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Prediction of Polymer Composite Material Products using Neural Networks

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Abstract

This article contains results of mathematical modeling of technological processes for manufacture of pre-production polymer composite prototypes having certain performance characteristics conducted with application of engineering analysis software using artificial neural networks. Based on mechanical testing results, the following material strength characteristics mathematical models were defined: ultimate strength (at room temperature); modulus of elasticity (at room temperature); compressive strength (at room temperature); compressive strength (at $T=150^{\circ}\text{C}$); ultimate strength (shear in the sheet's plane); modulus of elasticity (shear in the sheet's plane); ultimate strength (interlayer shear).

The first step was to evaluate the statistic importance of outside parameters which influence on materials' properties. The main task was to obtain the function of dependence of the mechanical properties from the outside factors.

Key words: technological process, analysis, modelling, control, neural network.

1. INTRODUCTION

The basic aim of the conducted works was a multiple-factor study of technological processes (TP) for manufacture of pre-production prototypes made from polymer-matrix composite materials (PCM) comprising a carbon reinforcement filler and a meltable matrix. The problem was stated as a study of TP factors influence on the matrix material content, surface density, and mechanical properties of the prototypes [1]. The results presented in this article were obtained in the frame of the program for "Research and development of the automated technological process for polymer composite products manufacture exemplified by the IL-76MD-90A airplane engine nacelle doors" conducted by Voronezh Aircraft Production Association (VASO) OJSC. Applied scientific research (ASR) is carried out by Voronezh State Technical University (VSTU) in accordance with

the federal target program "Research and development activities in priority areas of the Russian Federation scientific and technological complex for 2014 – 2020", in the field of "Transportation and space systems".

2. THE TASK

Manufacturing technology for prepregs based on unidirectional carbon tapes and meltable matrixes is schematically presented in Figure 1.

Manufacturing technology can be conventionally divided into several stages:

- line preparation and auxiliary materials placement;
- preparation and placement of the main materials: the reinforcement filler and the matrix;
- impregnation process.

The prepreg is a unidirectional carbon tape using the Formosa 12K carbon filament as a warp yarn and the VMPS-8 glass filament as a weft yarn. The tape is impregnated with the T-107 (and/or T-6815) adhesive (meltable) epoxy-based matrix at a given ratio by the method of matrix film application to a carbon tape. One of the practical objectives of this paper was to create the tooling for automated control of carbon tape

and meltable matrix TP factors providing maximum performance characteristics of the manufactured materials [2].

The input data used for solving this task were material types and parameters, and operational characteristics of processes realized in the considered TP on VASO base.

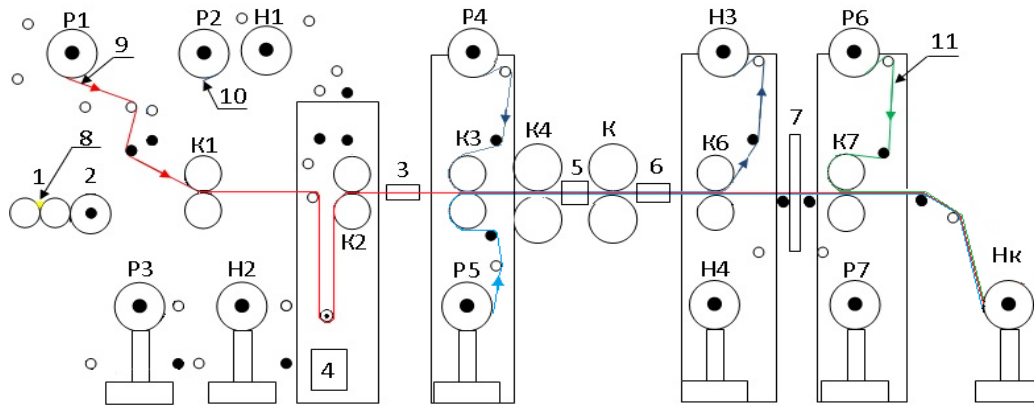


Figure 1. Schematic representation of the tape and auxiliary materials placement

1 – metering shafts, 2 – lamination shaft, 3 – IR furnace, 4 – matrix material bath, 5 – heating panel, 6 – cooling table, 7 – prepreg quality control system QMS-12 MAHLO, 8 – matrix material, 9 – cloth, 10 – paper, 11 – film, P1-P7 – unwinders, H1-H4 – winders, K1-K7 – calenders, ● – strain sensors, ○ – auxiliary shafts or rollers

At the experiment planning stage, the following variation ranges of the external factors were set: line speed $V = 0,5 \div 2$ m/min, lamination shaft clearance $B2 = 50 \div 150$ μm , calibration $K = -50 \div -20$ %.

The Optimal Space Filling Design experiment was planned with application of the DesignXplorer module for parametric studies and non-linear optimization integrated into the ANSYS Workbench computer analysis engineering platform [3].

Matrix content in prepreg (H) and surface density (ρ , R_0) were used as the quality criteria determined by results of experimental studies of hot melt prepreg manufacturing technology.

Figure 2 shows schematic interpretation of the adhesive prepreg mechanical testing results obtained in different technological conditions taking into account the experiment plan.

Based on mechanical testing results, the following material strength characteristics were defined:

- ultimate strength (at room temperature), SigR1;
- modulus of elasticity (at room temperature), SigR2;
- compressive strength (at room temperature), SigS1;
- compressive strength (at $T=150^\circ\text{C}$), SigS2;
- ultimate strength (shear in the sheet's plane), SigC1;
- modulus of elasticity (shear in the sheet's plane), SigC2;
- ultimate strength (interlayer shear), SigC3.

3. MULTI-FACTOR ANALYSIS

Multiple factor studies were conducted using the STATISTICA engineering system, including a mathematical module using neural network technology. Neural networks are the universal approximation tool of the multivariate nonlinear dependences, capable "to be arranged" under the appearing of the new information of the researched process, i.e. they can serve as the intellectual tool of monitoring which is constantly complemented and clarified [4]. Figure 3 presents the graphical notation of the computing artificial neural network (ANN) structure illustrating the process of intra-network computations.

The input signals or the values of input variables are distributed and "move" along the connections of the corresponding input together with all neurons of the hidden layer. They may be amplified or weakened through multiplying by the corresponding coefficient (called the weight of connection). The signals arriving to one or another of the neurons in the hidden layer are summed up and subjected to nonlinear transformation by using the so-called function of activation.

They proceed further to the network outputs that may be several in number. In this case the signals are also multiplied by a definite weight; it is the sum of the weighted values of neuron outputs in the hidden layer that represents the result of the neural network operation. The artificial neural networks of such a structure possess the universal approximating ability, i.e., make it possible to approximate the arbitrary continuous function with any accuracy desired.

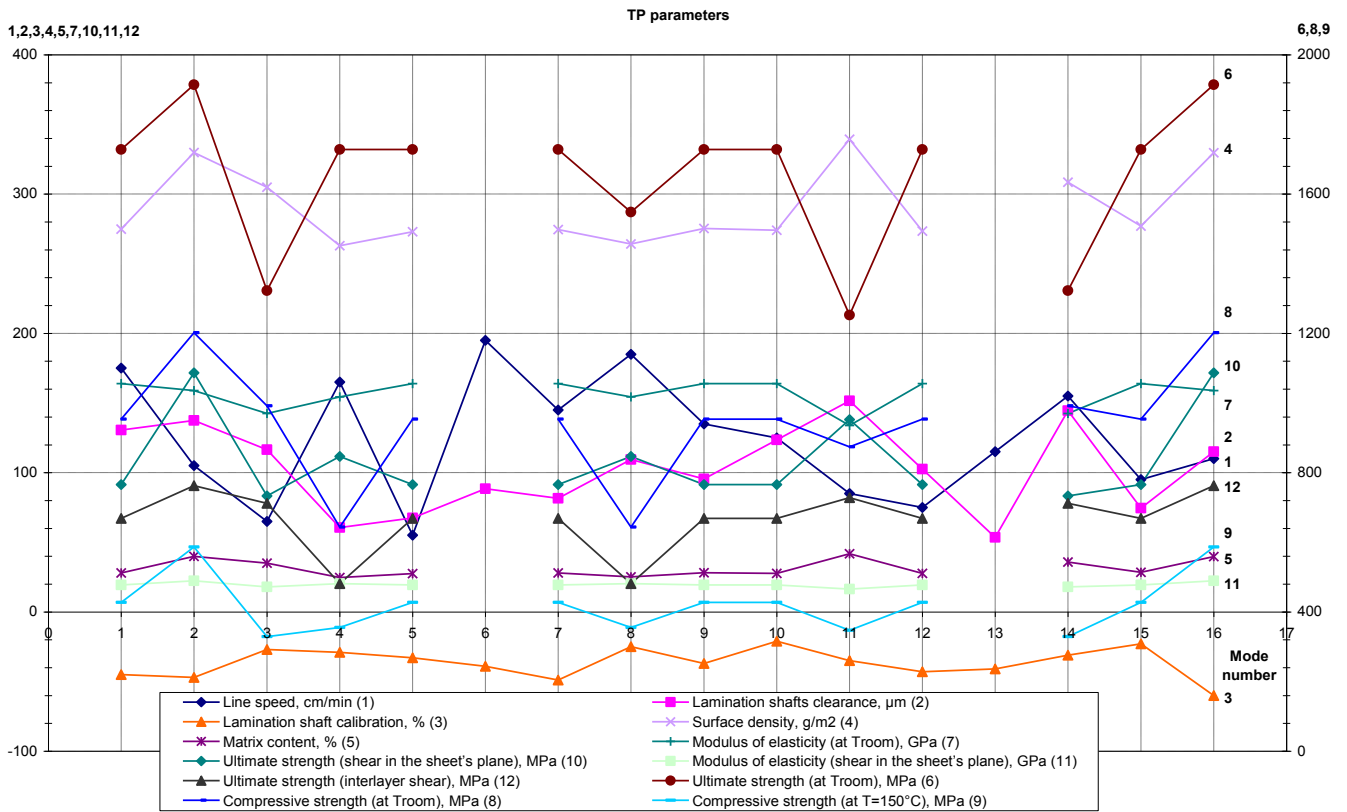


Figure 2. The results of TP execution

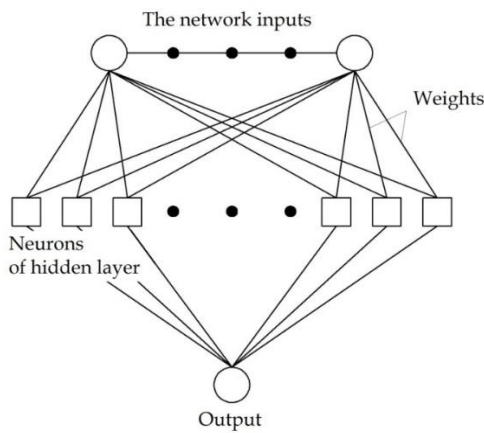


Figure 3. Neural network computing structure

To investigate the ANN approximated capabilities the perceptron with the single hidden layer (SLP) has been chosen as a basic model which performs nonlinear transformation of the input space into the output space in accordance with the formula⁶:

$$y(\mathbf{w}, \mathbf{x}) = \sum_{i=1}^q v_i f_{\sigma} \left(b_i + \sum_{j=1}^n w_{ij} x_j \right) + b_0 \quad (1)$$

where $\mathbf{x} \in \mathbf{R}^n$ – network input vector, made up of the values x_j ; q – the neuron number of the single hidden

layer; $\mathbf{w} \in \mathbf{R}^s$ – all weights and network thresholds vector; w_{ij} – weight entering the model nonlinearly between j -m input and i -m neuron of the hidden layer; v_i – output layer neuron weight corresponding to the i -neuron of the hidden layer; b_i, b_0 – thresholds of neurons of the hidden layer and output neuron; f_{σ} – activation function (in our case the logistic sigmoid is used). ANN of this structure already has the universal approximation capability, in other words it gives the opportunity to approximate the arbitrary analog function with any given accuracy.

The main stage of using ANN for resolving of practical issues is the neural network model training, which is the process of the network weight iterative adjustment on the basis of the learning set (sample) $\{\mathbf{x}_i, y_i\}, \mathbf{x}_i \in \mathbf{R}^n, i = 1, \dots, k$ in order to minimize the network error – quality functional

$$J(\mathbf{w}) = \sum_{i=1}^k Q(f_{\varepsilon}(\mathbf{w}, i)) \quad (2)$$

where \mathbf{w} – ANN weight vector; $Q(f_\varepsilon(\mathbf{w}, i)) = f_\varepsilon(\mathbf{w}, i)^2$ – ANN quality criterion as per the i -training example; $f_\varepsilon(\mathbf{w}, i) = y(\mathbf{w}, \mathbf{x}_i) - y_i$ – i -example error. For training purposes the statistically distributed approximation algorithms may be used based on the back error propagation or the numerical methods of the differentiable function optimization.

To solve the tasks of ANN training, it is important to attain good generalizing properties of the network, i.e. its capability to predict the values, which do not belong to the training sample. Thus, at the stage of training ANN, having a fixed structure, the problem arises in evaluating a certain functional of ANN performance, which is generally represented as the total quadratic error for a specified training sample, and the degree of correspondence to some subjective prior information about the type of the neuron-network response surface. This determines the necessity for regularization of fixed-structured ANN training.

In the absence of the ideal and infinitely large training set, the regularization of the training procedure is necessary, aimed at averting the network overtraining, so as to obtain the correct solution of the problem of the fixed-structured ANN synthesis. With sufficient amount of experimental data, the problem can be successfully solved by cross check, when part of the data is not used in the procedure of ANN training, but it serves for independent control of the training results.

When the training algorithm is complemented by additional information about the neuron-network function properties (i.e. limitation, smoothness and monotony), it leads to modification of the goal function, and necessitates the minimization of two or more training criteria. There is a well-known Bayesian approach, based on noisy data interpolation. The method of Bayesian regularization consists in the use of subjective assumptions about the function being investigated, and can be applied both at the stage of ANN structural optimization and during training. For example, the method is known, in which regularization is achieved by representation of the goal function in the form of convolution:

$$F = \beta \cdot E_D + \alpha \cdot E_W \tag{3}$$

where E_D is the total quadratic error, and E_W is the sum of the squares of network weights.

Here, the emphasis is made on the problem of specifying the correct values of the goal function parameters, α and β , and their selection determines the topology of the neuron-network approximating function. At the same time, there is a possibility of altering the regularization criterion in the formula 3, based on the analytical evaluation of the approximating response

surface curvature. Let us introduce the energy factor,

$$K = \sum_{s=1}^L \left(\frac{\partial^2 y}{\partial (x^s)^2} \right)^2$$

which will be presented as

for the training set $(x^s, y^s), s = \overline{1, L}$. The conducted computational experiments show that the adequacy of neuron network approximation for the available set of experimental data will enhance, if the model ensures the required energy factor value, besides the accuracy in proximity to the available empirical results [5-8].

Let us present the algorithm of combined back propagation (CBP), as part of the concept of fixed-structured ANN training for obtaining the response surfaces of minimal curvature, and for enhancing the robust properties of the developed theory for creating the ANN of optimal structure. To illustrate the computations, let us examine the functioning of the SHLP with one terminal.

Let us select the total quadratic mean error for internal points of the training sample $s = 2, \dots, L-1$ as the

$$\text{basic goal function of training: } E = \frac{1}{2} \sum_s (y^s - d^s)^2$$

. Let us assume the energy factor

$$K = \frac{1}{2} \sum_i \sum_s \left(\frac{\partial^2 y}{\partial (x_i^s)^2} \right)^2$$

as an additional goal function.

Let us represent the goal functions as complex SHLP parametric functions, and calculate all the components of their gradients using the formula, specified for complex functions. Thus, the network output is calculated as $y(\mathbf{x}^s) = \sum_j v_j f_j(\mathbf{x}_i)$, where \mathbf{x} is the

vector of inputs, s is the number of a point in the training sample, $f(\mathbf{x})$ is the function of activation, v_j

is the weight of the output neuron, and j is the number of a neuron in the hidden layer. Let us consider the logistic sigmoid function (Fermi's function) as the

$$\text{function of activation: } f_j(\mathbf{x}) = \frac{1}{1 + e^{-t_j(\mathbf{x}, b_j)}}$$

Here b_j is the threshold of the hidden-layer neuron j , and the function $t_j(\mathbf{x}, b_j)$ has the form of:

$$t_j(\mathbf{x}, b_j) = \sum_i w_{ij} \cdot x_i - b_j$$

where w_{ij} is the weight of neurons in the hidden layer. Let us write down the detailed expression for the summands of the energy factor:

$$\frac{\partial^2 y}{\partial (x_i^s)^2} = \sum_j (v_j w_{ij}^2 (f_j(\mathbf{x}^s, b_j) - 3f_j^2(\mathbf{x}^s, b_j) + 2f_j^3(\mathbf{x}^s, b_j))) \tag{4}$$

During the training process, we will correct the ANN parameters at each iteration (epoch), in the direction of the antigradient of the goal function. Each epoch will consist of two stages. At the first stage, steps are taken in the direction of $-\nabla E(\mathbf{v}, \mathbf{w}, \mathbf{b})$. The iterations of the first stage are achieved for all the points of the training sample. The iterations of the second stage are performed in the direction of the antigradient of the energy factor $-\nabla K(\mathbf{v}, \mathbf{w}, \mathbf{b})$, and, at that, it is easy to obtain the analytical expressions for the gradient components of the goal function.

The developed algorithm is the modification of the back propagation algorithm, which is essentially the method of stochastic approximation.

The expressions, obtained for the energy factor (4), may be used instead of E_w in the convolution (3). In this case, the energy factor must be represented by the

$$K = \sum_s \left(\nabla^2 f_{NET}(\mathbf{w}, \mathbf{x}^s) \right)^2$$

, i.e. this will be the

integral curvature parameter. With large dispersion K^s of the statistic sampling points, the efficiency of the use of total curvature as the goal function of training may be low, in contrast with using the algorithm of combined back propagation, which adjusts network parameters at certain experimental data points [9-11].

The model's sensitivity to different factors was analyzed with the aid of the DesignXplorer module. At the first stage, statistical significance of external conditions for material properties was estimated with application of dispersion analysis based on Pareto chart. It was found out that V and B2 factors are the most statistically significant for all parameters. The significant parameters were then used for building of the response surface charts and contour charts with the surface level lines marked on them. Typical charts using SigS1 parameter as an example are shown in Figure 4.

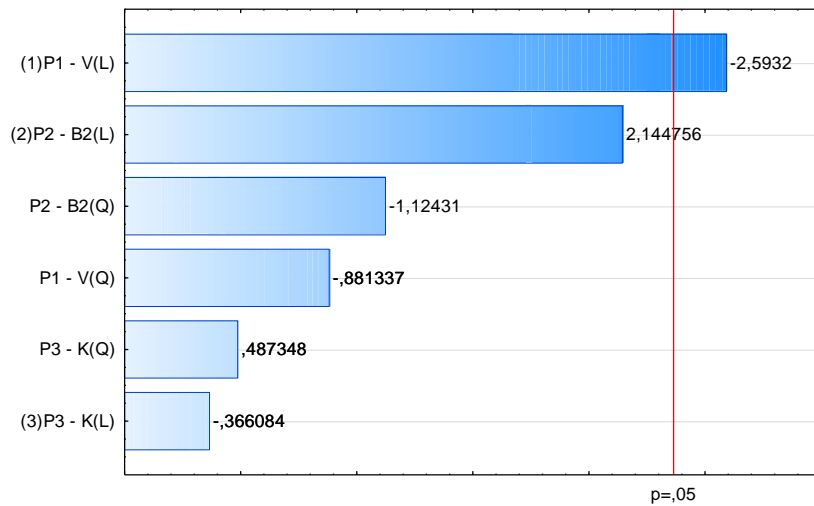


Figure 4. Pareto chart for SigS1

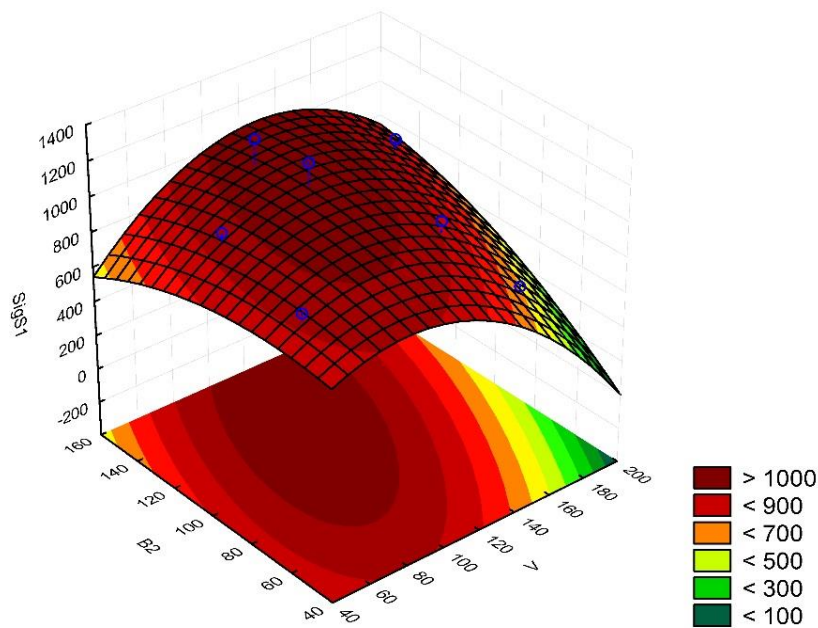


Figure 5. Response surface chart for SigS1

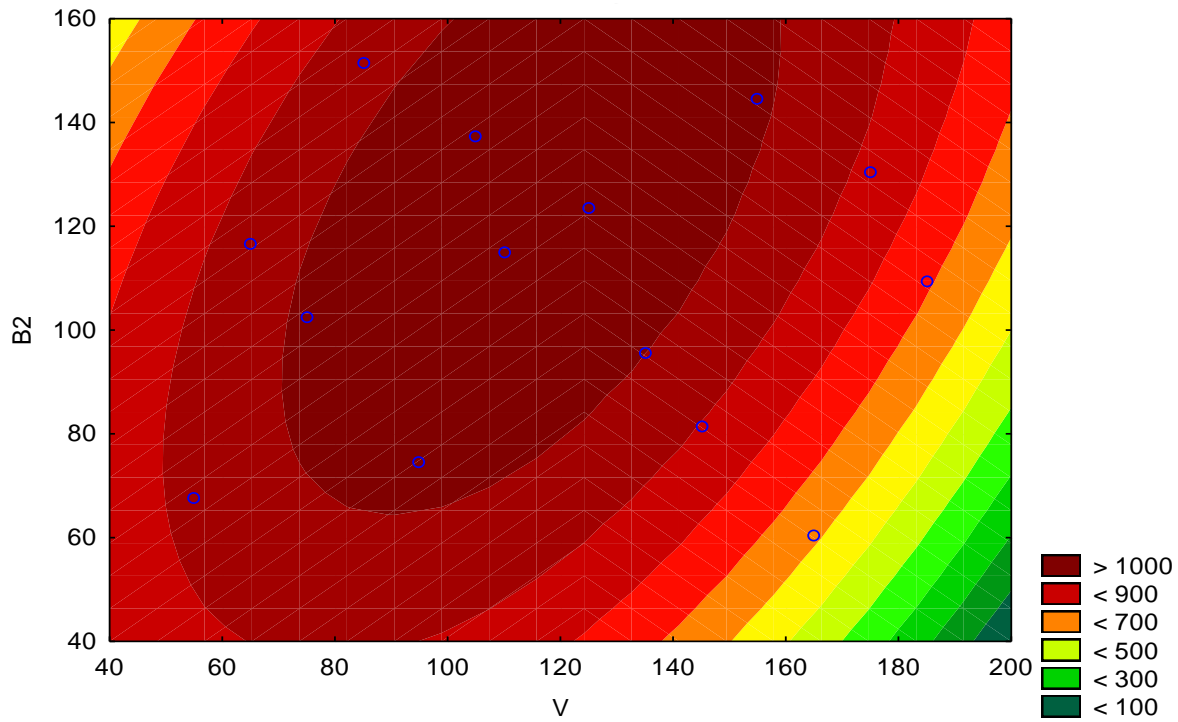


Figure 6. Surface level lines for SigS1

The main task was to establish dependencies of the mechanical properties on the external factors using procedures of multidimensional regression based on

the full quadratic polynomial. Table 1 contains determination coefficients of the obtained multiple factor regression models.

Table 1. Determination coefficients of regression models

Property	Sig_R1	Sig_R2		Sig_S1	Sig_S2	Sig_C1	Sig_C2	Sig_C3
R ²	0,786	0,734		0,823	0,767	0,887	0,805	0,983

Multiple regression results provided a base for definition of mathematical dependencies that allow prediction of the material's mechanical properties:

$$\text{SigR1}=1654,689-211,458 \cdot V+27,252 \cdot B2-137,537 \cdot K-447,135 \cdot V^2-16,722 \cdot B2^2+563,955 \cdot K^2+425,999 \cdot V \cdot B2+413,836 \cdot V \cdot K-890,851 \cdot B2 \cdot K. \quad (5)$$

$$\text{SigR2}=159,7009-18,7264 \cdot V+10,6514 \cdot B2-5,7387 \cdot K-33,3873 \cdot V^2-4,5060 \cdot B2^2+41,9386 \cdot K^2+29,3424 \cdot V \cdot B2+34,1372 \cdot V \cdot K-70,9805 \cdot B2 \cdot K. \quad (6)$$

$$\text{SigS1}=988,697-302,234 \cdot V+308,779 \cdot B2-45,646 \cdot K-397,782 \cdot V^2-355,211 \cdot B2^2+73,161 \cdot K^2+288,604 \cdot V \cdot B2-158,280 \cdot V \cdot K-292,151 \cdot B2 \cdot K. \quad (7)$$

$$\text{SigS2}=408,192-82,866 \cdot V+42,877 \cdot B2-45,940 \cdot K-128,903 \cdot V^2-143,277 \cdot B2^2+141,709 \cdot K^2+96,407 \cdot V \cdot B2+84,380 \cdot V \cdot K-236,965 \cdot B2 \cdot K. \quad (8)$$

$$\text{SigC1}=93,7963-35,8558 \cdot V+53,4977 \cdot B2-59,9834 \cdot K+6,5937 \cdot V^2+35,3655 \cdot B2^2+55,6043 \cdot K^2-39,5631 \cdot V \cdot B2+74,7243 \cdot V \cdot K-86,6989 \cdot B2 \cdot K. \quad (9)$$

$$\text{SigC2}=19,96278-0,26587 \cdot V+0,16148 \cdot B2-2,2236 \cdot K-1,11729 \cdot V^2-0,25707 \cdot B2^2+1,73786 \cdot K^2+0,87253 \cdot V \cdot B2+3,85354 \cdot V \cdot K-5,44637 \cdot B2 \cdot K. \quad (10)$$

$$\text{SigC3}=75,6566-21,9163 \cdot V+29,3265 \cdot B2-22,9902 \cdot K-47,4452 \cdot V^2+5,2717 \cdot B2^2+4,1305 \cdot K^2+27,4317 \cdot V \cdot B2-39,112 \cdot V \cdot K+3,6708 \cdot B2 \cdot K. \quad (11)$$

Practically all dependencies have extremums in the considered area of the factor space.

Then, using the DesignXplorer module, sensitivity coefficients at average parameter values were calculated (Figure 7).

It was found out that ρ , H, Sig_R2 and Sig_S1 criteria at the average parameter values are sensitive to variation of the external conditions V, B2, K; Sig_R1 and Sig_S2 criteria – to variation of V, B2 parameters. Typical results of analysis for the ρ criterion are presented in Figure 8.

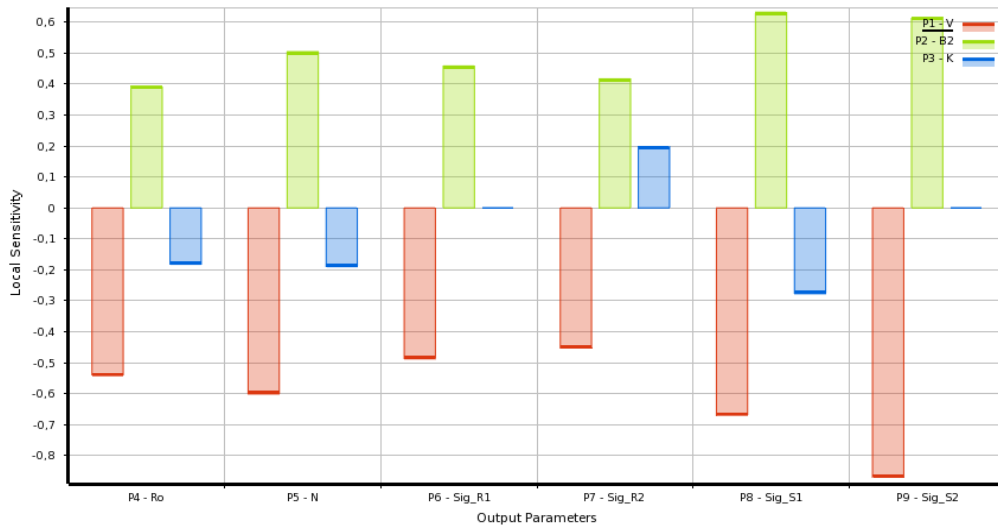


Figure 7. Calculated coefficients of sensitivity at average parameter values

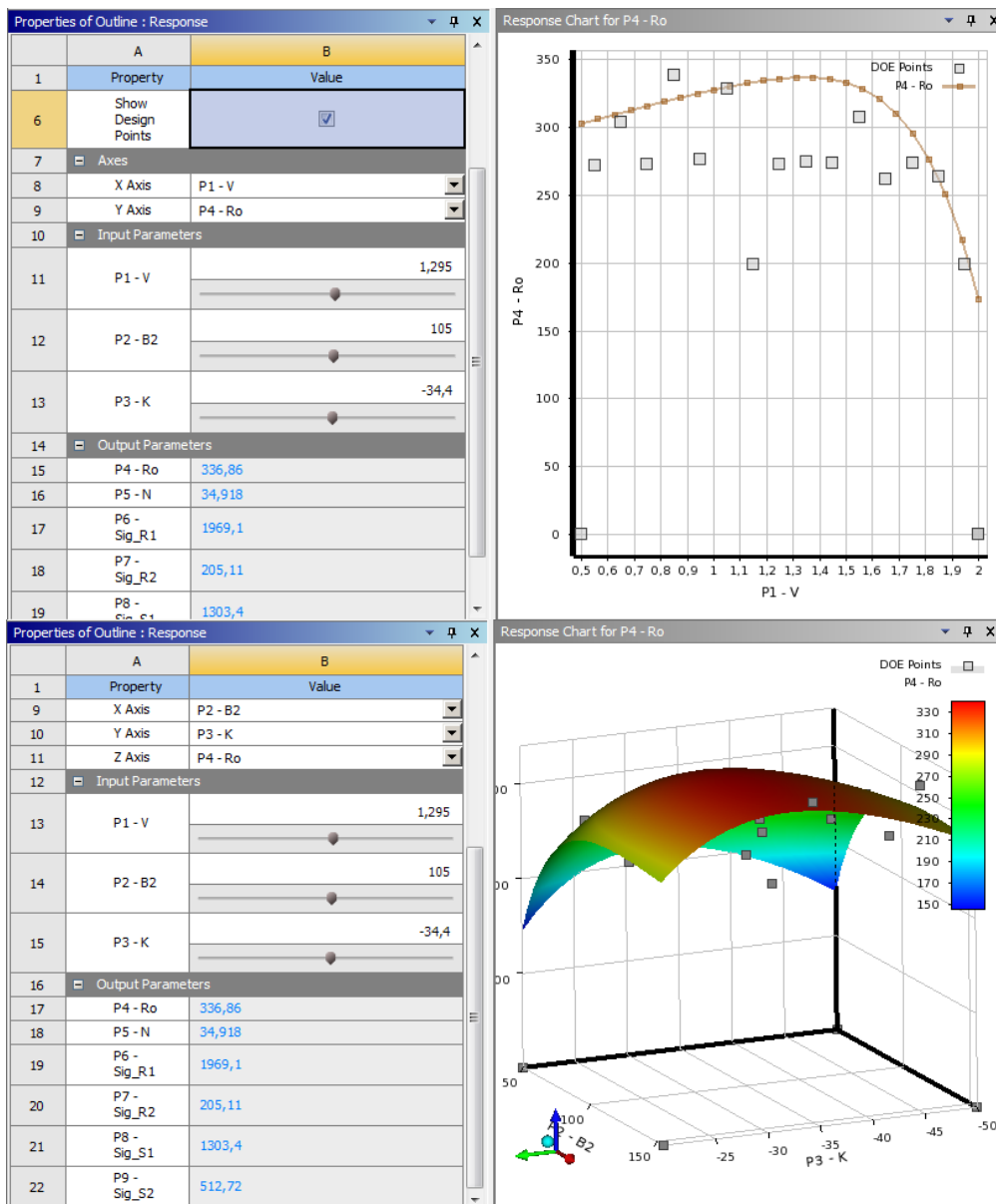


Figure 8. Dependencies obtained for the p criterion

The presence of extremums in the considered area of the factor space became a reason for optimization studies, including those in multicriteria statement. Optimal values of input parameters V, B2 and K were defined with the aid of the DesignXplorer module.

Sig_R1, Sig_R2, Sig_S1 and Sig_S2 characteristics were used as the optimized criteria. Representative results and some Pareto-optimal points of the factor space are shown in Figure 9 (in process of optimization, the Screening method was used with analysis settings for 10000 points and selection of the three best results).

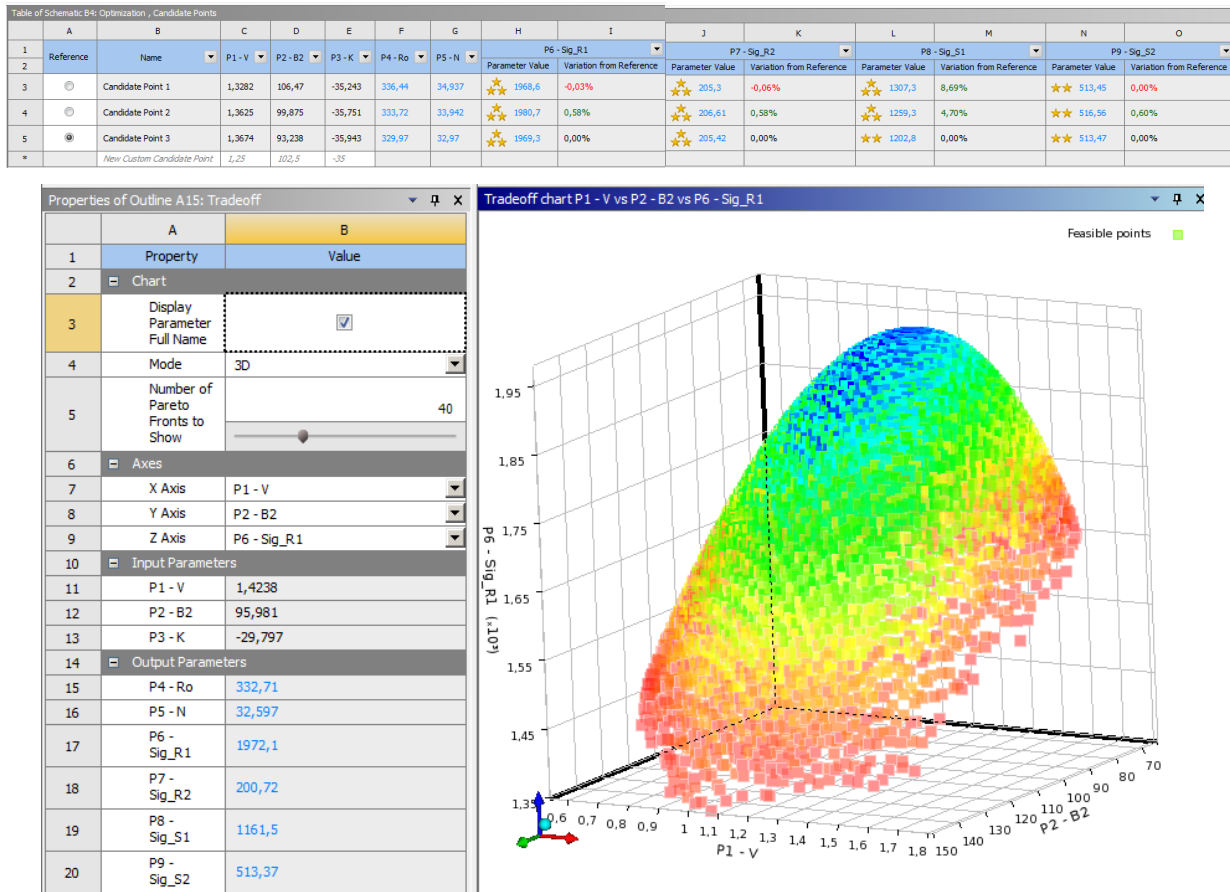


Figure 9. Results of multicriteria optimization

4. CONCLUSION

This paper contains results of the multiple factor study and mathematical modeling of technological processes for manufacture of pre-production polymer composite prototypes having the specified performance characteristics. The study and modeling have been conducted applying specialized software for parametric studies and non-linear optimization using artificial neural networks. The algorithm of combined back propagation, as part of the concept of fixed-structured ANN training for obtaining the response surfaces of minimal curvature, and for enhancing the robust properties of the developed ANN of optimal structure that make it possible to approximate the arbitrary continuous function with any determination coefficients desired. During the research, we have found which of the outside parameters have the largest impact on the results of these TP. The mathematical models were designed to forecast the results of the TP, which are now extremely unpredictable and stochastic.

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Predviđanje proizvoda od polimernih kompozitnih materijala pomoću neuronskih mreža

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Abstrakt

Ovaj članak sadrži rezultate matematičkog modeliranja tehnoloških procesa za proizvodnju predproizvodnih polimernih kompozitnih prototipova sa određenim karakteristikama performansi koje se sprovode uz primenu softvera inženjerske analize pomoću veštačkih neuronskih mreža. Na osnovu rezultata mehaničkih ispitivanja definisani su sledeći matematički modeli karakteristika čvrstoće materijala: konačna čvrstoća (na sobnoj temperaturi); modul elastičnosti (na sobnoj temperaturi); čvrstoća na pritisak (na sobnoj temperaturi); čvrstoća na pritisak (na $T=150^{\circ}\text{C}$); konačna čvrstoća (smicanje u ravni ploče); modul elastičnosti (smicanje u ravni ploče); konačna čvrstoća (smicanje međusloja).

Prvi korak je bio da se proceni statistička značajnost spoljašnjih parametara koji utiču na svojstva materijala. Glavni zadatak je bio dobijanje funkcije zavisnosti mehaničkih osobina od spoljašnjih faktora.

Ključne reči: *technološki proces, analiza, modeliranje, kontrola, neuronska mreža.*