Verification of mathematical models to optimize the composition of radio-absorbing polymer composite materials

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Abstract. At present, radio-absorbing dispersed-filled polymer composite materials have become widespread in aviation technology. These materials are used to protect electronic units of on-Board equipment from electromagnetic radiation. The article considers the need to develop mathematical models of the dependence of the composition of radio-absorbing polymer composite materials on their physical and mechanical properties. The article deals with the optimization of a group of physical and mechanical properties described by mathematical models in order to obtain the optimal composition of a radio-absorbing dispersed-filled polymer composite material based on heat-resistant low-molecular synthetic rubber with the addition of untreated ferric oxide as a filler. The research method is optimization by the method of successive concessions. Computer experiments were carried out to optimize the composition of materials. The performed calculations were checked by experimental data, the adequacy of the obtained models was checked.

1. Introduction
The development of aviation technology, the constant improvement of the control system of aircraft and the metrological characteristics of instruments for monitoring air-speed flight parameters, the widespread introduction of microprocessor technology lead to a change in the approach to the protection of electronic blocks from all kinds of electromagnetic interference. Their effect negatively affects the process of controlling the trajectory of the aircraft. Therefore, electronic components must be protected by structures made of radio-absorbing materials, which can be dispersed-filled polymer composite materials (DFPCM) [1]. To give them the properties of radio absorption, the composition of these materials includes trivalent iron oxide. By varying the amount of this filler, it is possible to give the DFPCM the necessary radio-absorbing properties. However, Ferric oxide changes the mechanical properties DFPCM. Using in aircraft structures, the most important quality indicators are: hardness, tensile strength and tensile elongation. The relevance of the development of mathematical models describing the relationship between the mechanical properties and composition of DFPCM is beyond doubt [2].

2. Materials and methods
SKTN A is used as a polymer binder (component \( x_1 \)) – synthetic rubber heat-resistant low-molecular weight, easy-flowing (grade A). The percentage of the polymer together with the silicone oligomer
(plasticizer component $x_3$) ranges from 30% to 70%. The silicone oligomer is one fifth of the mass content of the polymer binder. Trivalent iron oxide (without mechanochemical treatment) was taken as a filler (component $x_2$), with a percentage of 30% to 70%.

To verify the mathematical models describing the mechanical properties of DFPCM, depending on its composition, samples were made with radio absorption properties (RP.1 – RP.7) in accordance with GOST R 54553-2019 [3] with the following composition: polymer binder (with a content from 30% to 70%), filler (from 30% to 70%), silicone oligomer (makes up one-fifth of the mass fraction of the polymer). The total content of the components is 100%.

The results of measuring the hardness of the manufactured samples are presented in table 1.

**Table 1. Hardness measurement results.**

| Sample № | Content of polymer binder from plasticizers, wt% | Content of filler, wt. % | Filler processing | Hardness, conventional units | Average value, conventional units |
|----------|-----------------------------------------------|-------------------------|------------------|----------------------------|---------------------------------|
| RP.1     | 70                                            | 30                      | no               | 30 35 34 32 33             | 32.8                            |
| RP.2     | 60                                            | 40                      | no               | 40 41 40 43 44             | 41.6                            |
| RP.3     | 50                                            | 50                      | no               | 42 40 43 40 45             | 42                              |
| RP.4     | 45                                            | 55                      | no               | 55 50 46 45 48             | 48.8                            |
| RP.5     | 40                                            | 60                      | no               | 46 50 50 52 50             | 49.6                            |
| RP.6     | 35                                            | 65                      | no               | 58 57 53 59 56             | 56.6                            |
| RP.7     | 30                                            | 70                      | no               | 60 62 60 60 60             | 60.4                            |

Implementation and data processing were performed using the Minitab software. The parameters of the plan from the settings when selecting a mixture of three components are shown in figure 1.

**Figure 1.** Selecting a constrained plan and number of components.

Quadratic and special cubic multiple regression models are used to obtain mathematical models.
The vector of coefficients of the mathematical model is determined using the least squares method in matrix form according to the following formula:

$$B = (F^T F)^{-1} F^T Y,$$

where $B$ is the vector of the required coefficients, $Y$ is the column of experimental values of the dependent variable, and $F$ is the matrix of the experiment plan.

Dispersion uniformity test reproducibility, the adequacy of the model, the significance of the polynomial coefficients in the case of using a nonlinear second-order model is carried out according to the same scheme as in the case of a full factor experiment [4-5].

The mathematical model for hardness ($\tilde{y}_{\text{hard}}$) is:

$$\tilde{y}_{\text{hard}} = 157.4x_1 + 105.2x_2 + 172.1x_3 - 298.8x_1x_2 - 775.4x_1x_3$$

The results of measuring the tensile strength and elongation at break of the samples are presented in table 2 (the average values for the tests of five samples are indicated).

**Table 2.** Average values of tensile strength and elongation at break of samples.

| Sample No | Content of polymer binder from plasticizers, wt% | Content of filler, wt. % | Filler processing | Tensile strength, MPa | Elongation at break, % |
|-----------|-----------------------------------------------|--------------------------|------------------|-----------------------|------------------------|
| RP.1      | 70                                            | 30                       | no               | 0.031                 | 7                      |
| RP.2      | 60                                            | 40                       | no               | 0.932                 | 6                      |
| RP.3      | 50                                            | 50                       | no               | 0.851                 | 9                      |
| RP.4      | 45                                            | 55                       | no               | 0.332                 | 8                      |
| RP.5      | 40                                            | 60                       | no               | 0.237                 | 7                      |
| RP.6      | 35                                            | 65                       | no               | 0.309                 | 14                     |
| RP.7      | 30                                            | 70                       | no               | 1.004                 | 8                      |

The mathematical model for ultimate tensile strength ($\tilde{y}_{\text{str}}$) has the form:

$$\tilde{y}_{\text{str}} = -6.42x_1 - 0.02x_2 - 12.4x_3 + 16.87x_1x_2 + 32.27x_1x_3$$

The mathematical model for elongation at break ($\tilde{y}_{\text{el}}$) has the form:

$$\tilde{y}_{\text{el}} = 27.8x_1 + 44.6x_2 - 33.5x_3 - 107.4x_1x_2 + 9.8x_1x_3$$

To optimize the physical and mechanical characteristics of the polymer composite material, the radio-absorbing property provided by the percentage of the filler is not taken into account in the calculations. A decrease in the radio absorption coefficient during the optimization process is unacceptable. The mechanical properties of the polymer composite material are optimized using the successive concessions method. It is most suitable for the case when mathematical models describing the correlation "the composition of RP DFPSCM – properties of RP DFPSCM" can be ordered in descending order of their importance [6-8].
The maximum Shore hardness value is 60.378 conventional units with the following percentage of the components:

- $x_1 - 24\%$
- $x_2 - 70\%$
- $x_3 - 6\%$

After finding the maximum value of the first criterion in importance in the range of admissible solutions, the maximum value of the next most important criterion (strength limit) is found. However, in this case, the following condition must be met: the value of the first criterion (Shore hardness) should not deviate from its maximum value by more than the value of the permissible concession (in this case, $\delta_1 = 12$).

Thus, the following problem is solved

$$Z_2(\bar{X}) \rightarrow \text{max}$$
$$Z_1(\bar{X}) \geq 48.378, \quad (2)$$

When solving it, the maximum value of the ultimate strength is $116.1 \cdot 10^4$ Pa with the following percentage of the components:

- $x_1 - 34\%$
- $x_2 - 60\%$
- $x_3 - 6\%$

The next step is to use the value of the assignment $\delta_2$ according to the second criterion, which, together with the first assignment, is applied when finding the conditional maximum of the third particular criterion.

$$Z_3(\bar{X}) \rightarrow \text{max}$$
$$Z_1(\bar{X}) \geq 38.356$$
$$Z_2(\bar{X}) \geq 0.961 \cdot 10^6, \quad (3)$$

The maximum tensile elongation is 17.980% with the following percentages of components:

- $x_1 - 24\%$
- $x_2 - 70\%$
- $x_3 - 6\%$

The value of the percentage of components obtained at the last stage is optimal. This result is displayed in the software tab "Optimization of the composition of radio-absorbing polymer composite materials".

3. Results and discussion

As a result of multicriteria optimization, the percentage composition of DFPCM was calculated, in accordance with which samples for experimental studies were made, and the values of the characteristics that should be achieved with such a ratio. The target values of the functions (the values that tend to be obtained in practice) and the calculated optimal ratio of the components are given in tables 3 and 4, respectively. The output of the results is shown in figure 2.
**Table 3.** Target values of functions.

| Z1     | Z2     | Z3     |
|--------|--------|--------|
| 60.378 | 1.000  | 17.980 |

**Table 4.** Percentage of components.

| x1 | x2 | x3 |
|----|----|----|
| 0.24 | 0.70 | 0.06 |

**Figure 2.** Output of results

As a result of multicriteria optimization, it was calculated that to obtain a new radio absorbing dispersed-filled polymer composite material with a hardness value of 60.378 units, a tensile strength of $1.000 \times 10^6$ Pa, and a tensile elongation of 17.980%, the following components is required:

- silicone rubber type SKTN A (matrix) – 24%;
- iron oxide (powder filler) – 70%;
- silicone oligomer – 6%.

**4. Conclusion**

Based on the results of carrying out and processing the experimental data, nonlinear mathematical models of Shore hardness, ultimate tensile strength, elongation in tension of radio-absorbing DFPCM based on silicone rubber with ferric iron oxide were obtained. Optimization of the composition was carried out using the developed mathematical models as target functions. Thus, the optimization by the method of successive concessions can be successfully applied to obtain the optimal composition of a new material in an enterprise engaged in the creation of new functional materials.

Further research in this area should be aimed at developing a scientifically grounded methodology for choosing the value of the concession (permissible deviation) when optimizing the quality indicators of DFPCM with radio-absorbing properties.

The developed and verified mathematical models describing the mechanical properties of the created radio-absorbing DFPCM depending on their composition, make it possible to predict the properties of the materials created with subsequent optimization of the composition. It helps to determine the compositions of future materials with specified quality indicators.
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