Approaches to predicting the characteristics of fireproof materials

T Eremina, D Korolchenko and F Portnov
Moscow State University of Civil Engineering, Yaroslav shosse, 26, Moscow 129337, Russian Federation

E-mail address: wastingtimefilmart@gmail.com

Abstract. Planning an experiment is a new approach to research in which mathematical methods are given an active role. Based on the a priori information about the process under study, the researcher chooses some optimal research methodology. The results of the new approach to solving extreme problems depend to a large extent on the optimization of planning for a particular class of problems. The test plan presents a shortened plan of complete factor tests and can be considered acceptable due to the small correlation between affecting factors (AF) and output parameters (OP). The peculiarities of design of new composite materials to ensure safety in the operation of buildings and structures under conditions of man-caused and biogenic threats have been determined. The result of the article is the research using the method of forecasting the characteristics of fireproof materials.

1. Introduction
Many studies carried out in physics, chemistry and metallurgy come down to solving extreme problems aimed at finding optimal conditions for the processes or optimal choice of composition of multi-component systems. There are two different approaches to solving such problems. It may be required that the solution of extreme problems be preceded by a comprehensive study of both the process mechanism and the properties of substances. As a rule, systems to be optimized turn out to be so complex that they cannot be theoretically studied within a reasonable time. In most cases, extreme problems are solved experimentally with incomplete knowledge of the phenomena’ mechanism.

Classical regression analysis is based on processing the results of so called "passive experiments". It is assumed that the researcher observes some uncontrolled spontaneously changing process or makes experiments in some arbitrary way, choosing experimental points in the factor space, based on intuition or any random circumstances.

Experience has shown that the classical regression analysis, despite a well developed theory, has not found any wide application for solving extreme problems in physics, chemistry and metallurgy. In solving such problems, we have to deal with a very large number of independent variables. In this case, the method becomes extremely cumbersome. Here, we have to deal with almost insurmountable difficulties associated, on the one hand, with the need to set a very large number of independent variables and, on the other hand, with difficulties associated with the interpretation of the regression equation.

Planning an experiment is a new approach to research in which mathematical methods are given an active role. Based on the a priori information about the process under study, the researcher chooses some optimal strategy to manage the experiment. The research process is usually divided into separate
stages. After each step, the researcher receives new information that allows them to change the research strategy [1-3].

2. Building mathematical model

In mathematical language, the task of planning the experiment is formulated as follows: at each stage of the study, the researcher has to choose the optimal, in some sense, location of points in the factor space in order to get some idea about the response surface. The choice of the optimal criterion is to a large extent arbitrary. Here, it is necessary to take into account both the setting of the problem by the experimenter and the real situation in which this problem has to be solved. In setting extreme experiments, it is natural to formulate the problem at the first stage of the study as follows: it is necessary to find the direction of movement to the area where the process conditions are optimal. To solve this problem, it is enough to investigate the response surface in a small area, limited to linear approximation. After reaching the area where the optimum is located the problem will be formulated differently. Here, the researcher needs to get a much better idea of the response surface by approximating it with polynomials of the second and sometimes even third order. In many cases, the research has to start with the so-called screening experiments, the purpose of which is to identify the dominant effects among a very large number of the potentially possible.

Experience shows that the success of the new approach to solving extreme tasks largely depends on how well we have been able to formulate an optimal planning criterion for solving a particular class of tasks.

The main idea of the new method - possibility of optimal experiment management with incomplete knowledge - is relative to those prerequisites on which the cybernetics is based. Appearance of cybernetics - science of control, including consideration of such complex objects as biological systems, only became possible after it was realized that optimal control in case of incomplete knowledge is possible [4-10].

Figure 1. Presentation of the investigated complex system as a "black box" with m inputs and n outputs.

To build a mathematical model of a complex multifactor multiparameter system (figure 1), we need to perform the following actions:

1. make a list of m most significant affecting factors (AF) \([x_1,...,x_m]\) and n most informative output parameters (OP) \([y_1,...,y_n]\);

2. make a plan of active multifactorial tests in the form of matrix \(X\), containing m columns (by number of AF) and n rows (by number of tests), the main requirements to which are:
   a) the absence of correlation between AF (the coefficient of paired correlation \(r_{xkl}\) between factors \(x_k\) and \(x_l\) must be close to 0);
   b) full coverage of the factor space (at least, the condition: \(n > m\) must hold);
   c) feasibility - i.e. compliance with the capabilities of the experimental base;
   d) all experiments (AF combinations) in matrix \(X\) are equal.

3. carry out active tests, in the course of which to vary the AF combinations according to the plan (matrix \(X\)) and to determine (measure) the AF values, thus forming the matrix \(Y\) containing n rows (by
the number of tests) and \( n \) columns (by the number of OP). At the same time, the condition of unambiguosity of the result must be observed, i.e., when repeating the experiment (reproducing the same combination of AF), the spread of OP values must be insignificant;

4. perform mathematical processing of the results of active tests, which implies:
   a) determining the relationship between OPs by finding paired correlation coefficients between OPs (the values of \( r_{k,l} \) between the \( y_k \) and \( y_l \) parameters must be close to 0, otherwise one of the OP \( y_k \) or \( y_l \) can be replaced by another OP);
   b) estimating the correspondence of a sample of experimental values of each \( j \)-th OP \([y_{j1}, \ldots, y_{jN}]\) to the normal (Gaussian) distribution, in particular, by coefficients of asymmetry \( A'' \) and excess \( E_x \) (i.e., the condition \( A'' = E_x = 0 \) must be observed);
   c) building an adequate mathematical model

\[
y_j = f_j(x_1, \ldots, x_m) \quad j \in [1,n]
\]

which in this paper will take the form of a quasi-linear regression equation:

\[
y_j \approx \sum_{k=1}^{M_j} a_{jk} z_{jk} \quad j \in [1,n]
\]

where \( a_{jk} \) is the desired regression coefficient which is a component of vector \( A_j \),
\( z_{jk} \) is the \( k \)-th conditional factor, which is a component of the \( Z_j \) matrix and represents a function from \( \Phi x_1, \ldots, x_m \);
\( M_j \) is the number of regression coefficients or conditional factors (\( M_j < N \)).

d) using regression equations (2) for applied purposes:
   - interpretation of OP dependence on AF;
   - prediction of OP values in combinations of AF, different from those included in matrix \( X \);
   - estimation of the significance of the influence of AF on OP;
   - construction of the working area on the set of AF, in which each \( j \)-th OP lies within permissible limits.

Conditional factors \( \{z_{jk}\} \) are selected by the forced search method during the construction of the regression equation (2), and the vectors of the regression coefficients \( A_1, \ldots, A_m \) are calculated on the basis of the minimum dispersion condition of the regression equation (the least squares method)

\[
D_j = (N - M_j)^{-1} \sum_{i=1}^{N} (y_{ji}^e - y_{ji}^b)^2 \rightarrow \min, j \in [1,n]
\]

where \( y_{ji}^e, y_{ji}^b \) – values of \( j \)-th OP, respectively obtained in the course of the \( i \)-th experiment and calculated from the regression equation (2) for the \( i \)-th combination of AF.

The adequacy of regression equations (2) can be estimated by the Fisher criterion, for which we need to calculate the value of

\[
F_j = \frac{D_{je}}{D_j} \quad j \in [1,n]
\]

where \( D_{je} \) – experiment dispersion calculated by expression

\[
D_{je} = (N-1)^{-1} \sum_{i=1}^{N} (y_{ji}^e - y_{ju})^2
\]

\[
y_{ju} = N^{-1} \sum_{i=1}^{N} y_{ji}^e \quad j \in [1,n]
\]

If the value of \( F_j \) calculated by expression (4) is greater than the tabular value at degrees of freedom \( N-1 \) and \( N-M_j \), the equation of regression (2) is considered adequate with the corresponding confidence probability \( \alpha \) and can be used to solve the above applied problems. It is possible to take with engineering accuracy \( \alpha = 95\% \) at \( F_j > 10 \).
For the quasi-linear regression equation (2), condition (3) is reduced to matrix-vector expression:

$$A_j = (Z_j^T Z_j)^{-1} Z_j^T Z_j \quad j \in [1,n]$$  \hspace{1cm} (7)

where $Z_j$ – the conditional factor matrix, containing $N$ rows (by the number of tests) and $M_j$ columns (by the number of conditional factors);

$^T$ - symbol of matrix transposition;

$Y_j$ – $N$-dimensional vector of the values of the $j$-th OP.

Calculation of vector $A_j$ as well as selection of conditional factors $[z_{j1},..., z_{jM_j}]$ presents some difficulty overcome by using computer technologies.

It seems also expedient to use the multi-model principle, according to which the dependence of $j$-th OP on AF can be described not by one adequate equation, but by several such equations.

It is necessary to construct a mathematical model of a complex system in the form of quasi-linear regression equation (2), containing five OPs ($n = 5$), which are influenced by seven AF ($m = 7$). For this purpose was built a specialized plan of nine tests ($N = 9$) - matrix $X$, given in table 1.

The test plan (Matrix $X$, Table 1) presents a shortened plan of complete factor tests. According to this plan, the system was tested, resulting in a matrix $Y$, shown in table 1.

| № | $X_1$ | $X_2$ | $X_3$ | $X_4$ | $X_5$ | $X_6$ | $X_7$ | $Y_1^{**}$ | $Y_2^{**}$ | $Y_3^{**}$ | $Y_4^{**}$ | $Y_5^{**}$ |
|---|--------|--------|--------|--------|--------|--------|--------|------------|------------|------------|------------|------------|
| 1 | 0.5    | 0.5    | 0.5    | 0.5    | 0.5    | 0.5    | 0.5    | 12         | 2          | 1          | 0          | 6.9        |
| 2 | 1.5    | 1.5    | 0.5    | 1.5    | 1.5    | 0.5    | 0.5    | 12         | 1          | 5          | 1          | 2.0        |
| 3 | 1.5    | 0.5    | 1.5    | 1.5    | 0.5    | 1.5    | 0.5    | 27         | 1          | 7          | 1          | 2.0        |
| 4 | 0.5    | 1.5    | 0.5    | 1.5    | 0.5    | 1.5    | 0.5    | 37         | 2          | 1          | 0          | 6.9        |
| 5 | 1.5    | 0.5    | 1.5    | 0.5    | 1.5    | 0.5    | 1.5    | 30         | 1          | 5          | 1          | 3.4        |
| 6 | 0.5    | 1.5    | 0.5    | 1.5    | 0.5    | 1.5    | 0.5    | 20         | 2          | 3          | 2          | 5.6        |
| 7 | 0.5    | 1.5    | 1.5    | 0.5    | 1.5    | 0.5    | 1.5    | 40         | 2          | 1          | 2          | 5.6        |
| 8 | 1.5    | 1.5    | 1.5    | 0.5    | 0.5    | 0.5    | 0.5    | 36         | 1          | 5          | 1          | 3.4        |
| 9 | 1.5    | 1.5    | 1.5    | 1.5    | 1.5    | 1.5    | 1.5    | 25         | 1          | 7          | 3          | 6.9        |

$x_{\text{max}}$ = 24; $x_{\text{min}}$ = 10

* - formulation components of a flame retardant,
** - $y_1$-intumescence ratio, $y_2$-adhesion, $y_3$-service life, $y_4$-hazard class, $y_5$-flushability of film.

Pre-processing of $X$ and $Y$ matrices allowed determining the following pair correlation coefficients: $r_{x12}=r_{x13}=0.074$; $r_{x14}=0.102$; $r_{x15}=0.097$; $r_{x16}=0.917$; $r_{x24}=-0.217$; $r_{x25}=0.692$; $r_{x34}=0.428$; $r_{x35}=0.577$; $r_{x45}=0.107$; $r_{x12}=r_{x13}=r_{x14}=r_{x15}=r_{x16}=r_{x17}=r_{x23}=r_{x24}=r_{x25}=r_{x26}=r_{x27}=r_{x34}=r_{x35}=r_{x36}=r_{x37}=r_{x45}=r_{x56}=r_{x57}=r_{x67}=0.1$.

Thus, the test plan can be considered acceptable due to the small correlation between the AF. But among some OPs there is a significant correlation – $y_2$ and $y_3$ are closely connected, which allows one of them to be removed from consideration, thus simplifying the system analysis. The same conclusion can be made with respect to OP $y_5$, which is quite closely connected with OP $y_3$ and $y_5$. The values of coefficients $A_j$ and $E_j$ were found (table 1), which indicate some deviation of experimentally obtained values of OP from the normal law. Nevertheless, adequate quasi-linear regression equations (2) were obtained for all OP.
calculations. To quantify the relationship between the influence and output parameters, as shown in the results of formulation was developed, the characteristics of which are shown above. Quantitative optimization of the composition of the compositions was made and the fire retardant thickness of 1 mm. Efficiency time is 45 minutes according to the NSA 236-97 (4 group) with an average coating of the bend is 2 mm, the strength for the impact is 40 cm, the shelf life is 1.5 years, the fire retardant drying time is 24 hours, the resistance to the effects of variable temperatures is 15 cycles, the strength adhesion to the primed surface - 1 point, multiplier - 54 mm, the average density is 1.300 kg/m^3. Resistant fire retardant coating for metal structures has the following properties: life - 10 years, is produced by AF1, it was found that it is only affected by AF1, and the effect is negative. The greatest positive influence on OP y1 is produced by AF x1, and the greatest negative influence is produced by AF x2; the greatest positive influence on OP y2 is produced by AF x3, x4 and x5; the greatest negative influence on OP y1 is produced by AF x1, and the greatest positive influence is produced by OP x2, x3, x4 and x5.

As a result of the data confirmed by calculations: the optimal formulation of long-lasting weather-resistant fire retardant coating for metal structures has the following properties: life - 10 years, adhesion to the primed surface - 1 point, multiplier - 54 mm, the average density is 1.300 kg/m^3, the drying time is 24 hours, the resistance to the effects of variable temperatures is 15 cycles, the strength of the bend is 2 mm, the strength for the impact is 40 cm, the shelf life is 1.5 years, the fire retardant efficiency time is 45 minutes according to the NSA 236-97 (4 group) with an average coating thickness of 1 mm.

3. Conclusions
As a result of the study, methods were chosen to predict the characteristics of fire retardant materials to determine the main properties of fire retardant materials, including toxic effects on the human body. Based on the calculations carried out using the mathematical planning method of the experiment, quantitative optimization of the composition of the compositions was made and the fire retardant formulation was developed, the characteristics of which are shown above.

A mathematical multifactor model has been developed, experimentally by the calculation method to quantify the relationship between the influence and output parameters, as shown in the results of calculations.

Table 2. Comparison of experimentally obtained values of the 1st system OP with the results of calculations using regression equations

| № | y1 | y1a | y1b | y1c | y1d | y1e | y2 | y2a | y2b | y2c | y2d | y2e | y3 | y3a | y3b | y3c | y3d | y3e | y4 | y4a | y4b | y4c | y4d | y4e |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 12 | 16.8 | 14.7 | 11.2 | 11.8 | 2 | 2 | 1 | 1.63 | 1.33 | 0.95 |
| 2 | 12 | 6.98 | 14.6 | 11.9 | 11.8 | 1 | 1 | 5 | 4.90 | 5.40 | 4.93 |
| 3 | 27 | 27.0 | 27.1 | 26.2 | 25.8 | 1 | 1 | 7 | 6.52 | 5.87 | 6.99 |
| 4 | 37 | 35.3 | 39.9 | 40.1 | 36.8 | 2 | 2 | 1 | 2.17 | 1.49 | 1.02 |
| 5 | 30 | 30.2 | 28.3 | 31.5 | 29.4 | 1 | 1 | 5 | 4.77 | 5.20 | 4.93 |
| 6 | 20 | 20.8 | 20.2 | 20.1 | 19.7 | 2 | 2 | 3 | 3.38 | 3.41 | 3.01 |
| 7 | 40 | 39.5 | 37.0 | 35.7 | 40.0 | 2 | 2 | 1 | 1.77 | 1.44 | 1.02 |
| 8 | 35 | 35.3 | 34.2 | 34.6 | 35.8 | 1 | 1 | 5 | 5.31 | 5.34 | 5.16 |
| 9 | 25 | 25.0 | 24.3 | 25.8 | 26.4 | 1 | 1 | 7 | 6.52 | 6.76 | 6.99 |

From the analysis of table it follows, that in particular, that the factors x3 and x4 have a positive effect on OP y1 (i.e. with their increase OP y1 also increases), and AF x3 has a negative effect. As for OP y2, it was found that it is only affected by AF x1, and the effect is negative. The greatest positive influence on OP y1 is produced by AF x1, and the greatest negative influence is produced by AF x2; the greatest positive influence on OP y2 is produced by AF x3, x4 and x5; the greatest negative influence on OP y1 is produced by AF x1, and the greatest positive influence is produced by OP x2, x3, x4 and x5.

As a result of the data confirmed by calculations: the optimal formulation of long-lasting weather-resistant fire retardant coating for metal structures has the following properties: life - 10 years, adhesion to the primed surface - 1 point, multiplier - 54 mm, the average density is 1.300 kg/m^3, the drying time is 24 hours, the resistance to the effects of variable temperatures is 15 cycles, the strength of the bend is 2 mm, the strength for the impact is 40 cm, the shelf life is 1.5 years, the fire retardant efficiency time is 45 minutes according to the NSA 236-97 (4 group) with an average coating thickness of 1 mm.
Further research may allow us to assess the performance of durability and fire retardant properties of coatings with the best performance of fire retardant efficiency.

Acknowledgments
This work was financially supported by the Ministry of Science and Higher Education of the Russian Federation (Project: Theoretical and experimental design of new composite materials to ensure safety during the operation of buildings and structures under conditions of technogenic and biogenic threats #FSWG-2020-0007).

References
[1] Telichenko V I and Roitman V M 2010 Ensuring the resilience of buildings and structures with combined special impacts involving fire is a basic element of the integrated safety system
[2] Roitman V M 2009 Resilience of buildings and structures against progressive collapse with combined special impacts involving fire Moscow State University Herald 2 p 37-59
[3] Roitman V M 2009 Basics fire safety high-rise buildings (Moscow: MSSU) p 107
[4] Nalimov V V 1960 Application of mathematical statistics in substance analysis (Moscow: Fizmatgiz) p 430
[5] Nalimov V V 1971 Theory of Experiment (Moscow: Nauka - Fizmatgiz Library of the Engineer) p 208
[6] Brodsky V Z 1976 Introduction to factor planning of experiment (Moscow: Nauka) p 423
[7] Born M and Kun H 1958 The dynamic theory of crystal lattices (Moscow: Foreign Literature Publishing House) p 488
[8] Akhnazarova S L and Kafarov V V 1985 Methods of optimization of experiment in chemical technology (Moscow: Vyshch.shk) p 327
[9] Nalimov V V and Chernova N A 1965 Statistical methods for planning extreme experiments (Moscow: Nauka) p 338
[10] Markova E V and Lisenkov A N 1945 Combinatorial plans in problems of multifactor experiment (Moscow: Nauka) p 345