Method of mathematical modeling for the experimental evaluation of fire retardant materials parameters

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Abstract. In experiment planning research, mathematical methods play an active role. The main task of the researcher is to choose the optimal methodology for conducting the experiment. The experiment is an abbreviated design of full factorial tests and can be considered acceptable due to the small correlation between influencing factors and outputs. The features of the formulations of new composite fire retardant materials have been investigated. The main physical and chemical properties of the materials have been determined to provide fire protection.

1. Introduction
Experiment planning uses mathematical methods to choose some optimal strategy for experiment control. The research process contains separate stages. After at each stage, the researcher receives new information that allows to change the research strategy. In mathematical language, the problem of planning an experiment is formulated as follows: at each stage of the study, researcher needs to choose optimal location of points in the factorial space in order to get some idea of response surfaces. To solve this problem, it is enough to investigate response surface in a small area, limited to a linear analysis. The task is formulated differently after reaching the area where is the optimum. Here the researcher needs to get significantly more understanding of the response surface, approximating it by polynomials second, and sometimes even third order. In many cases, researcher has to start with the setting of the so-called screening experiments aimed at highlighting the dominant effects among a very large number of potential ones.

2. Mathematical model
To build a mathematical model of a complex multifactor multiparameter system, the following actions should be fulfilled:

1. Make a list of the m most significant influencing factors (IF) \([x_1,\ldots,x_m]\) and of the n most informative output parameters (OP) \([y_1,\ldots,y_n]\);

2. Make a plan of active multifactorial tests in the form of a matrix X, containing m columns (by the number of IF) and N rows (by the number of tests), the main requirements for which are:
a) lack of correlation between IF (pair correlation coefficient $r_{kl}$ between factors $x_k$ and $x_l$ should be close to 0);
b) the completeness of the coverage of the factor space (at least it should be: $N > m$);
c) practicability - i.e. compliance with the capabilities of the experimental bases;
d) all experiments (combinations of IF) in matrix $X$ are equivalent.

3. Run active tests, during which IF combinations are varied according to the plan (matrix $X$) and determine (measure) the values of the IF, forming thus, a matrix $Y$ containing $N$ rows (according to the number of tests) and $n$ columns (by the number of OP). In this case, the unambiguity of the result should be provided, i.e. when repeating an experiment (reproducing of the same IF combination), the spread of the OP values should be insignificant;

4. Carry out mathematical processing of the results of active tests, which assumes:
a) determining the relationship between the OP by calculating the coefficients pair correlation between OP (values of $r_{kl}$ between parameters $y_k$ and $y_l$ must be close to 0, otherwise one of the OP at $y_k$ or $y_l$ can be replaced by another OP);
b) assessment of the correspondence of the sample of experimental values of each $j$-th OP $[y_{j1},...,y_{jN}]$ to normal (Gaussian) distribution, in particular, according to asymmetry coefficients $\Delta_s$ and kurtosis $\Delta_k$ (i.e., condition $\Delta_s = \Delta_k = 0$);
c) building an adequate mathematical model
\[ y_j = f_j(x_{j1},...,x_{jm}) \in [1,n], \] (1)
which in this paper will be in the form of a quasilinear equation regression:
\[ y_j = \sum_{k=1}^{M_j} a_{jk} Z_{jk} \cdot j \in [1,n]. \] (2)
where $a_{jk}$ is the regression coefficient, which is a component of the vector $A_j$,
$z_{jk}$ is the $k$-th conditional factor, which is a component of the matrix $Z_j$ and representing function of IF $x_{j1},...,x_{jm}$;
$M_j$ is the number of regression coefficients or conditional factors ($M_j < N$).
d) using regression equations (2) for applied purposes:
- interpretation of the dependence of OP from IF;
- evaluating the values of OP for combinations of IF that differ from included in the matrix $X$;
- assessment of the significance of the influence of IF on OP;
- construction of the working area on the set of IF, in which each $j$-th OP is within acceptable limits.

Conditional factors $\{z_{jk}\}$ are chosen by accelerated choice method within the constructing the regression equation (2), and the vectors of the regression coefficients $A_1,...,A_m$ are calculated based on the condition of minimum variance for regression equations (least squares method):
\[ D_j = (N - M_j)^{-1} \sum_{i=1}^{N} (y_{ji} - \hat{y}_{ji})^2 \rightarrow min, j \in [1,n]. \] (3)
where $y_{ji}, \hat{y}_{ji}$ - the values of the $j$-th OP, respectively, obtained during the $i$-th experiment and calculated by the regression equation (2) for the $i$-th combination of IF.

The adequacy of the regression equations (2) can be assessed by the criterion Fisher.

It appears expedient to use also multimodel principle, according to which the dependence of the j-th OP on the IF can be described not by one adequate equation (2), but by several such equations.

It is required to construct a mathematical model of a complex system in the form of quasilinear regression equation (2) containing four OP ($n = 4$) on which affect eight IF ($m = 8$). For this specialized design of nine trials ($N = 9$) - matrix $X$ was built.

Pre-processing of the $X$ and $Y$ matrices made it possible to determine the following pair correlation coefficients:
\[ r_{x12} = r_{x13} = r_{x14} = r_{x15} = r_{x16} = r_{x17} = r_{x23} = r_{x24} = r_{x25} = r_{x26} = r_{x27} = r_{x34} = r_{x35} = r_{x36} = r_{x45} = r_{x46} = r_{x56} = r_{x57} = r_{x67} = 0,1 \]

\[ r_{y12} = -0.276; r_{y13} = -0.231; r_{y14} = 0.173; r_{y23} = 0.703; r_{y24} = -0.576; r_{y34} = -0.841. \]

Y1 - expansion ratio,
Y2 - adhesion,
Y3 - durability,
Y4 - water resistance.

### Table 1. Plan and test results of the 2nd system.

| № | x_1 | x_2 | x_3 | x_4 | x_5 | x_6 | x_7 | x_8 | Y_1 | Y_2 | Y_3 | Y_4 |
|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 1 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 0.5 | 10  | 120 | 15  | 1   |
| 2 | 1.5 | 1.5 | 0.5 | 0.5 | 1.5 | 1.5 | 0.5 | 0.5 | 10  | 48 | 15 | 1   |
| 3 | 1.5 | 0.5 | 1.5 | 0.5 | 1.5 | 1.5 | 0.5 | 0.5 | 10  | 48 | 15 | 1   |
| 4 | 0.5 | 1.5 | 0.5 | 0.5 | 1.5 | 1.5 | 0.5 | 1.5 | 10  | 24 | 5  | 2   |
| 5 | 1.5 | 0.5 | 0.5 | 1.5 | 1.5 | 1.5 | 0.5 | 1.5 | 10  | 24 | 5  | 1   |
| 6 | 0.5 | 1.5 | 0.5 | 1.5 | 1.5 | 1.5 | 0.5 | 1.5 | 30  | 24 | 3  | 2   |
| 7 | 0.5 | 0.5 | 1.5 | 1.5 | 1.5 | 1.5 | 0.5 | 1.5 | 10  | 24 | 3  | 2   |
| 8 | 1.5 | 1.5 | 1.5 | 1.5 | 0.5 | 0.5 | 0.5 | 1.5 | 50  | 48 | 15 | 1   |
| N=9 | 1.5 | 1.5 | 1.5 | 1.5 | 1.5 | 1.5 | 1.5 | 1.5 | 80  | 24 | 3  | 2   |

As=0.94

\[ x_{max} = 0.5 + (x_{k1} - x_{s1}) / (x_{kmax} - x_{s1}), \text{iC}[1.8]; iC[1.9]. \]

Applied to the 1st OP, in accordance with the principle of multi-model, four regression equations were obtained:

\[ y_{1a} = 4.622z_{1a} + 5.652z_{2a}. \]  
\[ y_{1b} = 9.407 z_{1b} + 6.537 z_{2b}. \]  
\[ y_{1c} = 12.97 z_{1c} - 0.6064 z_{2c} + 6.019 z_{3c}. \]  
\[ y_{1d} = -4.066 z_{1d} + 1.379 z_{2d} + 3.892 z_{3d} + 4.172 z_{4d} + 1.023 z_{5d}. \]

Where \[ z_{1a} = x_1 x_2 x_3 \] \[ z_{1b} = x_1 x_2 x_3 x_4 x_5 \] \[ z_{1c} = (x_1 x_2 x_4)^2 \] \[ z_{1d} = (x_1 x_2 x_3 x_4 x_5)^2 \] \[ z_{2} = x_2 x_3 x_6 / (x_2 x_3 x_4)^2 \] \[ z_{3} = x_1 x_3 (x_2 x_4 x_5)^2 / x_7 \] \[ z_{4} = x_2 x_3 x_4 x_5 / (x_1 x_2 x_3 x_6)^2 \] \[ z_{5} = x_3 x_4 x_5 / (x_1 x_2 x_3 x_6)^2 \]

Comparison of the experimentally obtained values of the OP for the 2nd system with the results of calculations using the regression equations.

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where x_{k}=0.5+(x_{k1}-x_{s1})/(x_{kmax}-x_{s1}), kC[1.8]; iC[1.9].
Table 2. Comparison of the experimentally obtained values.

| №  | y₁  | y₂  | y₃  | y₄  | y₅  | y₆  | y₇  | y₈  | y₉  | y₁₀ | y₁₁ | y₁₂ | y₁₃ | y₁₄ | y₁₅ | y₁₆ | y₁₇ | y₁₈ |
|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 1  | 0.43| 10.6| 18.9| 6.84| 1   | 1.03| 0.997|
| 2  | 6.20| 20.5| 10.4| 8.22| 1   | 0.959| 0.999|
| 3  | 20.7| 13.0| 9.03| 7.85| 1   | 0.983| 0.997|
| 4  | 5.13| 11.4| 9.03| 10.2| 2   | 2.0| 1.98 |
| 5  | 28.8| 20.3| 27.1| 31.2| 1   | 1.05| 1.03 |
| 6  | 30.6| 20.5| 27.1| 29.8| 2   | 2.0| 1.99 |
| 7  | 3.83| 13.0| 9.03| 10.5| 2   | 2.0| 2.02 |
| 8  | 55.8| 59.7| 59.2| 60.1| 1   | 0.983| 1.03 |
| 9  | 81.3| 81.2| 80.7| 80.1| 2   | 2.0| 1.98 |
| F  | -   | 15.1| 12.7| 46.6| 136 | - | 277.6| 377.7|

3. Conclusions

Based on the selected data, a mathematical model of a complex system in the form of a quasilinear regression equation was built.

As a result of the study, methods were chosen for determination of the main properties of fire retardant materials.

Changes in the fire-retardant efficiency of the agent with taking into account the operational properties of various buildings were investigated.

Based on the research of components, a series of formulations has been developed fire retardants with stable properties.

The main physical and chemical properties of the materials have been determined to provide fire protection.

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