

## EXPERIMENTAL-STATISTICAL MODELING OF INFLUENCE QUANTITY AND CHEMICAL COMPOSITION OF ADDITIVES ON THE PROPERTIES OF BUILDING COMPOSITES

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**Relevance of research.** Optimization of formulations and modes of obtaining building composites is carried out on experimental and statistical models most effectively [1]. Experimental and statistical models allow to consider simultaneously a large number of factors in a given production until binding to the careers of raw materials. Experimental and statistical models allow to held a deep analysis of a specific situation, taking into account features of the mechanisms of hydration and structure formation.

**State of the problem.** With the use of the methods of computer materials developed by the information-analytical units of experimental-statistical models is held the analysis of the significance of the effects of interactions between the parameters of the structure and properties. Such a technique allowed in the computational experiments to conduct systematic analysis of the transformation of these relationships and to identify the most sensitive to management factors for materials' producing with desired properties.

**Purpose of work.** With using experimental and statistical modeling to investigate the influence quantity and chemical composition of additives on the properties of building composites.

**The results obtained.** On the basis of the previously obtained data of natural studies [2], a basis for performing experimental and statistical modeling was formed. Experimental-statistical modeling [1] using polynomial models and correlation of coefficients was carried out to determine the influence of additives 1 and 2 on the strength characteristics of 28-day hardened building composites. First, the experimental-statistical models are constructed in the form of polynomial equations based on experimental results. For this purpose, the percentage of the calcined clays in the range of 0%-60% was normalized to encrypted data from -1 to +1 into dependence  $-1x_i + 1$  by applying typical equation  $x_i = (X_i - X_{0i})/X_i$ . The experimental- statistical models describing the

effects of the reactive oxide molar ratios and the reactive-phase content ( $x$ ) of the calcined clays on the 28-day, as the response ( $Y$ ), have the following expression:

$$Y = b_0 + b_1x + b_{11}x^2 \quad (1)$$

Coefficients of the experimental-statistical models calculated based on encrypted data are listed in Table 1. Coefficients of the experimental-statistical models and the corresponding variables calculated for the maximum 28-day hardened composites are listed in Table 2.

Table 1.

Coefficients of models based on encrypted data

| Coefficients of models | Ca/Si  | Ca/Al  | Na/Si | Na/Al  | Si/Al  | Amorphous content (%) | 28-day compressive strength (MPa) |
|------------------------|--------|--------|-------|--------|--------|-----------------------|-----------------------------------|
| Additive 1             |        |        |       |        |        |                       |                                   |
| $b_0$                  | 0.749  | 2.507  | 0.16  | 0.533  | 3.306  | 88                    | 27.23                             |
| $b_1$                  | -0.26  | -2.352 | 0.011 | -0.231 | -1.604 | -12                   | -15.47                            |
| $b_{11}$               | 0.08   | 0.916  | 0     | 0.096  | 0.622  | 0                     | -11.81                            |
| Additive 2             |        |        |       |        |        |                       |                                   |
| $b_0$                  | 0.846  | 3.415  | 0.18  | 0.729  | 3.994  | 80.6                  | 23.16                             |
| $b_1$                  | -0.216 | -2.055 | 0.035 | -0.12  | -1.301 | -22.16                | -15.18                            |
| $b_{11}$               | -0.036 | 0.33   | 0.005 | 0.021  | 0.319  | -3.56                 | -7.98                             |

Subsequently, numerical tests were designed to evaluate the significance for determining the effect of the amount and chemistry of the reactive phase on 28-day of the hardened composites. To calculate the coefficients, the variables were normalized to  $-1 < x_i < +1$  dependence. The main factors were Ca/Si ( $x_1$ ), Si/Al ( $x_2$ ), and Na/Si ( $x_3$ ) ratios, and the amorphous-phase portion ( $x_4$ ).

Table 2.

Coefficients of experimental-statistical models calculated with respect of maximum 28-day harden composites

| Ratio of building compositions | Ca/Si  | Ca/Al | Na/Si | Na/Al  | Si/Al | Amorphous content (%) | 28-day compressive strength (MPa) |
|--------------------------------|--------|-------|-------|--------|-------|-----------------------|-----------------------------------|
| 88.5/11.5                      | 0.9536 | 4.558 | 0.153 | 0.7255 | 4.623 | 89.64                 | 32.3                              |
| 99.5/0.5                       | 1.026  | 5.8   | 0.15  | 0.87   | 5.614 | 96.68                 | 30.3                              |

Accordingly, two-factor models were constructed in pairs of  $x_1$ - $x_4$ ,  $x_2$ - $x_4$ , and  $x_3$ - $x_4$  and had showed following forms for the hardened composites with additive 1:

$$R_{b_1\{Ca/Si:Am.ph\}} = 29.40 - 7.44x_1 - 7.01x_1^2 \pm 0x_1x_4 - 7.44x_4 - 7.0x_4^2 \quad (2)$$

$$R_{b_1\{Si/Al:Am.ph\}} = 29.87 - 7.37x_2 - 7.24x_2^2 + 0.01x_2x_4 - 7.72x_4 - 5.86x_4^2 \quad (3)$$

$$R_{b_1\{Na/Si:Am.ph\}} = 27.16 - 7.72x_3 - 5.86x_3^2 + 0.004x_3x_4 - 7.72x_4 - 5.86x_4^2 \quad (4)$$

For the hardened composites with additive 2, the models had the following expressions:

$$R_{b2\{Ca/Si;Am.ph\}} = 20.60 - 7.66x_1 - 2.68x_1^2 + 0.07x_1x_4 - 7.66x_4 - 2.68x_4^2 \quad (5)$$

$$R_{b2\{Si/Al;Am.ph\}} = 24.90 - 7.42x_2 - 4.88x_2^2 \pm 0x_2x_4 - 7.42x_4 - 4.88x_4^2 \quad (6)$$

$$R_{b2\{Na/Si;Am.ph\}} = 22.08 - 7.63x_3 - 3.44x_3^2 + 0.03x_3x_4 - 7.63x_4 - 3.44x_4^2 \quad (7)$$

Figs. 1 present response surfaces for 28-day of hardened composites for the following pairs: (1) molar reactive ratios Ca/Si and amorphous-phase content, (2) Si/Al and amorphous-phase content, and (3) Na/Si and amorphous-phase content.

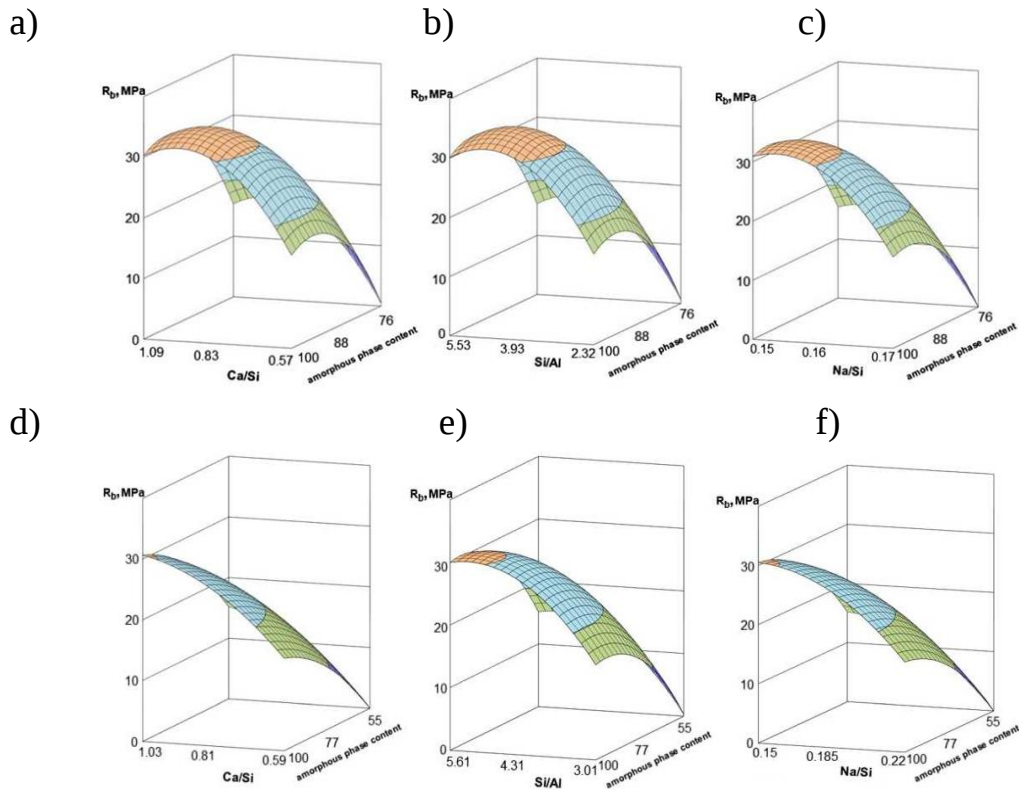


Fig 1. Response surfaces for 28-day hardened composites with additives 1 and 2: (a, d) Ca/Si-amorphous phase content; (b, e) Si/Al-amorphous phase content; and (c, f) Na/Si-amorphous phase content

Subsequently, correlation analysis was performed to rank the statistical significances and analyze the contributions of the reactive Ca, Si, Al, and Na oxides to the 28-day CS of the hardened composites. The computation experiment involved reproduction of a set of experimental data using the obtained experimental-statistical models [3]. The graphical representation of the correlation analysis (Fig. 3) shows differences in the ordering of the reactive oxide ratios, contributing to the strength of the composites.

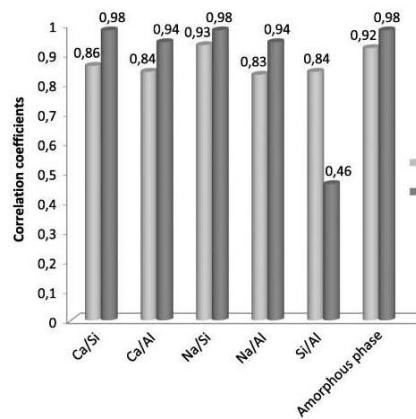


Fig. 9. Correlation coefficients versus reactive molar oxides ratios and amorphous phase.

As result, for composites, the significance of the reactive components evaluated using correlation coefficients  $r$  presented the following sequence:  $[r\{\text{Na/Si; reactive-phase content; } R\}] > [r\{\text{Ca/ Si; } R\}] > [r\{(\text{Ca/Al, Si/Al}); R\}] > [r\{\text{Na/Al; } R\}]$  and for additives 2:  $[r\{(\text{Ca/Si, Na/Si, reactive-phase content; } R\}] > [r\{(\text{Ca/Al, Na/Al}); R\}] > [r\{\text{Si/Al; } R\}]$ .

### Анотація

Досліджено особливості властивості будівельних композитів з добавками залежно від змісту та складу аморфної фази. Встановлено, що добавка, що містить 60% фази, придатна для використання як додатковий алюмосилікатний компонент до шлаку. В результаті досліджень отримано композиційне в'язуче з міцністю при стисканні у віці 28 діб до 30 МПа. Методами експериментально-статистичного моделювання встановлено, що найбільш значущими факторами у формуванні міцності композиційного в'язучого є вміст аморфної фази та співвідношення оксидів.

### REFERENCES

1. Lyashenko, T., and V. Voznesensky. 2017. *Composition-process fields methodology in computational building materials science*. [In Russian.] Odessa: Astroprin.
2. Rakhimova Nailia R. *Blended Alkali-Activated Cements Based on Blast-Furnace Slag and Calcined Clays: Statistical Modeling and Effect of Amount and Chemistry of Reactive Phase* / N. R. Rakhimova, V. P. Morozov, A.A. Eskin, Y.S. Lutskin, O.S. Shynkevych // *Journal of Materials in Civil Engineering*. June 2022. Volume 34, Issue 6. Online publication: March 26, 2022: *J. Mater. Civ. Eng.*, 2022, 34(6): 04022112.
3. Lutskin, E., and E. Shinkevich. 2015. *Analysis of the relationship between microstructure and properties of activated lime-silica composites on the basis of experimentally-statistical modeling*. *Technol. J.* 9 (1): 27.