
9	0.08	0.096	0.11	0.04	0.13	0.04	0.256	0.07	0.10	1.7	0.04	0.180
10	0.08	0.136	0.11	0.04	0.13	0.04	0.296	0.07	0.12	1.7	0.04	0.200
11	0.08	0.196	0.11	0.04	0.13	0.04	0.356	0.07	0.15	1.7	0.04	0.230
12	0.08	0.296	0.11	0.04	0.13	0.04	0.456	0.07	0.20	1.7	0.04	0.280
13	0.08	0.012	0.11	0.00	0.13	0.04	0.092	0.07	0.05	1.7	0.04	0.130
14	0.08	0.046	0.11	0.00	0.13	0.04	0.126	0.07	0.08	1.7	0.04	0.160
15	0.08	0.069	0.11	0.00	0.13	0.04	0.149	0.07	0.10	1.7	0.04	0.180
16	0.08	0.092	0.11	0.00	0.13	0.04	0.172	0.07	0.12	1.7	0.04	0.200
17	0.08	0.126	0.11	0.00	0.13	0.04	0.206	0.07	0.15	1.7	0.04	0.230
18	0.08	0.183	0.11	0.00	0.13	0.04	0.263	0.07	0.20	1.7	0.04	0.280
19	0.08	0.055	0.11	0.00	0.13	0.04	0.135	0.07	0.05	1.7	0.04	0.130
20	0.08	0.115	0.11	0.00	0.13	0.04	0.195	0.07	0.08	1.7	0.04	0.160
21	0.08	0.155	0.11	0.00	0.13	0.04	0.235	0.07	0.10	1.7	0.04	0.180
22	0.08	0.195	0.11	0.00	0.13	0.04	0.275	0.07	0.12	1.7	0.04	0.200
23	0.08	0.255	0.11	0.00	0.13	0.04	0.335	0.07	0.15	1.7	0.04	0.230
24	0.08	0.355	0.11	0.00	0.13	0.04	0.435	0.07	0.20	1.7	0.04	0.280

For multilayer materials, the balance of heat-shielding and mechanical characteristics is important. Behavior of the studied materials in shells (Figure 3a) and pan floor (Figure 4) has been considered.

We take the thickness of individual layers δ_i* ≤ 0.04 m. From here, we can find the thickness of the variable central highly porous layer of the five-layer shell, which plays the main role in the thermal insulation of the five-layer model (Table 2).

Positions 13 – 24 of Table 2 reflect the properties of a five-layer model, in which one of the layers with the thermal conductivity coefficient of λ_2*= 0.11 W/(m·^{0}C) has a thickness of δ_2*= 0. In this case, the total thickness of the multilayer shell can be reduced without significant change values of the thermal conductivity coefficient.



a) b)

Fig.3. Five-layer model for the shell: a) shell structure; b) the structure of a five-layer material (1 – central layer; 2 – middle layers; 3 – surface layers).

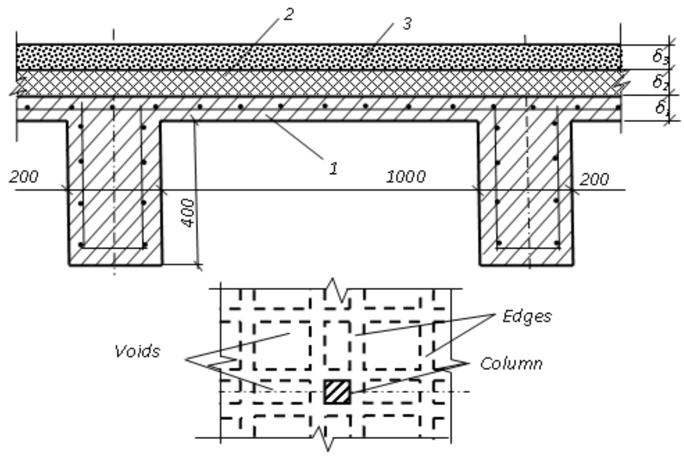


Fig.4. Pan floor: 1− heavy layer concrete; 2 – a layer of heat-insulation material; 3 – top protective layer.

Figures 5 and 6 illustrate the efficiency of using composite materials based on granular porous filler in the various types of floors. In numerical studies, the calculated vertical uniformly distributed load of P = 10 kN/m^2 was adopted on the walls of the shell and the pan floor. Strength calculations were performed by the finite element method in SCAD Office program using a multilayer shell finite element [22, 23]. Calculations confirm the advantages of using multilayer models of composite materials based on granular porous filler. Calculations show that the shell wall is subjected mainly to normal stresses; bending moments in the structure are small and can be neglected. Analysis of normal stress isofields (Figure 5a−b) indicates that the level of normal maximum stresses in a five-layer model made from composite material is three times lower than for a three-layer model of the same thickness. The level of vertical movements for the models compared is approximately equivalent and corresponds to the scheme (Figure 5c).

According to the calculations, the wall of the pan floor works in bending. The normal stresses in the wall are determined by the values of maximum bending moments. The use of a five-layer composite material in insulating layers (Figure 4) makes it possible to reduce the level of maximum bending moments by 25%; accordingly, the level of normal stresses will decrease by 25% compared to the three-layer model (Figure 6).

At the same time, vertical displacements are reduced by 20%, which is due to the increased deformability of the central layer and the violation of uniformity of the wall material made using a soft heat-insulating layer. To calculate the normal stresses, σ, using formula (8) from Figure 6c, it is assumed that the maximum bending moment for a five-layer model of a caisson slab 1 m wide is M_{max}= 0.04 t·m = 0.04·10^3 kg·m.

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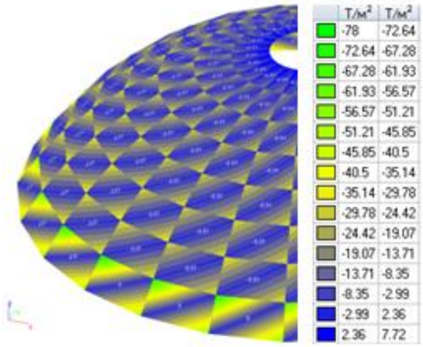

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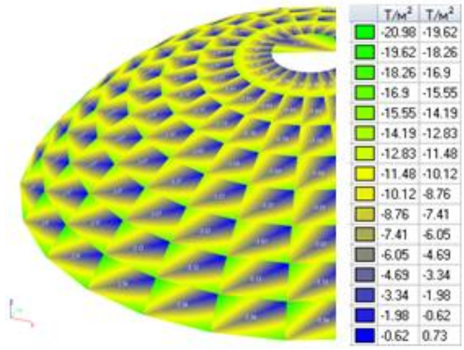

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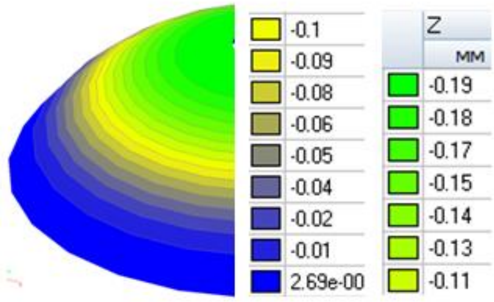
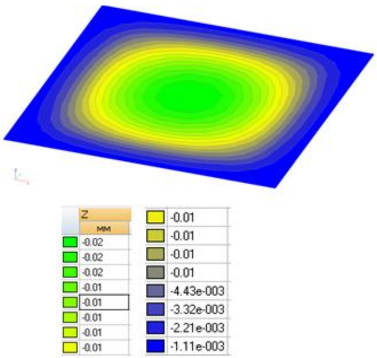


c)

Fig.5. Stress and strain isofields in the shell: a) normal stresses in a three-layer shell with a central layer of mineral wool; b) normal stresses in a five-layer composite shell; c) vertical movements in a three-layer shell.



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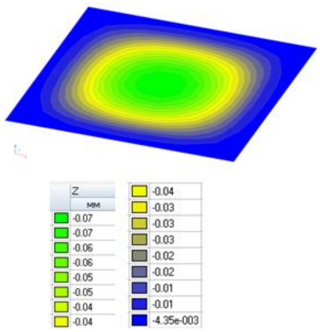

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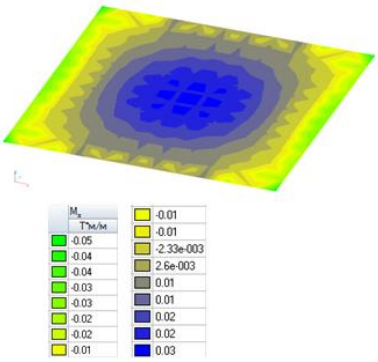

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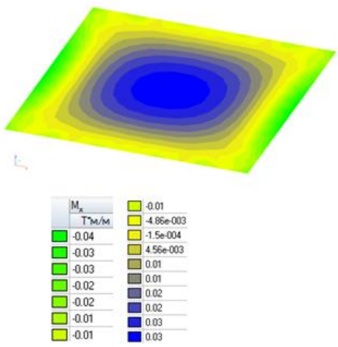

d)

Fig.6. Isofields of stresses and deformations in the wall of the pan floor: a) displacement isofields in a five-layer wall made from a composite material based on porous filler; b) displacement isofields in a three-layer wall based on mineral wool; c) isofields of bending moments in a five-layer wall made from composite material based on porous filler; d) isofields of bending moments in a three-layer wall based on mineral wool.

For the situation described in line 14 (Table 2), only one layer with a thickness of δ_0 = 0.126 − 0.03 = 0.096 m = 9.6 cm is accepted with a margin of safety:

$$\sigma = \frac{0.04 \cdot 10^3}{0.4 \cdot 10^2 \cdot 9.6^2} = 0.0108 \text{kN} / \text{cm}^2 = 0.11 \text{MPa} \le R_b.$$

According to building codes, the ultimate resistance of lightweight concrete of strength classes B2.5 − B12.5 varies from 0.18 to 0.59 MPa. Therefore, the necessary strength of the layer is provided. The calculated characteristics correspond with the results of experimental studies of composite materials [26].

Conclusion

Results of numerical studies made it possible to determine the nature of the change in heat-shielding and mechanical properties of multilayer materials and draw the following conclusions.

1. A technique for numerical determination of the thermal conductivity coefficient of a multilayer composite material with a variotropic structure based on porous granular filler has been developed. The results obtained correspond to the values obtained with the help of analytical dependencies.
2. The results of computer-aided design obtained for a flat model are in line with the data of an analytical calculation of composite materials' thermal conductivity coefficient for three-dimensional models.
3. Behavior of a composite material based on porous granular filler was studied by numerical methods in a spherical shell and a pan floor wall. The resulting stress and strain's isofields are comparable to the corresponding fields for a three-layer model containing dense load-bearing layers of heavy concrete and a central heat-insulating layer of mineral wool.
4. It has been revealed that with the same thermal characteristics and almost the same total thickness, the level of stresses and deformations in a multilayer shell made of a composite material based on porous granular filler is significantly lower than in a three-layer model made using heavy concrete. This is due to the absence of variotropic structure of abrupt change in layers' stiffness in the composite material, which is characteristic of a three-layer model of materials of different nature.
5. Computer simulation methods make it possible not only to predict technical characteristics of multicomponent systems, but also to carry out targeted development of effective composite materials with the desired properties.

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