DEVELOPMENT OF A METHODOLOGY FOR PREDICTING THE PROPERTIES OF MULTICOMPONENT HIGH-QUALITY CONCRETE TAKING INTO ACCOUNT THE SURFACE PROPERTIES OF MINERAL FILLERS AND STRUCTURAL SIMULATION MODELING

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Abstract: The results of theoretical and experimental research on the development of a scientifically based methodology for prescribing plasticizing chemical additives and mineral fillers in the selection of compositions of complex modified concrete (CMC) at the stage of their design are presented. A classification of plasticizing additives is proposed according to the degree of reduction in the surface tension of water upon their introduction and the activity of mineral additives according to the indicator of reduced hydration activity, which makes it possible to obtain highly economical BMPs with the required properties.

Key words: Concrete, classification of additives, modification, plasticizer, mineral filler, surface tension, adsorption centers, hydration activity

It is established that for the production of hollow floor slabs by the method of continuous formless molding, it is necessary to use concrete mixtures with a stiffness of about 90 c, which guarantees that the product retains its shape immediately after the vibration effect on the concrete mixture is completed. Therefore, the spatial framework should be formed according to the principle of selecting a rational grain composition of components.

When selecting the composition of concrete, the issues of ensuring the minimum consumption of cement from the conditions of reducing the energy intensity and cost of the mixture, ensuring workability and reducing defects associated with the collapse of the massif, as well as with the quality of the front surface were taken into account [1]. Effectiveproduction of products using this technology largely depends on the full involvement of local raw materials. When selecting concrete compositions, we used the accumulated experience of optimization from the conditions of minimal voidness with the replacement of part of the traditional raw **materials with soils of different nature and density.**

Purposeful optimization of the grain composition of concrete mixes was carried out at the expense of fillers.

Analysis of the research results of the authors [1-3-3] showed that mineral fillers with adsorption centers of intensities lying in the pKa region from -4 to 7 and more than 13 contribute to the catalytic activation of cement hydration. Active centers of mineral fillers in the areas of pKa from 7 to 13 contribute to accelerating the adsorption of water molecules from cement dough, thereby distracting from deeper participation in chemical interactions with the binder and thereby reducing the rate of hydration processes in the cement binder.

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Taking into account the above, we have proposed a new criterion - "indicator of reduced hydration activity", which, in our opinion, allows us to more accurately assess the contribution of the surface activity of mineral fillers to the course of interactions and transformations, occurring in a hydrated medium.

Table 1

Content of surface adsorption centers of mineral fillers

№ n /	a Name of mineral filler	Number of centers, 10^3 mg-eq/^{m2}				Total number of centers
		-4...0	0...7	7...12,8	>12,8	
		P_{ol}	P_{kb}	P_{ob}	P_{kl}	
1.	Sand Quartz Sand	8.04	9.11	8.75	1.88	27.78
2.	Sand dune	4.12	7.08	9.95	1.07	22.22
3.	Clay	13.22	16.47	10.08	2.87	42.64
4.	Basalt	23.41	22.15	11.16	1.96	58.68
5.	Zeolite containing rock	102.08	24.88	12.62	2.14	141.72

The proposed indicator is indicated by the symbol $-P_{pga}$ and is determined by the formula:

$$P_{pga}= P_{kv}+P_{kl}+0.33P_{ol}-0.1P_{ob}, \text{ where } (1)$$

P_{kv}, P_{kl}, P_{ol}, P_{ob} –the number of adsorption centers in the regions 0<pKa<7; pKa>13.0; -4<pKa<0; 7<pKa<13.0 in $10\text{-}3^{-3}$ mg-eq/g. co, respectively.

This criterion, which characterizes the acid-base properties of the surface of mineral fillers, allows us to scientifically classify mineral fillers according to the degree of their impact on cement systems. In general, the following classification of mineral fillers is proposed according to the $P_{pga\ criterion}$-an indicator of the reduced hydration activity (Table 2).

Table 2

Classification of mineral fillers according to the indicator of reduced hydration activity P_{pga}.

№ n /	a Type of mineral filler	Values of the $P_{pga\ criterion}$.	Potential efficiency in cement systems, cement savings in %
1.	Weakly	active from 0< to. <10	To 10%
2.	Moderately	active from 10< to. <25	10-20%
3.	Highly	active 25< to <50	20-30%
4.	Super	Active Over Up to >50	Up to 50%

For mineral fillers accepted for the study, the calculation of this criterion, i.e., the indicator of reduced hydration activity, is presented in (Table 3).

Comparative analysis of mineral fillers according to the $P_{pga\ criterion}$ allows predicting their effectiveness in cement systems and characterizing them by their degree of activity, such as: barkhany sand-weakly active; quartz sand, clay, SEP-moderately active; basalt, OMP, fly ash from the Angren thermal power plant-highly active and zeolite-containing rock-super active.

Table 3

Criterion P $_{pga}$ in mineral fillers

№ n/	a Mineral filler name	Converted data		Criterion $P_{pga.}$	Ey, MPa
		$0.33P_{ob}$	$0.1\ P_{ol}$		
1.	Sand Quartz Sand	2.65	0.87	12.77	200
2.	Dune sand	1.36	0.99	8.52	180
3.	Voronezh	4,36	1,01	22,39	120
4.	Basalt	7,72	1,12	30.71	290
5.	Zeolite containing rock	33.68	1.26	59.44	300

Теый developed Patent No . IAP 07520 allows determining **the composition** of filled cement systems with local mineral fillers, which makes it possible to design concretes with the necessary physical and mechanical properties for the technology of non - formwork molding using structural simulation modeling.

Конструктивные слои из смесей щебеночно-гравийно-песчаных, соответствующих ГОСТ 25607-94 и ГОСТ 3344-83

Материал слоя	Нормативные значения модуля упругости, E, МПа
Щебеночные/гравийные смеси (С) для покрытий:	
- непрерывная гранулометрия (ГОСТ 25607)	
при максимальном размере зерен: C_1 - 40 мм	300/280
C_2 - 20 мм	290/265
Смеси для оснований	
- непрерывная гранулометрия: C_3 - 80 мм	280/240
C_4 - 80 мм	275/230
C_5 - 40 мм	260/220
C_6 - 20 мм	240/200
C_7 - 20 мм	260/180
Шлаковая щебеночно-песчаная смесь из неактивных и слабоактивных шлаков (ГОСТ 3344)	
C_1 - 70 мм	275
C_2 - 70 мм	260
C_4 - 40 мм	250
C_6 - 20 мм	210

Geometric and physical parameters of the modeling object

Concrete macrostructure the structure of concrete that is visible to the eye or at low magnification. In the macrostructure of concrete, structural elements are distinguished: coarse aggregate, sand, cement stone, air pores. Sometimes the macrostructure of concrete is conventionally assumed to consist of two components: a coarse aggregate and a cement-sand mortar.

Matrix - a component of a two-component concrete system that represents the mortar part (in Figure2, the main field of the "plate" is represented by light dots).

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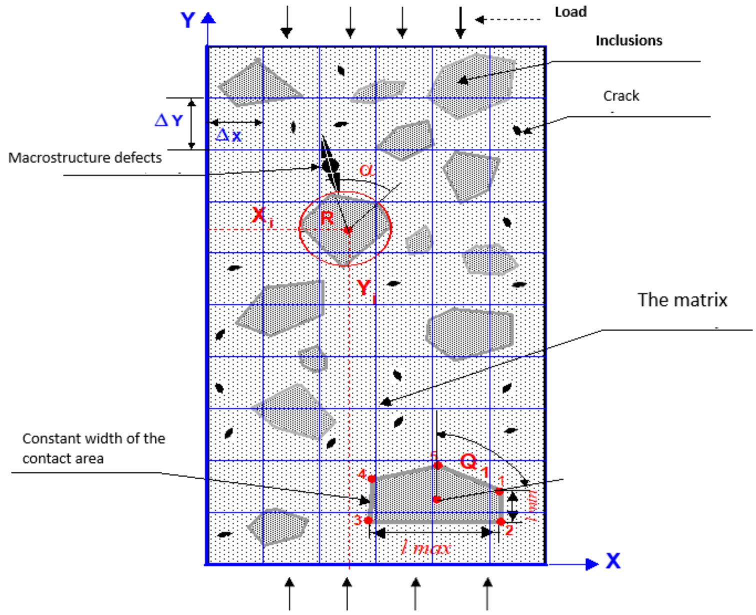

Figure 2. The simulated object and its components

Physical parameters of the matrix: - elastic modulus E_m, Poisson's ratio μ_m, critical coefficients of stress intensity at normal rupture $K^{\grave{I}}_{Ic}$ and plane shear $K^{\grave{I}}_{I}$ }}fixed values.

Initial defects in the macrostructure of concrete and its components (SSS) pores with collinear cracks (Fig.2).

Geometric parameters of the SSS: - r_{ij} – pore radius with coordinates X_iXi,Y_j – const, l_{oij} ––initial crack length = 0.184r, α_{ij} – crack orientation relative to the load vector, random-a value obeying the law of arbitrary distribution in the range from 0 to 2π, X_i, Y_j VAT coordinates, independent random variables distributed according to a uniform law over the area of the plate (simulated sample); N is the number of initial defects in the sample field (N_{min}= 30).

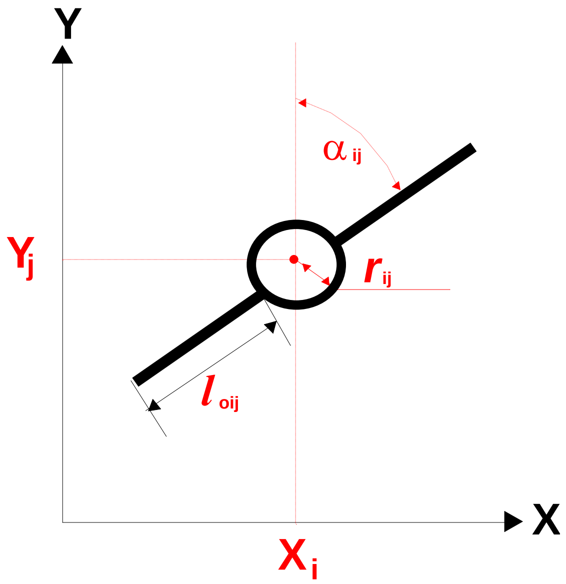

Figure 3. Geometric parameters of VAT.

Inclusions oϕ coarse aggregate grains. They are modeledby convex polyhedra (Fig. 4). Geometric parameters:

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- R_{ij} is the radius of the circle described around the polygon – const; n_{ij} is the number of vertices of the polygon ($n \le 6$) – Θ_k^m - orientation *of the k*-th vertex of the polygon *of the m*-th inclusion relative to the load vector – a random variable distributed according to a uniform law in the interval from 0 to 2π; X_i^M, Y_j^M ––coordinates of the center of the circumscribed circle *M*- th inclusion φ concentration of inclusions:

$$\varphi = \frac{\sum_{m=1}^{M} S_m^B}{S_{об}}, \qquad (2)$$

where S_m^B – is the area *of the m*-th inclusion, $S_{об}$ is the area of the sample.

––K_f–shape coefficient:

$$K_\Phi = \frac{L'_{max}}{L'_{min}}, \qquad (3)$$

where $L_{max} = L'_{max} = L_{max}\ \mathrm{Cos}\xi_1$, $L'_{min} = L_{min} \times \mathrm{Cos}\xi_2$; L_{max}, L_{min} are the maximum and minimum sides of the inclusion polygon, respectively (Fig.).

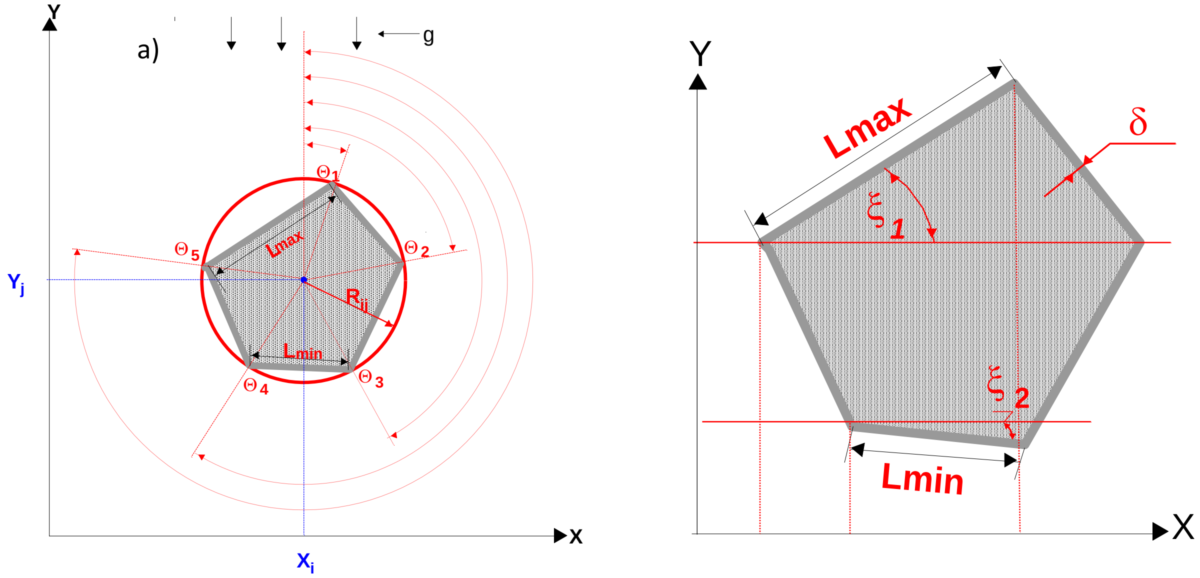

Fig. 4. Geometric parameters of switching on.

Physical activation parameters:

E_b elastic modulus - const; μ_b – Poisson's ratio - const; $K_{Ic}^{в}$ – stress intensity coefficient at normal rupture; $K_{IIc}^{в}$ –stress intensity coefficient at plane shear- const.

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