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Application of mathematical model methods for optimization tasks in construction materials technology

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Abstract. In this paper, the regression equations method for design of construction material was studied. Regression and polynomial equations representing the correlation between the studied parameters were proposed. The logic design and software interface of the regression equations method focused on parameter optimization to provide the energy saving effect at the stage of autoclave aerated concrete design considering the replacement of traditionally used quartz sand by coal mining by-product such as argillite. The mathematical model represented by a quadric polynomial for the design of experiment was obtained using calculated and experimental data. This allowed the estimation of relationship between the composition and final properties of the aerated concrete. The surface response graphically presented in a nomogram allowed the estimation of concrete properties in response to variation of composition within the x-space. The optimal range of argillite content was obtained leading to a reduction of raw materials demand, development of target plastic strength of aerated concrete as well as a reduction of curing time before autoclave treatment. Generally, this method allows the design of autoclave aerated concrete with required performance without additional resource and time costs.

1. Introduction
Currently, the development of science and technology is associated with advancement of traditional technologies as well as design of new technologies where the major stage is experimental study. Complex technological process initiates an increase of resource and time consumption as well as application of up-to-date IT-technologies for data processing. A design of experiment application leads to improvement in quality of experimental studies and final products. Design of experiment enables one to develop polynomial equations which demonstrate a correlation between input and output parameters [1, 2].

Normally, mathematical simulation is applied for design of the experiment. The method of the polyfactorial experiment is realized in several stages: previous study of an investigating object; design of the mathematical model and its analysis. Completion of technological tasks using the design of the experiment during production of construction materials and structures is relevant because the production technology is a complex and multi-stage process [2–5].

The principle of design of the experiment and statistic analysis during designing the construction composites consists of mathematical correlation between input and output parameters such as characteristics and consumption of raw materials as well as technological factors [6]. This allows a

complete monitoring and optimization of the technological process with reduced resource costs [7–11] and development of highly efficient construction materials with required performance [12–14].

2. Methods

In this study, the experimental procedure was realized using the regression equations method. It is based on design of experiment including a number of varied input parameters as well as the task object [15]. All input parameters $(X_1, X_2, ..., X_n)$ were varied at the following three levels: basic-level (0), low-level (-1), top-level (1) with variability interval (ΔX_i) between the levels. According to the designed experiment the compositions of the aerated concrete were prepared.

Processing of the experimental results was performed using mathematical statistics methods. As a result, the polynomial equations were developed showing a correlation between input and output parameters [1, 16].

The regression equation for the two-factorial experiment was developed (eq. 1):

$$y = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_1^2 + b_4 x_2^2 + b_5 x_1 x_2; \tag{1}$$

Calculation of coefficients for the regression equations was done with equations (2)–(5):

$$b_0 = T_1 \sum_1^N y_u - T_2 \sum_1^K \left(\sum_1^N x_{iu}^2 y_u \right); \tag{2}$$

$$b_i = T_3 \sum_1^N x_{iu} y_u; \tag{3}$$

$$b_{ii} = T_4 \sum_1^N x_{iu}^2 y_u + T_5 \sum_1^K \left(\sum_1^N x_{iu}^2 y_u \right) - T_2 \sum_1^N y_u; \tag{4}$$

$$b_{ij} = T_6 \sum_1^N x_{iu} x_{ju} y_u, \tag{5}$$

where $T_1...T_6$ are reference data [17];

y_u is an experimental value of the output parameter. An average value was used in case of row-wise matrix duplication of the matrix;

u is a point number;

x_i is a coded form of i-factor;

N is a total number of points in the matrix.

According to the experimental procedure, the statistical verification of the coefficient relevance, as well as feasibility assessment of the designed regression equation to describe a correlation between the studied parameters, was accomplished.

Feasibility assessment and efficiency of the designed regression equation is normally determined by calculation of the followings parameters [1, 18]:

a) Arithmetical average value.

An arithmetical average value for output parameter $\overline{y}_u$ was calculated with eq. (6) in terms of row-wise matrix duplication of the matrix:

$$\overline{y}_u = \frac{y_{u1} + y_{u2} + ... + y_{ur}}{r}, \tag{6}$$

where r is a number of row-wise duplicated matrices.

In the same way, the value of the output parameter was calculated for the experiment in zero-points.

b)   Error mean-square for the output parameter was calculated with eq. (7) in case of row-wise matrix duplication of the matrix and with eq. (8) in case of experiment completion in zero-points:

$$S^2_{(yu)} = \frac{\sum\limits_{1}^{N}\sum\limits_{1}^{r}(y_{ui} - \bar{y}_u)^2}{N(r-1)}, \tag{7}$$

where $\sum\limits_{1}^{r}$ is the matrix row sum;

$\sum\limits_{1}^{N}$ is the matrix column sum.

$$S^2_{(y_0)} = \frac{\sum\limits_{1}^{n_0}(y_{ou} - \bar{y}_o)^2}{n_o - 1}, \tag{8}$$

where n_o is a number of zero-points.

c)   Mean-square deviation for the output parameter, associated with the experimental error, was calculated with eq. (9) in terms of the experiment matrix dublication and with eq. (10) in terms of the experiment in zero-points:

$$S_{(y_u)} = \sqrt{S^2_{(y_u)}}; \tag{9}$$

$$S_{(y_o)} = \sqrt{S^2_{(y_o)}}; \tag{10}$$

d)   Mean-square error for the coefficient determination was calculated with eq. (11)–(14) in terms of row-wise matrix-duplication:

$$S_{(b_o)} = T_7 S_{(y_u)}; \tag{11}$$

$$S_{(b_i)} = T_8 S_{(y_u)}; \tag{12}$$

$$S_{(b_{ii})} = T_9 S_{(y_u)}; \tag{13}$$

$$S_{(b_{ij})} = T_{10} S_{(y_u)}. \tag{14}$$

For the experiment in zero-points using eq. (11)–(14) $T_7 ... T_{10}$, the reference values instead $S_{(y_u)}$ were applied.

e) Calculated Student criterion value t_c for each coefficient was calculated with regression equations (15)–(18) from a minimum to maximum value:

$$t_{p(b_0)} = \frac{|b_0|}{S_{(b_0)}}; \tag{15}$$

$$t_{p(b_i)} = \frac{|b_i|}{S_{(b_i)}}; \tag{16}$$

$$t_{p(b_{ij})} = \frac{|b_{ij}|}{S_{(b_{ij})}}; \tag{17}$$

$$t_{p(b_{ii})} = \frac{|b_{ii}|}{S_{(b_{ii})}}. \tag{18}$$

The calculated coefficient was relevant if the Student criterion value $t_p > T_n$ considering a required level of significance and the number of degrees of freedom f(y). In engineering design, the relevant level is normally, 0.05 or 0.1. A number of degrees of freedom were calculated with eq. (19) in terms of row-wise matrix duplication and with eq. (20) in terms of the experiment in zero-points:

$$f(y) = N(r-1); \tag{19}$$

$$f(y) = n_0 - 1, \tag{20}$$

where n_o is a number of zero-points excluded of the matrix.

e) In the second-order matrix, any coefficients (relevant and non-relevant) for quadratic term were included in the regression equation.

f) Residual dispersion S_{ag}^2 was calculated with eq. (21) and (22) to revise adequacy of the obtained regression equation and with eq. (23)–(24) in terms of row-wise matrix-duplication.

$$S_{ag}^2 = \frac{\sum_{1}^{N}(y - y_u)^2}{N - m - (n_0 - 1)}; \tag{21}$$

$$S_{ag}^2 = \frac{\sum_{1}^{N}(y - y_u)^2}{N - m}; \tag{22}$$

$$S_{ag}^2 = \frac{r\sum_{1}^{N}(y - y_u)^2}{N - m - (n_0 - 1)}; \tag{23}$$

$$S_{ag}^2 = \frac{r\sum_{1}^{N}(y - y_u)^2}{N - m}, \tag{24}$$

where y is a calculated value of the output parameter;

m is a number of relevant coefficients in the regression equation.

If the matrix contained zero-points, the residual dispersion was calculated with eq. (21) and (23); in terms of absence of zero-points eq. (22) and (24) were applied.

g) Fisher's criterion F_p was calculated with eq. (25) in terms of $S_{ag}^2 > S_{(y)}^2$ and with eq. (26) in terms of $S_{ag}^2 < S_{(y)}^2$

$$F_p = \frac{S_{ag}^2}{S_{(y)}^2}; \tag{25}$$

$$F_p = \frac{S_{(y)}^2}{S_{ag}^2}, \tag{26}$$

where $S_{(y)}^{2}$ is an error mean square for the output parameter. The reference value of the Fisher's criterion F_{ref} depends on the accepted confidence factor of 90–95 % and the number of degrees of freedom f(y) that was calculated with eq. (27)–(28) for the non-pure quadratic equation.

$$f_{ag} = N - m; \tag{27}$$
$$f_{ag} = N - m - (n_0 - 1); \tag{28}$$

In terms of $F_p < F_{ref}$ the obtained regression equation was considered to be an adequate. Otherwise the equation was non-adequate. In this case the experiment should be performed again or the variability interval should be corrected or other matrix should be designed. The required adequacy can be achieved by replacement of some parameters with logarithmic values or the polynomical equation.

Thus, the regression equation allows working with inter- and extrapolation functions, making nomograms and quick calculation of the output parameter, considering the variation of input parameters [17].

3. Enhancement of aerated concrete composition using design of experiment

In this paper, the regression equation method was used to develop the binder for energy saving autoclave aerated considering the replacement of traditionally used quartz sand by a coal mining by-product such as argillite. Development of plastic strength in aerated concrete before autoclave curing was studied. Normally, the curing time before autoclave treatment is significant during the production process for the formation of physical and mechanical characteristics to happen.

Calculation of the results using regression equation was made with the SigmaPlot software. The software interface was presented by logic sections for inserting input data and variation of output parameters interactively according to the used mathematical model. The program algorithm included the followings procedures: determination of coefficients for the response function; statistical analysis; visual representation of the mathematical model.

Table 1. Factors level sand matrix range

Input parameters		Variation level			Variation interval
Origin form	Coded form	-1	0	1	
Argillite content, %	X_1	5	25	45	20
Curing time of the aerated concrete before autoclave treatment, min	X_2	30	120	210	90

In order to estimate the effect of input parameters on physical and mechanical characteristics of the developed binder the calculation was completed by the linear interpolation method using eq. (29) and (30):

$$X_1 = \frac{A - 25}{20}; \tag{29}$$

$$X_2 = \frac{\tau - 120}{90}; \tag{30}$$

where A and X_1 are argillite content in origin and coded forms, respectively;

τ and X_2 are curing times of the aerated concrete before autoclave treatment in origin and coded forms, respectively.

To obtain the required data for the design of experiment, the specimens of aerated concrete were prepared followed by plastic strength testing of the specimens at different age.

The reference composition of aerated concrete was consisted of lime (11.6 %); quartz sand (68.3 %); portland cement (20 %); gas forming agent (aluminum paste) (0.1 %) with water/solid ratio (0.5).

Argillite was incorporated into the concrete mixture partially replacing quartz sand. Results of the experiment are presented in Table 2.

Table 2. Effect of replacement quartz sand by argillite on plastic strength (MPa) at different age

Curing time of the aerated concrete before autoclave treatment, min	Argillite content,%					
	0	5	15	25	35	45
30	0.0086	0.0092	0.010	0.0095	0.0070	0.0044
60	0.010	0.017	0.018	0.010	0.0075	0.0053
90	0.018	0.019	0.024	0.014	0.0083	0.0059
120	0.024	0.028	0.032	0.026	0.017	0.0064
150	0.028	0.032	0.039	0.034	0.027	0.0085
180	0.043	0.049	0.053	0.041	0.032	0.013
210	0.087	0.094	0.13	0.066	0.037	0.025

Data from Table 2 were the input parameters for the matrix in the regression equation method (Table 3). Nine sets of experiments were performed.

Table 3. Matrix of design of experiment

№	X_1	X_2	Curing time of the aerated concrete before autoclave treatment, min	Argillite content, %	Y_{exp}	Y_{cal}
1	−1	−1	30	5	0.0092	0.01
2	1	−1	210	5	0.094	0.09
3	−1	1	30	45	0.0044	0.01
4	1	1	210	45	0.025	0.03
5	0	0	120	25	0.026	0.02
6	0	1	120	45	0.0064	0.00
7	0	−1	120	5	0.28	0.03
8	1	0	210	25	0.066	0.07
9	−1	0	30	25	0.0095	0.01

The SigmaPlot software controlled automatically the input data, calculated coefficients for the designed mathematical model and formed the response function in the form of regression equation (31) for compressive strength R_{comp} as the output parameter:

$$Y(R_{comp}) = 0.024 + 0.27X_1 - 0\,X_2 + 0.015\,X_1^2 - 0{,}006\,X_2^2 - 0\,X_1X_2 \qquad (31)$$

Development of the mathematical model was followed by revision of relevancy of the coefficients (they should be non-zero) and the model validity using eq. (6)–(28). The response function for the designed binder and relevant aerated concrete is presented in Fig. 1.
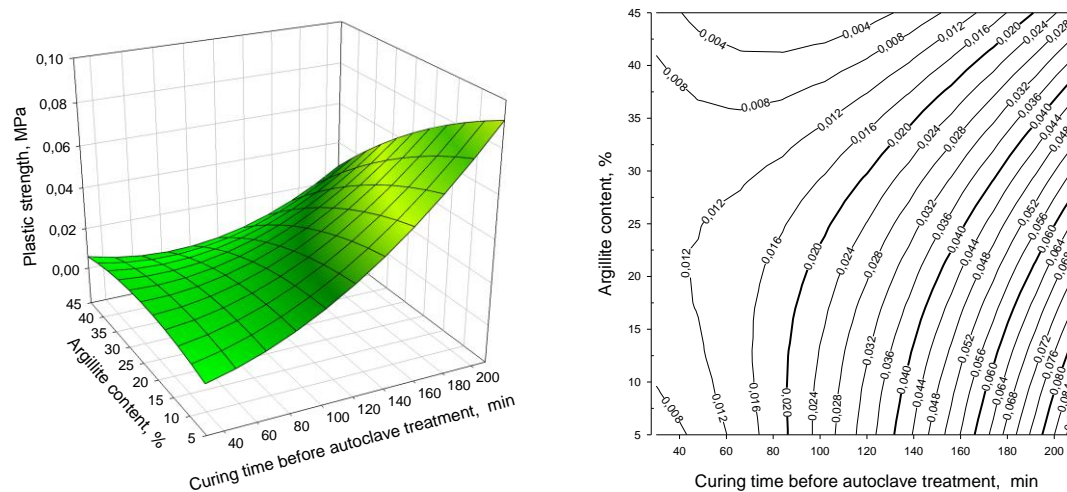
Figure 1. The response function for the designed binder plastic strength vs variation of argillite content and curing time of the aerated concrete before autoclave treatment

Discussions

During production of aerated concrete, the development of required plastic strength before cutting procedure is significant. Under production conditions, plastic strength can reach up to 0.03–0.08 MPa after 3 hours of curing. Analysis of the response function for the required plastic strength of the binder demonstrated that the most effective argillite content was 15 %. In this case, the minimal time for the required plastic strength to develop was reduced from 3 hours to 90 min. In this regard, varying the argillite content in the aerated concrete mixture allows monitoring a total production process for autoclave aerated concrete. By increasing argillite content up to 35 %, the time of plastic strength development was elongated up to 3 hours. However, a further increase of argillite content leads to such negative effect as inhibition of setting time.

Conclusions

The regression equation method was applied to study the effect of composition and curing time before autoclave treatment for plastic strength of autoclave aerated concrete. The step-by-step procedure, when mathematical model design including a design of regression equations, statistic analysis and development of a response surface was represented by a nomogram (in 3-D coordinate system), was presented. The obtained nomogram allowed a visual analysis of effect of argillite content and curing time before autoclave treatment as input parameters on resulting plastic strength as an output parameter. The designed model can be used when design autoclave aerated concrete with the required characteristics and minimal resource and time consumption.

Acknowledgements

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