Optimal dry mixes simulating

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Abstract. When applying mortar mixes in thin layers on porous substrates, moisture is released from the mortar mix. As a result, such operational characteristics of the solution as bending strength, compressive strength, adhesion strength and crack resistance can be reduced. The introduction of modifying additives, such as: dispersed mineral additive, powder polymers and fibers, allows providing these indicators at the required level. In order to simulate the composition of the dry mix with modifying additives, multivariate design of the experiment was carried out, regression equations were obtained, statistical analysis of the proposed equations was carried out, which confirmed their significance. The verified model showed a high degree of correspondence between the values calculated by the regression equations and experimental data. The procedure of regression equations maximizing made it possible to determine the optimal composition of dry construction mixes depending on their functional purpose, hardening conditions and operation.

1. Introduction

Due to the literature data, water migrates to the base or evaporates into the atmosphere when ordinary solutions are applied with a thin layer on porous substrates. Therefore, hydration processes can occur unevenly along the thickness of the solution, which leads to a significant decrease in strength, cracking and the appearance of internal stresses in the structure of the material. In addition, there is a selection of moisture with a base and partial evaporation at the beginning of conventional Portland cement hardening more than 45 minutes (usually 1.5 - 2.5 hours). All this complicates the use of thin-layer technologies for mortar mixes applying [1-4].

High requirements are made on finishing mixes that are used in difficult conditions when it is necessary to have high adhesion, low water absorption, water repellent effect, high vapor permeability, wear resistance, crack resistance, impact resistance, low shrinkage (facade coatings, adhesive plasters and putties, self-leveling screeds for the floor, waterproofing compounds for gluing insulation and reinforcing mesh, glue for laying tiles in wet rooms, etc.). These requirements can be met by introducing modifying additives into the dry building mix [5-10].

We used the available recommendations [11-13], took into account the study results of physic mechanical parameters of solutions modified with a dispersed mineral additive, powder polymers and fibers, as well as the functional purpose of dry mixes, the conditions for their hardening and operation, compiling dry construction mixes.
2. Research methods

In order to select the optimal composition of dry mix, we used the method of multi-factorial planning of the experiment. It helped us find the relationship between the components of dry mix and its final properties [14-17].

To obtain a solution the dry mixture was mixed with water. Bending strength, adhesion at separation from the base and cracking resistance were determined as the three main properties of the solution. Using the method of multi-factorial design of the experiment, a mathematical model was constructed for each property in the form:

\[ Y = f(X_1, X_2, \ldots, X_n) + \varepsilon, \]  

where \( Y \) – response function, random variable, \( X_1, X_2, \ldots, X_n \) – variation factors, \( f(X_1, X_2, \ldots, X_n) \) – unknown function \( X_1, X_2, \ldots, X_n \), \( \varepsilon \) – random model error.

The following factors were taken as variation factors: \( x_1 \) – amount of re-dispersible polymer powder (RPP), \( x_2 \) – amount of hydrated lime, \( x_3 \) – amount of methylcellulose, \( x_4 \) – amount of fibers.

The experiment design was set in the form of a planning matrix with \( 2^i \times i \) dimension, where \( i \) was the number of factors (\( 16 \times 4 \) in our case). Each row of the planning matrix determined the recipe parameters; each column determined the values of factors corresponding to this recipe. Table 1 shows the experiment planning matrix, and the values of four factors at three variation levels are in table 2.

| Table 1. Experiment planning matrix. |
|--------------------------------------|
| Composition Number | Planning Matrix | Composition Number | Planning Matrix |
| x₁ | x₂ | x₃ | x₄ | x₁ | x₂ | x₃ | x₄ |
| 1 | -1 | -1 | -1 | -1 | 9 | -1 | -1 | -1 | +1 |
| 2 | +1 | -1 | -1 | -1 | 10 | +1 | -1 | -1 | +1 |
| 3 | -1 | +1 | -1 | -1 | 11 | -1 | +1 | -1 | +1 |
| 4 | +1 | +1 | -1 | -1 | 12 | +1 | +1 | -1 | +1 |
| 5 | -1 | -1 | +1 | -1 | 13 | -1 | -1 | +1 | +1 |
| 6 | +1 | -1 | +1 | -1 | 14 | +1 | -1 | +1 | +1 |
| 7 | -1 | +1 | +1 | -1 | 15 | -1 | +1 | +1 | +1 |
| 8 | +1 | +1 | +1 | -1 | 16 | +1 | +1 | +1 | +1 |

| Table 2. Factors’ values. |
|----------------------------|
| Factor | Designation | Values of Variation Factors |
|       |             | -1 | 0 | +1 |
| Amount of RPP, % wt. | \( x_1 \) | 0.3 | 0.4 | 0.5 |
| Amount of hydrated lime, % wt. | \( x_2 \) | 15 | 20 | 25 |
| Amount of methyl cellulose, % wt. | \( x_3 \) | 0.2 | 0.3 | 0.4 |
| Amount of fibers, % wt. | \( x_4 \) | 0.4 | 0.6 | 0.8 |

A mix of the following composition was prepared: binder – 313 kg, sand – 1400 kg, water, a mineral additive (limestone) – 7% by weight of cement. The amount of water was selected, based on the solution mobility.

It was studied whether the linear regression can be used [18,19]:

\[ y = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_3 + b_4 x_4 \]  

(2)

Determining the optimal composition of dry mixes was to find the unknown coefficients of the regression model (2), where: \( x_1, x_2, x_3, x_4 \) – factors' values; \( b_0 \) – free term is equal to a response in the
absence of additives; \(b_1, b_2, b_3, b_4\) – regression coefficients indicates the influence of a factor on the process under study.

The test results were presented in the form of a 16×5 matrix, where the first column is the percentage of RPP by weight of cement; the second column is the hydrated lime percentage; the third – the methyl cellulose percentage; the forth – fiber fraction. The last column is the bending strength (MPa) or adhesion strength (MPa), or cracking resistance (hr) obtained in experiments. These values (responses) are shown in table 3.

| Composition Number | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  | 11  | 12  | 13  | 14  | 15  | 16  |
|--------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Bending Strength, MPa | 4.8 | 5.0 | 4.6 | 4.7 | 4.5 | 4.7 | 4.3 | 4.4 | 5.0 | 5.2 | 4.8 | 4.9 | 4.7 | 4.9 | 4.5 | 4.6 |
| Adhesion Strength, MPa | 1.4 | 1.6 | 1.3 | 1.5 | 1.5 | 1.7 | 1.4 | 1.6 | 1.4 | 1.6 | 1.3 | 1.5 | 1.5 | 1.7 | 1.4 | 1.6 |
| Cracking Resistance, hr | 3.0 | 3.5 | 3.25| 3.75| 3.25| 3.75| 3.5 | 4.0 | 4.0 | 4.5 | 4.25| 4.75| 4.25| 4.75| 4.5 | 5.0 |

24 measurements were performed for each composition to reduce random error. Thus, all values in table 3 were calculated as arithmetic means of 24 measurements.

Unknown coefficients in the regression (2) were found by the least squares method from the minimum of \(\sum (y_i - \hat{y}_i)^2\) functional. For bending strength, the equation:

\[
\hat{y}(x_1, x_2, x_3, x_4) = 5.075 + 0.75 x_1 - 0.025 x_2 - 1.5 x_3 + 0.5 x_4, \tag{3}
\]

for adhesion strength:

\[
\hat{y}(x_1, x_2, x_3, x_4) = 1.15 + x_1 - 0.01 x_2 + 0.5 x_3 - 3.35 \cdot 10^{-15} x_4, \tag{4}
\]

for crack resistance:

\[
\hat{y}(x_1, x_2, x_3, x_4) = 0.625 + 2.5 x_1 + 0.025 x_2 + 1.25 x_3 + 2.5 x_4. \tag{5}
\]

To check the statistical significance of calculated coefficients a value was determined:

\[
t_j = \frac{b_j}{s_{bj}}, \tag{6}
\]

where \(s_{bj}\) – standard error of the coefficient \(b_j\). Values \(t_j\) were compared with a critical value \(t(1 - \alpha/2, n-m) = 2.201\) for \(\alpha = 0.05\), \(n = 16\), \(m = 5\) \((m – \) the number of coefficients in regression). The comparison showed that for the coefficient \(b_4 = -3.35 \cdot 10^{-15}\) in (4) the condition \(|\hat{f}_j| > t(1 - \alpha/2, n-m)\) is not performed, therefore, it can be excluded from equation (4). All other coefficients of equations (3) - (5) at the significance level \(\alpha = 0.05\) are statistically significant.
In order to determine the quality of the proposed models, for each equation (3) - (5), the multiple determination coefficients $R^2$ and the advanced determination coefficient $\hat{R}^2$ were calculated:

\[
R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2},
\]

\[
\hat{R}^2 = 1 - \frac{n-1}{n-m} (1 - R^2).
\]

![Image showing graphs](image)

**Figure 1.** Graphs of the bending strength at a fixed percentage a) methylcellulose 0.3%; b) hydrated lime 20%; c) RPP 0.4%; d) fiber 0.6%; e) adhesion strength; cracking resistance at a fixed percentage of f) hydrated lime 20%; g) RPP 0.4%; h) fiber 0.6%; i) methylcellulose 0.3%.

Calculations showed that the values of $R^2$ and $\hat{R}^2$ for equations (3) - (5) vary from 0.98 to 0.995. This indicates that the developed mathematical model corresponds to experimental data.

Checking the statistical significance of equations (3) - (5) using the Fisher criterion showed that, at a significance level of 0.05, all equations are significant.
The equation analysis (3) showed that bending strength increased with the introduction of RPP and fibrous additives; it decreased with the addition of hydrated lime and methylcellulose. The adhesion strength (4) increased with the introduction of RPP and methylcellulose; decreased with the addition of hydrated lime. Resistance to cracking (5) increased with the introduction of hydrated lime, methylcellulose, polymer and fiber additives. The greatest contribution was made by the content of fiber additives and RPP.

Ternary graphs were constructed for a visual representation of separate factors influence on the responses (figure 1). The values of three factors were plotted on three axis of graphs; the factors’ values were normalized from 0 (in the planning matrix this corresponded to level -1) to 1 (level +1 in the planning matrix). Response values were digitized in pixels of different colors. If more than three factors were present in regression, then one of them was fixed at an average level, and the graph of the remaining three factors was plotted. Obtained 9 graphs graphically describes dependence of bending strength, adhesion strength, and crack resistance from the components of dry mix: RPP, hydrated lime and fiber additives.

3. Experimental results
The obtained regression equations make it possible to simulate the dry mix composition depending on the required indicators. The ratio of “banding: sand” remains unchanged, in volume it is 1: 3.2. The amount of additives varies within the limits showed in table 2. Thus, a broad formulation can be made depending on the required properties [20].

So, for example, the following composition of additives can be recommended for the plaster compositions used on the outside of the building: hydrated lime is not more than 25% by weight of cement; dispersed limestone is 7% by weight of cement; methyl cellulose is 0.4%; RPP is 0.5%; basalt fibers are 0.8%. The obtained solution from such a mix will have a bending strength – 4.625 MPa, adhesion strength – 1.6 MPa, resistance to cracking – 5 hours. This problem can be solved by equations (3) - (5) optimizing (maximizing).

So, the greatest bending strength (5.175 MPa) was obtained for a mix with the following composition: hydrated lime – not more than 15% by weight of cement; methylcellulose – 0.2%; RPP – 0.5%; basalt fibers – 0.8%.

For maximum adhesion strength (1.7 MPa), the following composition was calculated: hydrated lime – not more than 15% by weight of cement; methyl cellulose – 0.4%; RPP – 0.5%; basalt fibers – 0.4%.

The cracking resistance was greatest (5 hours) for the composition: hydrated lime – less than 25% by weight of cement; methylcellulose – 0.4%; RPP – 0.5%; basalt fibers – 0.8%.

In all the proposed compositions, there was a dispersed limestone additive – 7% by cement weight.

4. Conclusion
Regression equations were obtained because of multi-factorial design of the experiment and its mathematical processing. These regressions make it possible to simulate the composition of the dry mix depending on the required indicators. A statistical analysis of the proposed equations was carried out, confirming the equations significance.

Verification of the model showed a high degree of correspondence between the values calculated from regressions and experimental data. The performed procedure of the regression equations maximizing made it possible to determine the optimal composition of dry building mixes depending on their functional purpose, hardening conditions and operation.

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