Mathematical modeling of an effect of refractory metal nanopowders on the strength of concrete

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Abstract. The quality of concrete and the reliability of its exploitation in structures and structures are largely determined by such characteristic as strength. Additives increasing the strength can significantly improve the quality of concrete. The aim of this work is mathematical modeling of the effect of refractory metal nanopowders on the strength of concrete. Regression equations of the first and second orders are constructed, which adequately find the dependence of the compressive strength of concrete on the input parameters. For presented model the optimal values of the concentrations of refractory metal nanopowders have been calculated.

1 Introduction

The construction industry is one of the most dynamically developing segments of the Russian economy. Modern trends in the development of materials science in construction are closely related to the development of new resource-saving technologies for production concrete, with improved performance and durability. At the same time, the lack of material resources, developed in a number of regions, urgently requires increasing the profitability of the industry production of building materials due to the wide use as local resources and man-made materials. The downside of this trend is that the use of local substandard raw materials leads to a decrease in the strength of the cement construction composites.

At the same time, the quality of concrete and the reliability of its using in structures and structures are largely determined by such characteristic as strength. Strength is understood as the ability of a material to resist destruction as a result of external loading. This integral characteristic strongly depends on the mechanical and chemical properties of the material (concrete components), on the methods of concrete preparation and the exploitation of the structure. Some theoretical aspects of the dependence of the strength of composite materials on their physical and mechanical properties are considered in [1-4]. Nevertheless, in modern building materials science there is no complete theory that allows us to calculate its strength based on the given properties of concrete ingredients.

One of the possible solutions to the problem of improving the quality of concrete is the use of a limited number of highly active additives. As well known, concrete resists compression well and is much worse in tension. Due to this, additives, leading to an increase in strength can significantly improve the quality of the concrete. The experimentally demonstrated [5] that micro- and nanomodifiers (nanopowders) are the most promising

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among the possible additives. A significant limitation of this approach is the high cost of nanopowders, the lack of technologies for their mass production, which does not allow them to be used as additives on an industrial scale.

However, new technologies for the production of nanopowders make it possible to include the use of nanopowders in the cycle of concrete production in the future [6]. Thus, the aim of this work is mathematical modeling of the effect of refractory metal nanopowders on the strength of concrete.

2 Methods

The purpose of experimental studies is to study the effect of the addition nanopowders of refractory metal on the strength of a concrete sample (size $100\times100\times100mm$) at the age of 28 days of normal hardening (R^{28} , MPa) under compression in order to select the optimal amount of additives for which the concrete has the desired properties. Methods of mathematical planning of the experiment will make it possible to create a mathematical empirical model, depicting the influence of incoming parameters, that is, to form a response function in the form

$$y = f(x_1, x_2, ..., x_n),$$

where $x_1, x_2, ..., x_n$ - are the factors of the experiment.

It is usually assumed in experimental analysis of building structures that the response function (concrete compressive strength) is a random variable with a normal distribution law. On this basis, regression analysis methods are used when testing statistical hypotheses about the response function. Tables 1, 2 present the results of the characteristics of the homogeneity of concrete modified with various powders of refractory metals. It should be noted that statistical values are estimated as averages due to the limited sampling.

Table 1. Results of homogeneity characteristics of concrete modified with nanopowder WC, in strength.

Nanopowder content WC, %	The range of single values W_m	Average quadratic deviation S_m	The coefficient of variation V_m , %	Actual class, B_{ϕ}
0	0.711364	0.420925	4.088007	8.237275
1	1.514205	0.895979	6.961364	10.29659
2	0.302841	0.179196	1.344809	10.66
3	0.605682	0.358392	2.320455	12.35591

Table 2. Results of homogeneity characteristics of concrete modified with nanopowder WO₃, in strength.

Nanopowder content WO ₃ , %	The range of single values W_m	Average quadratic deviation S_m	The coefficient of variation V_m , %	Actual class, B_{ϕ}
0	0.711364	0.420925	4.088007	8.237275
1	0.605682	0.358392	3.034441	9.448639
2	0.302841	0.179196	1.461027	9.812048
3	0.908523	0.537588	4.863419	8.842957

The analysis of the homogeneity of concrete (tables 1, 2) showed, that the intra-batch coefficient of variation is in the range of less than 5%. Thus, the quality of production and testing of samples can be considered satisfactory.

3 Results of modeling

Let us carry out mathematical modeling of the influence of parameters on the strength of concrete under compression by the first-order planning method, where first-order polynomials $y = b_0 + b_1x_1 + b_2x_2 + ... + b_nx_n$ are chosen as approximating functions.

The working composition of concrete samples without additives had the following ratio: Cement (C): Sand (S): Crushed stone (St): Water (W) = 1: 2.4: 4.3: 0.6.

During the experiment the mixes with different contents of the modifier (H) have been prepared for the same ratio of the working composition of concrete. The following parameters

were selected as input parameters have effect on strength of concrete: x_1 – ratio $\frac{S + N}{C + St}$ in the range of 0.454 ... 0.458; x_2 – ratio $\frac{W}{C}$ within 0.59 ... 0.61. The number of experiences in first-order planning is $N_0 = 2^n = 4$. The first-order planning results are shown in Table 3.

Table 3. Experimental results with the addition of refractory metal nanopowder.

Experiment number	Initial values		Code values		$\bar{R}^{28}_{WC}$	$\bar{R}^{28}_{WO_3}$
	$\frac{S + N}{C + St}$	$\frac{W}{C}$	x_1	x_2		
1	0,454	0,59	-1	-1	12,870	11,810
2	0,458	0,61	+1	+1	15,445	10,448
3	0,458	0,59	+1	-1	15,444	10,447
4	0,454	0,61	-1	+1	12,871	11,811

The hypothesis of the homogeneity of the dispersion is verified by using the Cochran test, its value is calculated by the formula:

$$G_p = \frac{S_{\max}^2}{\sum_{k=1}^{N_0} S_k^2},$$

where S_k^2 is the estimate variance of experiment k , $S_{\max}^2$ is a maximum of the calculated variances.

The calculated value of the Cochran test is compared with the table value G_T ($G_p \leq G_T$), which is at confidence level P with degrees of freedom of numerator $f_1 = n - 1$ and denominator $f_2 = N_0$.

For the experiments, each of which included 3 parallel experiments $G_p = 0,788$, he hypothesis about the homogeneity of variances is can be accepted on 1% significance level, since the experimental value of the criterion does not exceed the tabular value.

Values of the coefficients b_i in the regression equation can be found as follows

$$b_i = \frac{\sum_{k=1}^{N_0} x_{ik} \bar{y}_k}{N_0} i = 0, ..., n ,$$

where x_0 is a fictive variable, which is introduced to obtain complete symmetry; $x_{0k} = +1$ for all values $k = 1, ..., N_0$.

Images of the surface were obtained (Fig. 1), described by objective functions. $Y_1 = R^{28}(WC)$ and $Y_2 = R^{28}(WO_3)$.

Fig. 1. Linear approximation of influence on the parameters on concrete strength.

Let us carry out mathematical modeling of the effect of parameters on the strength of concrete under compression by the second-order planning method, where second-order polynomials are chosen as approximating functions $y = b_0 + b_1x_1 + b_2x_2 + b_{12}x_1x_2 + b_{11}x_1^2 + b_{22}x_2^2$.

The number of second-order orthogonal compositional planning experiments is calculated by the formula $N = 2^n + 2n + 1$. Plan parameter values are calculated as following

$$a = \sqrt{\frac{N_0}{N}} , \quad \alpha = \sqrt{\frac{1}{2} \left(\sqrt{NN_0} - N_0 \right)}$$

is “star” shoulder.

Second order planning results $N = 9$ with parameters $a = \frac{2}{3}$, $\alpha = 1$ are given in Table 4.

Table 4. Experimental results with the addition of refractory metal nanopowder.

Experiment number	Code values		$x_1 x_2$	$x'_1 = x_1^2 - a$	$x'_2 = x_2^2 - a$	$\bar{R}^{28}, WC$	$\bar{R}^{28}, WO_3$
	x_1	x_2					
1	-1	-1	1	1/3	1/3	12,870	11,810
2	+1	+1	1	1/3	1/3	15,445	10,448
3	+1	-1	-1	1/3	1/3	15,444	10,447
4	-1	+1	-1	1/3	1/3	12,871	11,811
5	-1	0	0	1/3	-2/3	12,870	11,810
6	+1	0	0	1/3	-2/3	15,445	10,448

7	0	-1	0	-2/3	1/3	13,224	11,911
8	0	+1	0	-2/3	1/3	13,225	11,912
9	0	0	0	-2/3	-2/3	13,224	11,911

The above-mentioned formulas are used to calculate the coefficients of the second order regression equation.

The significance of the regression coefficients can be determined by the Student's t-test. For each coefficient, the calculated value of the Student's criterion is determined as following

$$t_{ip} = \frac{|b_i|\sqrt{N}}{S_{\bar{y}}},$$

where $S_{\bar{y}} = \sqrt{\frac{S_y^2}{m}}$, m is number of parallel experiments, $S_y^2 = \frac{\sum_{k=1}^N S_k^2}{N}$ is variance of a single measurement of the output parameter.

Calculated value of the Student's criterion is compared with tabulated t_T , which can be found with help of the confidence probability P and the number of degrees of freedom $f = N(m-1)$.

After verifying the significance of the coefficients, images of surfaces of the objective functions (Fig. 2) were constructed $Y_1 = R^{28}(WC)$ и $Y_2 = R^{28}(WO_3)$.

Fig. 2. Quadratic approximation of influence on the parameters on concrete strength.

4 Conclusions

The obtained regression equations of the first and second orders allow us to find adequately the dependence of the concrete compressive strength on the ratio of the input parameters x1 and x2. The optimal values of the concentration of nanopowders are calculated as: 2.95% WC , 1.72% WO_3 . According to presented modeling, nanopowder WC is the optimal additive to concrete that increases its operational properties.

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