MODELING OF CONCRETE MACROSTRUCTURE

MÔ HÌNH HÓA CẤU TRÚC VĨ MÔ CỦA BÊ TÔNG

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Abstract: *An imitating model of concrete is proposed in the form of a two-component system consisting of a matrix and inclusions - porous aggregate grains simulated by convex polygons. On their border, there is a zone of contact with properties other than the matrix and inclusions, and in the bulk of the material (in the matrix and inclusions), initial defects of the pore structure of various shapes and sizes are randomly located. Unlike concrete on porous aggregates in heavy concrete, the defectiveness of the macrostructure is due to the violation of the contact of granite rubble with the matrix.*

Keywords: *Concrete macrostructure, matrix and inclusions properties, structurally-simulated modeling.*

Classification number: *2.4*

Tóm tắt: *Một mô hình bắt chước của bê tông được xem xét dưới dạng một hệ hai thành phần bao gồm ma trận và các hạt cốt liệu–dạng hạt tổng hợp xốp được mô phỏng bởi các đa giác lồi. Trên biên của chúng có một vùng tiếp xúc có các đặc tính khác với đặc tính của ma trận và các hạt tổng hợp, và trong phần lớn vật liệu (trong ma trận và các hạt tổng hợp), các khiếm khuyết ban đầu của cấu trúc lỗ rỗng có các hình dạng và kích cỡ khác nhau được đặt ngẫu nhiên. Không giống như bê tông trên cốt liệu xốp trong bê tông nặng, độ khuyết tật của cấu trúc vĩ mô là do sự vi phạm tiếp xúc của đá dăm granite với ma trận.*

Từ khóa: *Cấu trúc vĩ mô của bê tông, ma trận và tính chất hạt tổng hợp, mô hình cấu trúc-mô phỏng.*

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1. Introduction

Production of highly efficient construction materials can be carried out most rationally on the basis of data on the influence of material parameters on its properties. However, in a full - scale experiment (*FSE*), it is difficult to establish the degree of influence of one or another parameter of the macrostructure of a material on its properties and it is often impossible because of their uncontrollability and interdependence. But such reliable information can be obtained in a computational experiment (*CE*), which is conducted on a model of a construction material, in particular, the model of concrete macrostructure.

2. Formulation of the problem

At the present stage of development of building materials science, a computational experiment (*CE*), which allows not only to shorten the duration of research and increase their reliability, but also to obtain results that are difficult to be achieved in a full - scale experiment (*FSE*) in a number of cases, occupies an important place in the study of the relationship between the structure and material properties [1].

This raises the problem of constructing a reliable structural - simulation model (*SS* - model) of a material that reflects the main features of its behavior under the load of one or another kind. In particular, the problem of obtaining high - strength lightweight concrete can be solved by conducting a *CE* on its design analogue model. The results of such an experiment are used to rank the macrostructure parameters by the degree of their impact on the strength of concrete and the choice of the most effective technological parameters for obtaining high - strength lightweight concrete.

3. Solution of the problem

An analogue model of concrete is a *SS*-model having geometric (dimensions of a sample, initial defects (*ID*), a filler (inclusions, etc.) and physical (moduli of elasticity of the matrix and inclusions, properties of the contact zone (*c.z.*, etc.) parameters close to the full - scale sample. In turn, samples of concrete and its components at the macrostructure level are modeled by a plate of unit thickness, the width A and the height H of which are equal to the standard dimensions of the samples.

The physical parameters of the matrix of concrete are: modulus of elasticity $E_м$, Poisson's ratio $\mu_м$, the critical stress intensity factors (*SIF*) for normal fracture $k_{ICм}$ and plane shear $k_{IICм}$. *ID* of concrete and its components at the macrostructure level ─ the pores, are modeled by round holes with two collinear cracks on the contour and have the following geometric parameters: The pore radius r_d, the initial crack length l_{0d}, and their orientation α_d relative to the load q, the defect coordinates on the plate x_d, y_d and their number. Radius of *ID* r_d in the model vary according to a given law of pore size distribution. The initial crack length l_{0d} is fixed and is $l_{0d} = 0{,}184\ r_d$ [2]. The orientation of *ID* with respect to the load q varies over the interval from 0 to 2π. The coordinates of the centers *ID* x_{id}, y_{id} are independent random variables.

The inclusions are modeled by convex polygons and have the following geometric parameters: the conditional radius R_b, the number of vertices n_b and their angle θ_b relative to q, the coordinates of the center X_b, Y_b, the concentration φ_b and the form factor $\kappa_{\varphi b}$ of inclusions, as well as physical parameters – modulus of elasticity E_b, Poisson's ratio μ_b, critical *SIF* for normal fracture K_{ICb} and plane shear K_{IICb}.

The conditional radius R_b, coordinates of the centers X_b, Y_b, number of vertices n_b and their orientation θ_b, form factor $\kappa_{\varphi b}$ of inclusions change randomly on the intervals $[R_{bmin}; R_{bmax}]$, $[A; H]$ $[3;6]$, $[0; 2\pi]$ and $[\kappa_{\varphi min}; \kappa_{\varphi max}]$ respectively. The concentration of inclusions in concrete φ_b is a constant value. The values of physical parameters of inclusions E_b, μ_b, K_{ICb} and K_{IICb} are random values that vary according to the law of distribution of the average density of porous fillers. The sides of polygons simulate *c.z.* of inclusions. Its geometric parameter is width $\delta_к$, and physical parameters – critical *SIF* for normal fracture $k_{ICк}$ and plane shear $k_{IICк}$.

The width of *c.z.* $\delta_к$ gets a constant or random value. Critical *SIF* for *c.z.* are taken in proportion to analogous parameters for the matrix – $k_{ICк} = \Delta_м k_{Iсм}$ and $k_{IICк} = \Delta_м k_{IIсм}$, where $\Delta_м$ – proportionality coefficient, equal to the microhardness of *c.z.* to the microhardness of the matrix.

Thus, the initial macrostructure of concrete is modeled by a plate of unit thickness (fig.1), on the surface of which there are *ID* and convex polygons, sides of which imitate *c.z.*, and the polygons – inclusions (fig.1a, b); for components of concrete on the surface of the plate only *ID* of the macrostructure are located(fig.1c).

Statistically independent geometric G and physical P parameters of the macrostructure of concrete and its components are characterized by a joint probability distribution function $F\ (G,\ P)$ or probability density $f\,(G, P)$.

The values of the geometric parameters of the macrostructure of the concrete are $G = G(r_d, l_{0d}, \alpha_d, x_d, y_d, N_d, R_b, n_b, \theta_b, X_b, Y_b, \kappa_{\varphi b}, \delta_к, \Delta_м)$ and its components $G = G(r_d, l_{0d}, \alpha_d, x_d, y_d, N_d)$ are assumed to be constant or random, corresponding to the given distribution laws. The physical parameters in the concrete model $P = P(M, B, К)$ for the matrix $M = M(E_м, \mu_м, k_{ICм}, k_{IICм})$ are constants, for inclusions $B = B(E_b, \mu_b, k_{ICb}, k_{IIcb})$ and *c.z.* $k = k\ (\Delta_м)$ can be taken depending on the conditions of a particular task as constant or random variables.

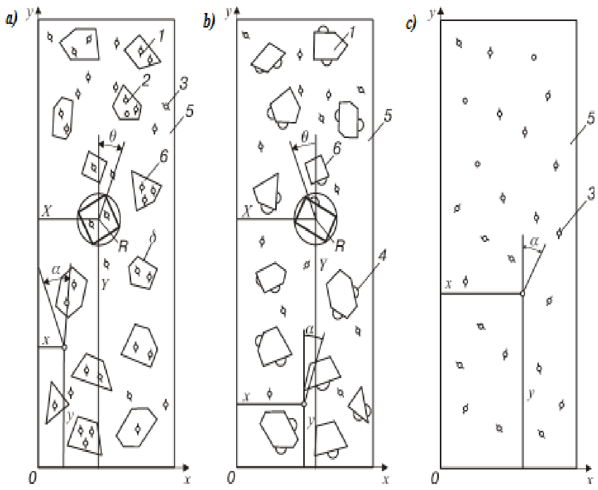

Figure 1. *Model of concrete samples on porous (a), dense (b) fillers and components of their macrostructure (c) – fillers and matrix:*

1 – inclusion;
2 – initial defect of inclusion;
3 – the same of the matrix;
4 – the same of the contact zone;
5 – matrix;
6 – c.z

The geometric characteristics of the parameters of concrete macrostructure were established by carrying out *CE*. The form of a large porous filler (slag pumice), was studied on polished sections of concrete. It was found out that almost all (about 96%) of the filler's contours are convex and, therefore, can be described by convex polygons. Statistical processing of the results of 460 measurements showed that 10% of the filler's sections can be described by triangles, 50% – by quadrangles, 30% – by pentagons and 10% – by hexagons. This ratio is practically not affected by the type, size and fractional composition of the filler.The results of measurements of the parameters of *c.z.* of the filler in concrete showed that its width is 18 - 640 μm in the pores, 10 - 5 μm in the interpore partitions, and its strength is 9 - 40% higher than the strength of *CSS*. Its parameters depend both on the chemical activity of the filler's surface and on the porosity: The presence of a relatively thick contact layer of cement stone in the pores is explained by more favorable (than in interpore partitions) hydration conditions when the absorbed moisture accumulates in the pores. In assessing the defectiveness of the macrostructure, it is established that in concrete on granitic rubble the main part of the defects is located in *CSS* and in the place of its contact with the dense filler. Unlike concrete on a dense filler, in lightweight concrete with the approach to the surface of a porous filler, the porosity (defectiveness) of the matrix is reduced, which at the contact point in ultraviolet light can be seen in the form of a thin strip fringing the filler. The main defect of such concrete is the pores located both in the matrix and in the inclusions. The physical characteristics of the parameters of the concrete model can be conveniently represented in the form of polynomial models "content – properties" for *CSS* (matrix) and regression equations "average density – properties" for the porous filler (inclusions).

Mathematical models (*MM*) of the properties of *CSS* were established by methods of planning of experiments using as variable factors: *C* – volume concentration of cement paste in solution, rel. units; $(W/C)_{true}$ – true water - cement ratio, rel. units and R_a – cement activity, MPa.

Below, there are the obtained polynomial models of the properties of CSS for variables on an encoded scale: Compressive strength R_M, MPa and tensile strength R_{ppM},MPa, initial modulus of elasticity E_M, MPa, Poisson's ratio μ_M, rel. units, limiting relative deformations under compression ε_{comM},, rel. units, critical *SIF* for normal fracture k_{IcM}, $MN/m^{3/2}$ and plane shear k_{IIcM}, $MN/m^{3/2}$, angle of internal friction ρ_M, degrees, and adhesion coefficient k_M, MPa:

$$R_M = 30{,}78 + 14{,}42x_1 - 2{,}19x_2 + 4{,}82x_3 - 13{,}36x^2{}_1 - 2{,}45x_1x_2 + 3{,}04x_1x_3 + 4{,}99x^2{}_2 + 0{,}86x^2{}_3; \quad (1)$$

$$R_{PPM} = 2{,}615 + 1{,}0x_1 - 0{,}447x_2 + 0{,}163x_3 - 0{,}675x^2{}_1 - 0{,}236x_1x_2 + 0{,}135x^2{}_2 - 0{,}025x^2{}_3; \quad (2)$$

$$E_M \cdot 10^{-4} = 1{,}748 + 0{,}164x_1 - 0{,}221x_2 + 0{,}122x_3 - 0{,}344x^2{}_1 - 0{,}026x_1x_2 + 0{,}202x^2{}_2 - 0{,}124x^2{}_3; \quad (3)$$

$\varepsilon_{comM}\cdot 10^{-5} = 243 + 99x_1 - 10,5x_2 + 2,7x_3 - 46,4x^2_1 - 5x_1x_2 - 14,5x_1x_3 + 13,1x^2_2 - 5,5x_2x_3 + 4,2x^2_3$; (4)

$\mu_M = 0,195 + 0,02x_1 - 0,015x_2 - 0,011x_3 + 0,007x_1x_3 + + 0,022x^2_2 + 0,009x_2x_3 - 0,006x^2_3$; (5)

$K_{IcM} = 0,466 + 0,09x_1 - 0,08x_2 + 0,01x_3 - 0,18x^2_1 - 0,03x_1x_2 - 0,02x_1x_3 + 0,02x^2_2 + 0,04x_2x_3$; (6)

$K_{IIcM} = 8,518 + 4,548x_1 - 0,883x_2 + 1,643x_3 - 3,268x^2_1 + 0,485x_1x_3 + 1,322x^2_2 + 0,71x^2_3$; (7)

$\rho_M = 54,5 + 5,7x_1 - 0,18x_2 + 1,2x_3 - 3,5x^2_1 - 0,5x_1x_2 - 0,6x_1x_3 + 2,8x^2_2 + + 0,7x_2x_3 + 4,8x^2_3$; (8)

$k_M = 5,28 + 1,95x_1 - 0,5x_2 + 0,28x_3 - 1,95x^2_1 - 0,24x_1x_2 + 0,53x^2_2 + + 0,18x^2_3$; (9)

MM of properties of inclusions of concrete (slag pumice), obtained by the methods of correlation analysis, are shown in fig.2 (in the numerator) with the indication of the number of single tests (in the denominator). A critical *SIF* for inplane shear k_{IIc} for slag pumice was determined by the equation [3]:

$$k_{IIcB} = k_{Ic_B} R_{comB} / 2R_{PPB} \qquad (10)$$

After substituting k_{Icb}, R_{comb} and R_{ppB} into which we find finally:

$$k_{IIcB} = 0,23\rho_{mB}^{4,004}\cdot 10^{-12} \text{ (MN/m}^{3/2}) \qquad (11)$$

In fig.2e, the dotted line shows the dependence of the modulus of elasticity of inclusions upon fracture E_B^{pr}, obtained from the equation $E_B^{pr} = R_{comB}/\varepsilon^{pr}_{comB}$. It is seen that the difference between the initial modulus of elasticity E_B and E_B^{pr} becomes significant at $\rho_{mB} > 1000$ kg/m^3 and reaches 27 - 30%.

Critical *SIF* k_{Ic_B} and k_{IIc_B} characterize the ability of a material to resist the propagation of tear and shear cracks in it, respectively. According to the results of the experiments, the ratio of these coefficients k_{IIc_B}/k_{Ic_B} for *CSS* is more than 5 (see (6) (7)), and for slag pumice – more than 2 (estimate of the lower boundary – see fig.2h), which determines mainly the separation mechanism of crack propagation in concrete.

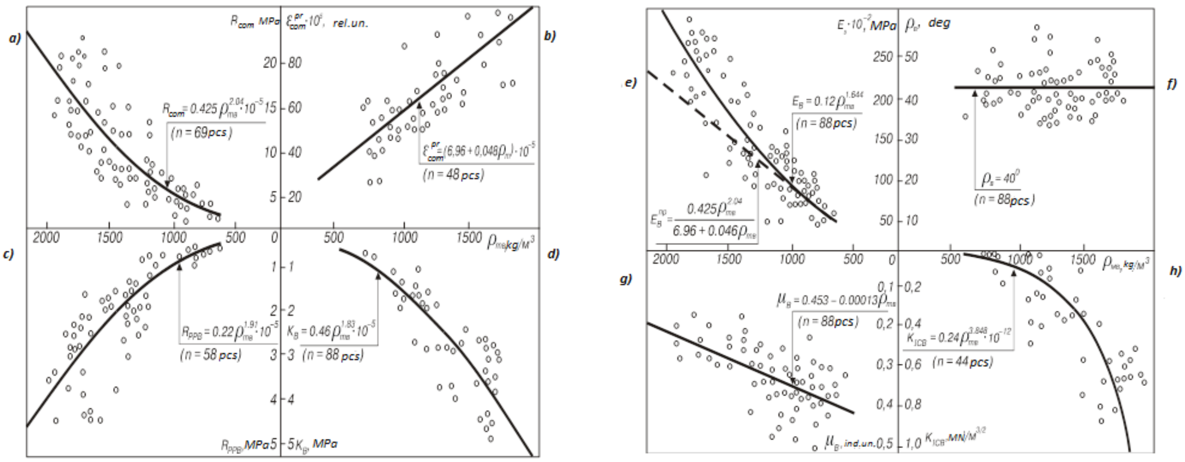

Figure 2. *Dependence of the properties of inclusions on their average density ρ_{mB}.*

a – compressive strength; b – limiting compressibility; c – tensile strength during splitting; d – coefficient of adhesion; e – modulus of elasticity; f – angle of internal friction; g – Poisson's ratio; h – critical stress ratio at normal fracture

On the other hand, the comparison of critical *SIF* for normal fracture for slag pumice (fig.2h) and *CSS* (see (6)) shows that the values of this coefficient for inclusions at $\rho_{mB} > 1500$ kg/m^3 are from 2 to 5 times higher than the similar indicator for the matrix. Consequently, such inclusions, being an obstacle to developing cracks, will be rounded by them, which leads to formation of zigzag - cracks. On the basis of the experiments carried out, the structure of lightweight concrete before the application of the load (in a static state) will be represented as a two - component system consisting of a matrix (*CSS*) and inclusions (porous filler's grains) – convex polygons. At the boundary of the matrix and inclusions, there is a contact zone with properties different from the matrix and inclusions, and initial defects of the structure − pores of various shapes and sizes − are randomly located in the material volume. In heavy concrete, the defectiveness of the inclusions can be neglected, since it is represented mainly by a loss of the contact of granite rubble with *CSS* due to sedimentation phenomena. However, under load, concrete exhibits already the properties of a dynamic system, the state of which changes in time from the moment the load is applied up to the destruction of the sample. This is due to the appearance of a new structural element in the form of micro - and macro - cracks.

The phenomena occurring under load in repeatedly structured dynamical systems refer to the processes of formation of a hierarchy of structures based on the following principles: a) when forming a structure at a certain level, the local stress field of the structural element of this level and the structural element corresponding to the structure of the previous level is determinant; b) the formation of the hierarchy of structures is completed at the level of the structure, unstable elements of which are limited by the natural boundaries of the material system [4].

Based on these provisions, the process of destruction will be modeled at the highest level – at the macrostructure level of concrete with the inclusion of structural elements of the given (matrix, inclusions, contact zone, macrocracks) and the previous (fields of the matrix and inclusions, microcrack) levels. Then, the destruction of the concrete sample will correspond to the moment of formation of an unstable structural element – a main crack that extends to the sides of the sample.

The process of destruction of a concrete sample is modeled on a plate of unit thickness. In case of uniaxial compression, this does not lead to significant errors in comparison with the actual volumetric stress state [2]. In addition, the accepted simplification makes it possible to use the known solutions of the two - dimensional theory of elasticity to describe the stressed state of structural elements of concrete [5].

The obtained *MM* of properties of the matrix and inclusions were used in the formation of the computational analogue model of concrete on porous fillers. As such a model, a plate of unit thickness with width $A = 100\ mm$ and height $H = 400\ mm$ was taken with the following geometrical and physical characteristics of the structural elements (see fig. 3a): The number of *ID* of the structure is $N = 50$; the laws of distribution of the dimensions of *ID* of the structure for the matrix r_M and the inclusions r_b, are taken from the table; the random values of the coordinates of the centers of *ID* (x_d, y_d) and the inclusions (X_b,Y_b) are uniformly distributed for x_d and X_b on the interval [0; A], and for y_d and Y_b – on the interval [0; H]; the law of distribution of the sizes of the inclusions R_b is taken from the table; the random orientations of *ID* α_d and the vertices of the inclusions θ_b relative to the load q are uniformly distributed on the intervals [$-\pi/6$; $\pi/6$] and [0; 2π]; the laws of the distribution of the number of vertices of inclusions n_b and the width of *c.z.* δ_κ are taken according to the table; the physical characteristics of the matrix are determined from the *MM* of properties of *CSS* (1) - (9) at the basic level of the variable factors: C = 0,625; $(W/C)_{true}$ is = $0,23$ and $R_a = 39$ MPa; the physical characteristics of inclusions are established from the correlation equations (see fig.2) under the distribution law ρ_{mB}, given in the table (for $\rho_{mB} = 1060\ kg/m^3$ and $\vartheta\rho_{mB} = 25\%$); the relative magnitude of microhardness of *c.z.* is the value of Δ_M = $1{,}087$; the form factor of inclusions $\kappa_{\varphi b}$, obeys the law of uniform distribution in the interval [$1{,}2$; 1.4]; the concentration of inclusions φ_b is $0{,}35$.

One of the realizations of development of cracks in the analogue model of concrete on porous fillers and, for comparison, in a natural sample is shown in fig. 3. Thus, a simulation model of concrete in the form of a two - component system consisting of a matrix (*css*) and inclusions (porous filler's grains) − convex polygons − is proposed. At the boundary of the matrix and inclusions, there is a contact zone with properties different from the matrix and inclusions, and initial defects of the structure − pores of various shapes and sizes − are randomly located in the material (in the matrix and inclusions). In heavy concrete, the defectiveness of the inclusions can be neglected and attributed to the contact zone, since it is represented mainly by a loss of the contact of granite rubble with *css* due to sedimentation phenomena that appear during vibration of the concrete mix.under load, concrete exhibits the properties of a dynamic system, the state of which changes in time from the moment the load is applied up to the destruction of the sample, which is caused by the appearance of a new structural element − micro and macro cracks.

Table 1. *Characteristics of the elements of the structure of the analogue model of concrete on porous fillers.*

Indicators	Ranks/frequency of indicators				
r_M, µm	1-25/0,15	25-50/0,17	50-100/0,37	100-250/0,25	250-500/0,06
r_b, mm	0,01-0,3/0,5	0,3-0,5/0,13	0,5-1/0,25	1-2/0,09	2-3/0,03
R_b, mm	10-15/0,5	15-18/0,3	18-20/0,2	–	–
n_b, pcs	3/0,1	4/0,5	5/0,3	6/0,1	–
δ_K, µm	10-50/0,5	50-640/0,5	–	–	–
$\rho_{mB}\cdot 10^2$, kg/m^3	6-8/0,22	8-10/0,18	10-12/0,30	12-14/0,18	14-16/0,12

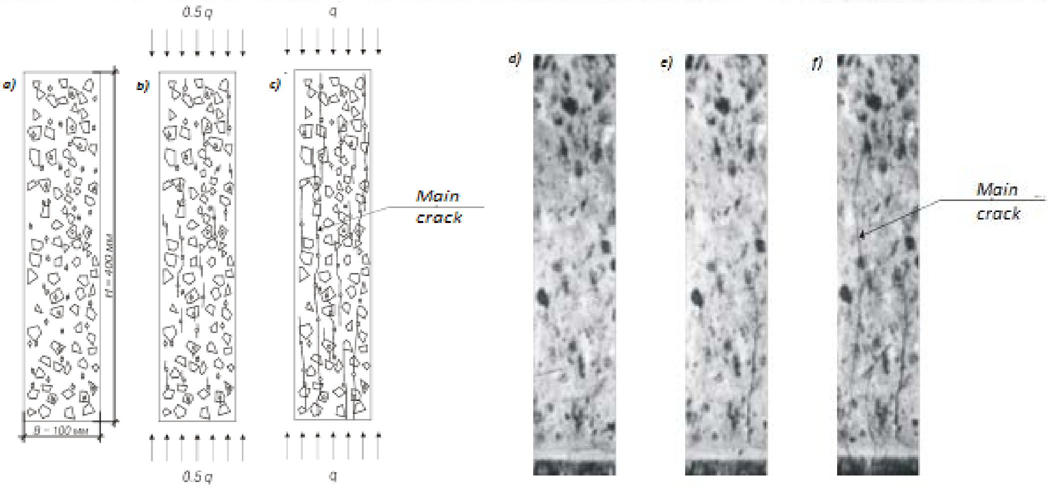

Figure 3. *Destruction of concrete on porous fillers on the analogue model (a - c) and the full - scale sample (d - e).*

Thus, the process of destruction is modeled at the level of the macrostructure of concrete with the inclusion of the structural elements of the given (matrix, inclusions, contact zone, macrocrack) and the previous (fields of the matrix and inclusions, microcrack) levels. Then, the destruction of a concrete sample on a model in the form of a plate of unit thickness corresponds to the moment of formation of an unstable structural element-a main crack that extends to the sides of the sample, which is the natural boundary for a given material system at the macrostructure level.

4. Conclusions and Recommendations

Thus, a simulation model of concrete in the form of a two - component system consisting of a matrix (*CSS*) and inclusions (porous filler's grains) − convex polygons − is proposed. At the boundary of the matrix and inclusions, there is a contact zone with properties different from the matrix and inclusions, and initial defects of the structure − pores of various shapes and sizes − are randomly located in the material (in the matrix and inclusions). In heavy concrete, the defectiveness of the inclusions can be neglected and attributed to the contact zone, since it is represented mainly by a loss of the contact of granite rubble with *CSS* due to sedimentation phenomena that appear during vibration of the concrete mix. The proposed model of concrete macrostructure is designed for conducting *CE* on assessment of the degree of influence of structural parameters on the strength of concrete to establish rational technological regimes for production of high - strength concrete ❑

References

[1] Chermashentsev, V. M. *Theoretical aspects of computer modeling of effective composite materials* [*Teoreticheskie aspekty komp'juternogo modelirovanija kompozicionnyh materialov*]. Izvestiya vuzov. Stroitelstvo, Iss. 3, 2002, pp. 33-40.

[2] Zaitsev, Yu. V. *Modeling of deformations and strength of concrete by the methods of fracture mechanics* [*Modelirovanie deformacii i prochnosti betona metodami mehaniki razrushenii*]. Moscow, Stroyizdat publ., 1982, 196 p.

[3] Cherepanov, G. P. *Equilibrium of a slope with a tectonic crack* [*Ravnovesie otkosa s tektonicheskoi treshchinoi*]. *Prikladnaya mehanika i matematika*, Vol. 40, Iss. 1, 1976, pp. 136 – 151.

[4] Goldstein, R. V., Osipenko, N. M. *Structures of destruction. Formation conditions. Echelons of cracks* [*Struktury razrusheniya. Usloviya formirovaniya. Eshelony treshchin*]. Institute of Strength Problems of the Academy of Sciences of the USSR. Preprint No. 110. Moscow, 1978, 59 p.

[5] Muskhelishvili, N. I. *Some basic tasks of the mathematical theory of elasticity* [*Nekotorye osnovnye zadachi matematicheskoi teorii uprugosti*]. Moscow, Nauka publ., 1966, 707 p.

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