Double Check of Optimization Results using Neural Network and Statistical Methods

Natalja Fjodorova, Marjana Novič

Abstract**—**The goal of optimization is to select the best elements (objects) with regard to some criteria from some set of available alternatives. The application of optimization methods in industry is of great importance nowadays. It contributes to the increasing of quality of product and the productivity as well as reduction of energy consumption, waste and operational costs. In the study the traditional designs of experiment (DOEs) based on statistical method (response surface design) was complimented with neural network (NN) mapping method which enables to get 2D image of studied technological process (as a 2 dimensional map of properties od product) and select multiple optima. The implementation of both methods supports the double check of optimization results and expands options for selection of multiple optima. The final solution can be taken on the basis of compromise decision. Implementation of neural network mapping technique together with parametric estimation models were demonstrated for improvement of technological process of pigment dying of high performance fibers. Proposed method is simple in use and not time consuming. It can be recommended for the use in different industries for improvement of existing (ongoing) process as well as at the stage of development of new product.

Keywords**—**design of experiment, feed forward bottle neck neural network, neural network mapping, optimization, surface response design.

I. Introduction

The reason for the popularity of experimental design strategies and optimization methods is the competitive environment of today's marketplace in many manufacturing and service industries.

The goal of design of experiment (DOE) is to find desired factor settings so that a process average or a quality characteristic of key product properties are close to the target (on aim) and the variability is as small as possible. In chemical engineering optimization can be used to improve the production, economic and environmental performance or other criteria and simultaneously meet the specification requirements. Different algorithms can be used to solve the optimization problem. The type of relationship between input parameters and output response (linear or non-linear) determines the choice of applied technique. A few examples of different approaches for optimization of different processes are represented in papers [1-4].

Some of the tools for optimization of non-linear processes using regression methods are described in the book [5]. Besides the regression methods (especially for non-linear processes) the neural network methods can be applied for solving optimization problems. Many papers [6-11] discuss the application of NNs for optimization with combination of other methods like genetic algorithm (GA).

The statistical regression method, particularly, response surface design (RSD) [12] has been applied in the study because it is widely used in industry and science. A relatively new method, namely, feed forward bottle neck neural network (FFBN NN) mapping technique for optimization was applied in this work. The basic goal of the optimization method using a neural network (NN) is to replace the model equations by an equivalent NN using mapping technique that allows one to identify multiple optima easily. A 2D map of output parameters (responses) overlapped with locations corresponding to the combinations of input parameters (setting points) enables visualization of optimal setting parameters of technological processes in the 2D map. Implementation of the FFBN NN mapping technique enables improvement of the quality of industrial products as well as findings multiple optimal solutions in the development of the new products. The application of FFBN neural network mapping technique for pigment dying of aramid and arimid fibers was published in the paper [13]. In this study we considered FFBN NN method versus RSD and compare obtained results for aramid fibers.

In our study, first, the FFBN NN was applied and several optimums were determined. Second, the RSD was performed and optimal setting parameters were found. Finally, the optimal setting parameters obtained using the FFBN NN method were checked in the regression model of RSD. The desirability of optimum parameter settings in both methods was compared and correlation between them was demonstrated. Implementation of both methods supports double check of process which is very important for reliability of settings.

II. Materials and Process

A. Aramid fibers

Poly-amide benzimidazole (PABI) fibers (in Russian literature known under the trade name SVM) [14] were used in the present study. These fibers relate to the group of aramid fibers based on aromatic para-aromatic polyamide with

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heterochains. The PABI fibers have extremely high modulus and strength, are heat resistant at the temperatures of 200-250°C and can be used at high operating temperature. Therefore, they are widely used in production of protective clothing (i.e. bulletproof vests) [15].

PABI fibers are generally undyeable by using classical methods. In the study we used continuous pigment dyeing process at the stage of formation of PABI fibers combined with thermo-spinning.

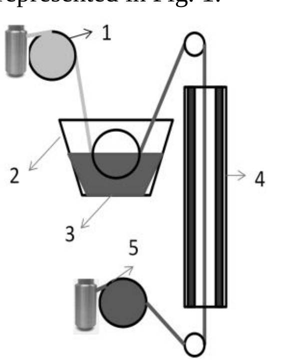
B. The pigment dyeing process

Pigment dyeing bath used in the study contains the following components: X1-pigment- phthalocyanine blue (highly thermostable); X2- binder latex on the bases of butadiene and vinylidene chloride in ratio (30:70); X3- anti-migration agent- manutex RS on the bases of sodium alginate; X4- dispersing agent- prevocell Wof. The process was performed at different temperatures X5. For the references see the patent [16]. The concentrations of components in dyeing bath used in the study and temperatures are represented in Table I.

TABLE I. CODED AND UNCODED VALUES OF INDEPENDENT INPUT VARIABLES AT 5 LEVELS (-2, -1, 0, 1, 2) FOR PIGMENT DYEING PROCESS OF ARAMID FIBER

Variables (factors)	Coded levels				
	-2	-1	0	+1	+2
X1- concentration of binder, %	10	15	20	25	30
X2- concentration of pigment %,	0,25	0,50	0,75	1,00	1,25
X3 - concentration of anti-migration agent, %	0,025	0,050	0,075	0,100	0,125
X4- concentration of dispersing agent, %	0,02	0,04	0,06	0,08	0,10
X5 - temperature, °C	300	350	400	450	500

The operation scheme of module for the continuous pigment dyeing of PABI fibers combined with thermo-spinning is represented in Fig. 1.



The distinctive feature of our proposed method is that first the fiber pass through the dyeing bath with pigment composition, thereafter the impregnated fibers go through the heat chamber with infrared radiation (heating) at the stage of thermo-spinning. The thermo-fixation of dye pigment composition here takes place at temperature of 350-500°C.

Fig. 1. The operation scheme of pigment dyeing module.

Note:1- let off roll with original arimid fiber; 2-pigment dye bath; 3- pigment dyeing suspension; 4- heat chamber with infrared radiation; 5-take up roller device for colored fiber.

The following three response variables (represented the quality of dyed fibers) were considered: y_1- color strength, y_2- tensile strength, y_3- elongation to break.

III. METHODS

A. The feed-forward bottleneck neural network

The FFBN neural network was applied in the study (so called auto associative neural network). For the references about this technique and its application see articles [17-22]. Multidimensional data sets are difficult to interpret and visualize. The FFBN neural network was used for compression and visualization of the data in 2D maps.

The input vector in the FFBN neural network can be represented as a vector of $xi= \{x_{i1}\ x_{i2}\ x_{i3}...\ x_{im}\}$, where "m" corresponds to the number of factors (m=5 in our model). In the FFBN each i-th object is projected onto a two dimensional map with coordinate h_{i1}/h_{i2}. In our model "*i*" corresponds to a number of run (from 1 to 32 in our case). See Fig. 2.

The FFBN neural network is formed by means of mapping and de-mapping the hidden layer. The signals in the two hidden nodes are taken as two coordinates for each input object, enabling a 2D projection of experimental objects onto a 2D map. In other words, the two neurons in the hidden layer produce, for each input object *xi*, a corresponding pair of coordinates ($H=\{h_1, h_2\}$). Thus, in our study we obtained the 2D map with distribution of 32 experimental settings (like was determined in the plan of experiment).

For each of the 32 experimental settings the corresponding value of Y (Y1, Y2, Y3) was determined in the course of the experiment. The projection of Y onto H1/H2 coordinate gave the contour plots of response Y (Y1, Y2, Y3). Overlapping the projection of 32 experimental objects (obtained from the FFBN neural network 2D map) with responses contour plots at the same coordinates (H1/H2) enables visualization and determining of optimal settings corresponding to the Y optimal values.

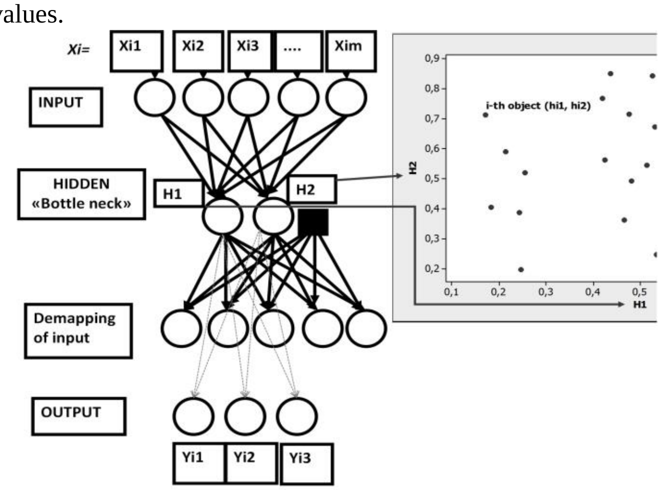


Fig. 2. The FFBN neural network mapping of i-th object.

B. The response surface methodology

Response surface methods (RSM) are used to examine the relationship between response variables (y_n) and a set of quantitative experimental factors (x_m). A general form of this

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type of response function can be represented as equation:

$y = f(x_1, x_2, ..., x_m)$,

where y is the response and $x_1, x_2, ..., x_m$ are quantitative levels of factors of interest. Function f here defines the response surface.

Response Surface Methodology (RSM) is the general term for collection of statistical techniques that are useful for analysing problems influenced by several variables where the objective is to understand curvature for the purpose of optimizing the response or tolerancing the Xs. Among the techniques are: central composite designs, method of steepest ascent, evolutionary operation, simplex, and numerous others.

The goal of the study was to determine the factor levels for which the response variables (y_1- y_3) are optimal (maximal in our case) or to find factors setting that simultaneously optimize several responses (so called generalized response Y_{n_gen}).

The generalized response $Y_{n\_ gen}$ as well as individual responses y_1, y_2, y_3 can be determined for five factors x_1-x_5 using the equations 1-4 in the course of RSD.

$$y_1 = f(x_1, x_2, ..., x_5) + \alpha \quad (1)$$

$$y_2 = f(x_1, x_2, ..., x_5) + \beta \quad (2)$$

$$y_3 = f(x_1, x_2, ..., x_5) + \gamma \quad (3)$$

$$Y_{n\_gen} = f(x_1, x_2, ..., x_5) + \varepsilon \quad (4)$$

where $x_1, x_2, ..., x_5$ are quantitative levels of considered factors.

The central composite design (CCD) [5, 12, 23] based on a quadratic model was used in the study.

Experimental data were analyzed using the response surface regression procedure using Minitab 15 software and fitted to a second-order polynomial model.

Minitab has a Response Optimizer that provides with an optimal solution for the input variable combinations and an optimization plot. This command in our study was based on the results of previously performed RSD.

The MINITAB's Response Optimizer identifies the combination of input variable settings that jointly optimize a set of responses. We examined Y1-Y3 as well as generalized response Y_{n_gen}. Joint optimization satisfies the requirements for all the responses in the set. The desirability (D) is a measure of how well you have satisfied the goals for considered responses.

The opportunity exists to check the desirability of any settings. Therefore, in the study we calculated the desirability of optimal settings obtained using FFBN neural network method. This was done to see how data obtained in both methods (RSD and FFBN) are correlated with each other.

IV. Results and Discussion

A. Plan of experimental design

Five independent variables (which affect the quality of pigment dyeing) namely concentration binder latex (x_1, (%)), concentration of pigment (x_2, (%)), concentration of anti-migration agent (x_3, (%)), concentration of dispersing agent (x_4, (%)) and temperature (x_5, (°C)) of thermo fixation were chosen.

Each of the 5 independent variables were explored at 5 levels: –2;– 1; 0; +1 and +2. The coded and uncoded values are given in Table 1. The design matrix with 32 runs (number of experiments) for Central Composite Design (CCD) was composed and represented in Table II. As the dependent variables we explored the following responses: y_1- color strength; y_2- tensile strength and y_3-% elongation to break for PABI fiber.

TABLE II. The experimental plan of CCD with five independent variables (X1-X5) in coded units and values of responses Y1-Y3 in the experiment with 32 runs

№ run	X1-pigment	X2-binder	X3-anti-migration agent	X4-dispersing agent	X5-temperature	Y1, color strength	Y2, tensile strength	Y3, elongation to break
1	+1	+1	+1	+1	+1	4.3	102.3	3.4
2	- 1	+1	+1	+ 1	- 1	3.3	90.2	3.9
3	+1	-1	+ 1	+1	- 1	4.3	91.6	3.8
4	- 1	-1	+ 1	+ 1	+ 1	4.6	100.5	3.5
5	+1	+ 1	- 1	+1	- 1	3.9	92.3	3.8
6	- 1	+ 1	- 1	+ 1	+1	4.2	101.2	3.6
7	+ 1	-1	- 1	+1	+1	4.7	102.7	3.5
8	-1	- 1	-1	+ 1	- 1	4.3	90.1	3.9
9	+ 1	+ 1	+ 1	- 1	- 1	3.6	91.7	3.8
10	- 1	+1	+1	- 1	+1	3.4	101.1	3.5
11	+1	- 1	+ 1	-1	+ 1	3.8	102.5	3.4
12	-1	-1	+ 1	- 1	- 1	3.5	91.1	3.9
13	+1	+ 1	- 1	-1	+ 1	3.9	102.6	3.4
14	-1	+ 1	-1	- 1	-1	3.4	90.6	3.8
15	+ 1	- 1	-1	- 1	- 1	4.9	102.3	3.5
16	- 1	- 1	- 1	-1	+ 1	4.7	101.9	3.4
17	-2	0	0	0	0	3.2	98.6	4.1
18	2	0	0	0	0	3.3	99.1	4
19	0	-2	0	0	0	5	97.9	4
20	0	2	0	0	0	3	98.3	4.1
21	0	0	-2	0	0	3.5	98.5	4
22	0	0	2	0	0	3.9	98.7	4.1
23	0	0	0	-2	0	3.5	98.6	4
24	0	0	0	2	0	3.9	98.7	4.1
25	0	0	0	0	-2	3.5	90.4	3.8
26	0	0	0	0	2	4.6	105.5	3
27	0	0	0	0	0	4.7	98.8	4.1
28	0	0	0	0	0	4.8	98.7	4.1
29	0	0	0	0	0	4.7	98.7	4
30	0	0	0	0	0	4.8	98.8	4
31	0	0	0	0	0	4.8	98.7	4.1
32	0	0	0	0	0	4.7	98.8	4

B. Analysis of FFBN neural network maps

The architecture of FFBN neural network applied in our work is shown in Fig. 3.

The neural networks use vectors for treatment of information. The input data in Fig. 3 (see left upper corner) is represented as 5 vectors. Each vector (X1-X5) represents an individual parameter (X1-X5) at different levels (-2, -1, 0, +1, +2) as determined by 32 experimental settings.

For the 5 factors (X1-X5) with independent variables (5 input parameters) a special architecture of error back-propagation neural network (5, 2, 5) was used, in which the data are fed into the 5-nodes input layer and then transferred through the 2- nodes hidden layer (so called bottleneck) to the 5-nodes output layer. The two hidden nodes of the hidden layer (bottle neck) produce two coordinates ($H=\{h_1, h_2\}$) for each input object Xi like was explained in section Methods.

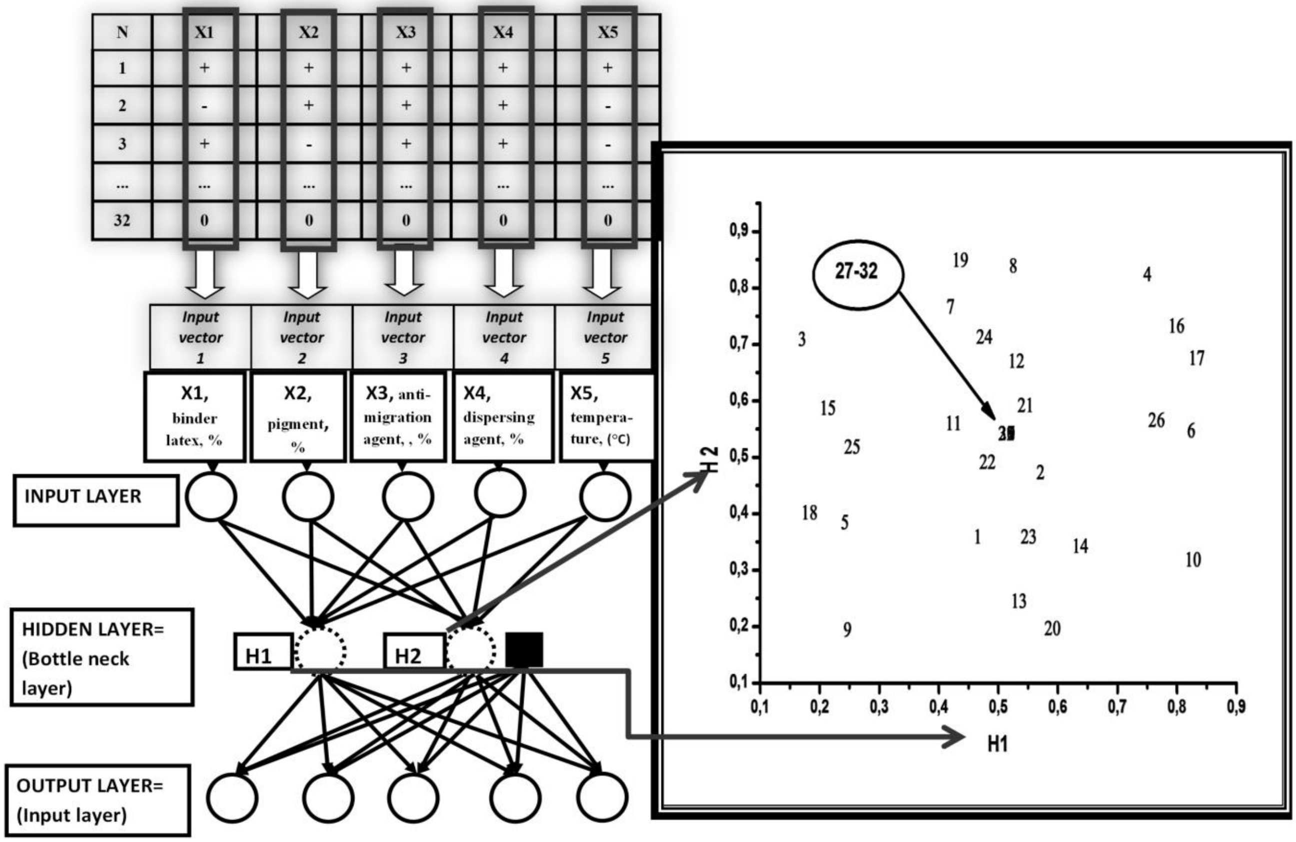

Fig. 3. The architecture of FFBN neural network applied in the study and projection of 32 objects (corresponding to the 32 experimental settings) from two hidden layers H1/H2 into 2D map.

The projection of 32 objects into the H_1/H_2 plot is shown on the right side in Fig. 3. This way the five-dimensional representation space was transformed into a 2D space (H_1/H_2) as the 32 varied data-points (32 experimental settings in design of experiment).

It should be highlighted that the distribution of the 32 setting points in the 2D map is independent from values of responses Y1-Y3, which is the intrinsic property of the considered neural network. Values of responses Y1-Y3 for 32 experimental settings were measured in the course of the experiment. Then the projection of Y values onto H_1/H_2 coordinates was made and the contour plots of Y were obtained overlapped with a 2D map with the 32 setting points. See Fig. 4, where (a)-corresponds to contour plot of generalized response Y_{n_gen}, (b) relates to individual response Y_{n1}- color strenth, (c)- to individual response Y_{n2}- tensile strenth and (d)- to individual response Y_{n3}- elongation to break. Overlapping the projection of 32 objects with responses contour plots enables the determination of multiple optima.

A. Determination of optimums using FFBN NN mapping technique

2D projection of setting points as well as responses related to the quality of studied product enables easy determination of several optima and understanding of the dynamic of the studied process. Take a look at Fig. 4. In the contour plots the dark grey area corresponds to maximum and the more light grey relates to the minimal values. The following optimums were investigated in the study: the central point (setting at zero level 0,0,0,0,0) corresponding to setting points 27-32 and setting points № 19, 16, 15, 7 and 4 marked with circles in Fig. 4 (a). The main goal of optimization in our study was to find the best color strength keeping in mind physical properties that should stay at the level that meets specification requirements for PABI fibers.

Fig. 4 (b, c, d) demonstrates that setting points 16, 15, 7 and 4 correspond to the best color strength while the elongation reduced sacrificing for increase of tensile strength.

Thus, the point № 19 belongs to the highest value of response (most dark grey area). The combination 19 gave the best color strength without significant reduction of mechanical properties of fibers (neither of elongation nor tensile strength). The point №19 corresponds to the following levels of parameters: X1=0, X2=-2, X3=0, X4=0, X=0. Therefore, the optimum was set for factors X1 and X3-X6 at zero level (0) and for factor X2 at minimal level (-2) that corresponds to the minimal concentration of pigment.

A few optima exist. A final decision should be based upon a compromise, taking into account expert opinion based on understanding the nature of the studied polymers, their mechanical properties and the mechanism of action between binder, pigment and fiber during the coloring process.

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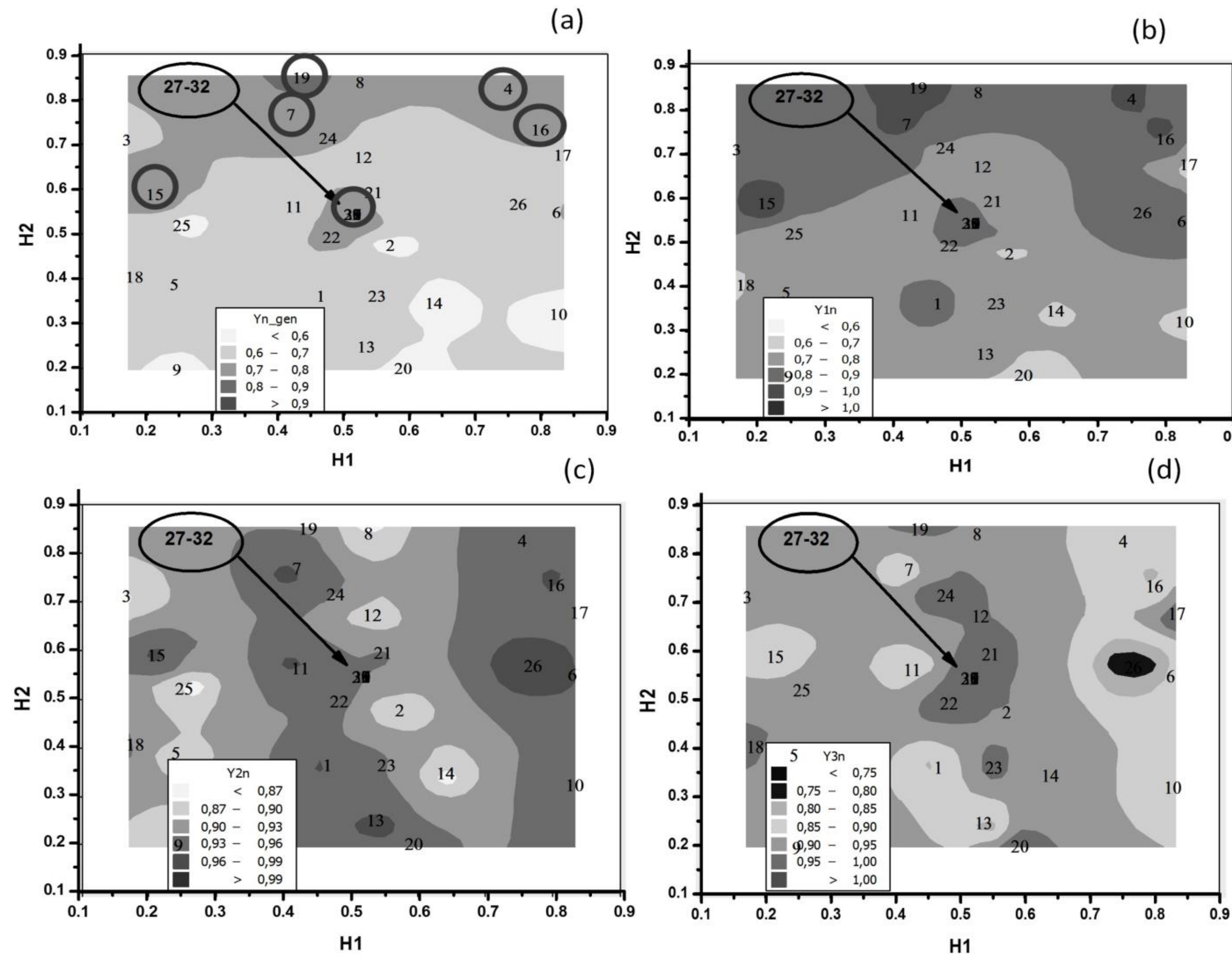

Fig. 4. The map of 32 factor settings (experimental condition) overlapped with contour plots of (a)-generalized response Yn_gen and individual responses: (b)- Yn1- color strenth, (c)- Yn2- tensile strenth and (d)- Yn3- elongation to break.

B. Analysis of response surface design (RSD)

The central composite design (CCD) with 5 factors, 32 total runs, 1 block, 16 cube runs and 6 total center points (replicates) was performed using the Minitab 15 software program. The simple and combined effects of five input variables (x_1-x_5) on the quality of dyed fiber (y_1-y_3) were determined. Minitab calculates regression coefficients for each Y (y_1, y_2, y_3) and p-values. The p-values were used as a tool to check the significance of each coefficient.

Reduced model equations (5-7) were obtained:

$y_1 = 4{,}648 - 0{,}733x_2 - 1{,}091x_1^2$ (5)

$y_2 = 98{,}965 + 1{,}858x_1 + 8{,}758x_5$ (6)

$y_3 = 4{,}097 - 0{,}358x_5 - 0{,}836x_5^2$ (7)

The obtained results show that for color strength y_1 of PABI fiber, only the concentration of pigment x_2 and square of concentration of binder latex x_1^2 have significant influence; for tensile strength y_2 the most significant parameters are concentration binder latex (x_1) and temperature x_5. Elongation to break y_3 appeared to be significantly dependent only on temperature x_5.

C. Determination of optima using RSD

Determination of optima using RSD was performed using the response optimizer option in Minitab 15. We are dealing with a predictive model here. The set of values for the independent variables (X1-X5) that correspond to the technological conditions of the product (for 32 setting points) are fed into the model while the response variables related to the product quality were determined in the course of experiment. The aim is to find a set of values for independent variables for which the predictive model yields the desired response. The program performs a search for response target in the independent variable space. For each selected set of independent values, the model prediction is evaluated and compared with the desired response.

In the first part of our study the RSD was used to find factor regions (parameters settings- (X1-X5)) that produce the best combinations of each of individual responses Y1-Y3. The optimization plot layout is represented in Fig. 5a and shows how the factors X1-X5 affect the predicted responses Y1-Y3. Minitab calculates optimal settings for the input variables along with desirability values to indicate how well those settings achieve the response targets. In Fig. 5a the composite desirability (0.87420) is fairly close to 1, which indicates the settings appear to achieve favorable results for all responses as

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a whole. The most important response is color strength y_1 of PABI fiber – more important than tensile strength of PABI fiber y_2 and elongation to break of PABI fiber y_3. The highest individual desirability equal to 1 was obtained for color strength y_1, the desirability for tensile strength y_2 was equal to 0.70212 and desirability for elongation to break y_3 was equal to 0.83182.

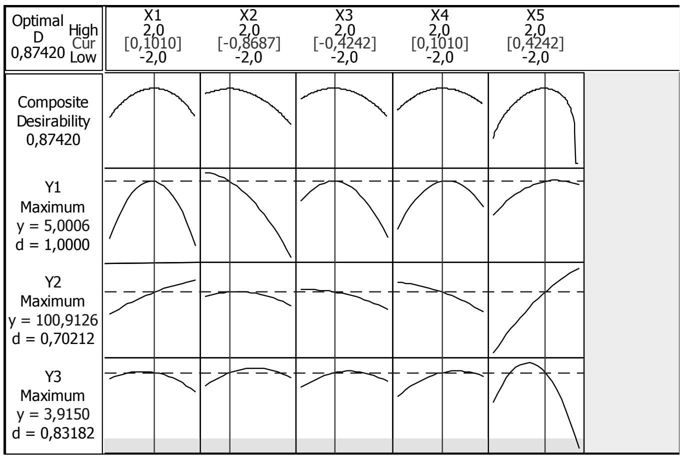

Fig. 5a. The optimization plot layout for factors X1-X5 (coded unites) for responses Y1-Y3.

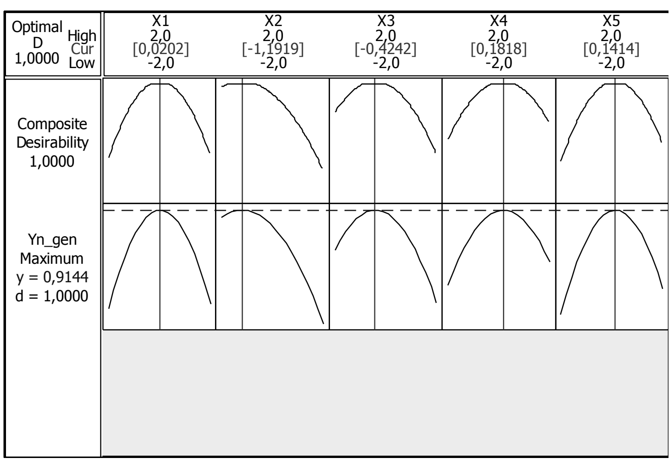

Fig. 5b. The optimization plot layout for factors X1-X5 (coded unites) for generalized response Yn_gen.

In the second part of our study, we examined the generalized value of response Y. At first we divided each of Y (y_1-y_3) on its maximal value and got y_{n1}- y_{n3} in coded units in the range 0-1. The goal of optimization was to reach the maximum for each of Y, therefore to get generalized value of Y (Y_{n_gen}) we multiply $y_{n1} * y_{n2} * y_{n3} = Y_{n\_gen}$

Fig. 5b represents the optimization plot layout for factors x_1-x_5 (coded unites) for generalized response Y_{n_gen} (coded units). The highest dezirability equal to 1 was obtained in this case.

The optimization plot is interactive; we can adjust input variable settings on the plot to search for more desirable solutions. The possibility exists to explore the desirability of settings obtained using the neural network method. We used this property to find desirability of results obtained in neural network method which is described below.

D. Comparison of optimal results in both methods (FFBN NN and RSD)

The optimization plot enables the changing of settings. We entered the optimal setting points obtained using the FFBN NN mapping method into the Minitab response optimizer. We considered the following points: **19, 16, 15, 7, 4** which correspond to the following combination of factors in coded units: **19** (0,-2, 0, 0, 0); **16** (-1,-1,-1,-1,+1), **15**(+1,-1,-1,-1,-1), **7**(+1,-1,-1,+1,+1), **4**(-1,-1,+1,+1,+1).

The desirability of different optimum settings is illustrated in Fig. 6.

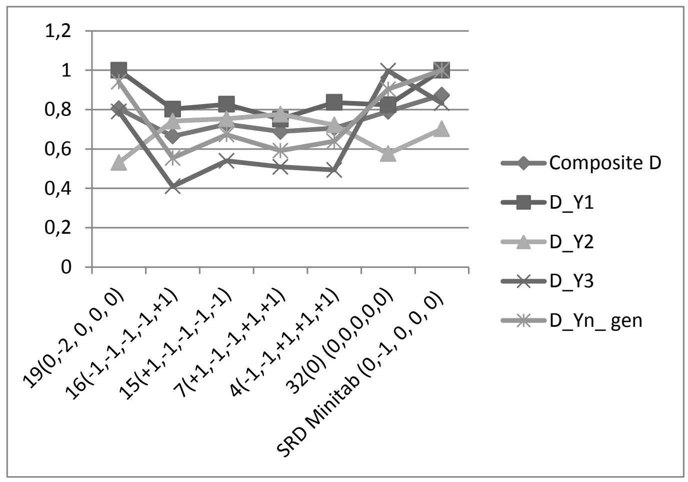

Fig. 6. Composite desirability (D) and desirability of different setting points related to studied optimums.

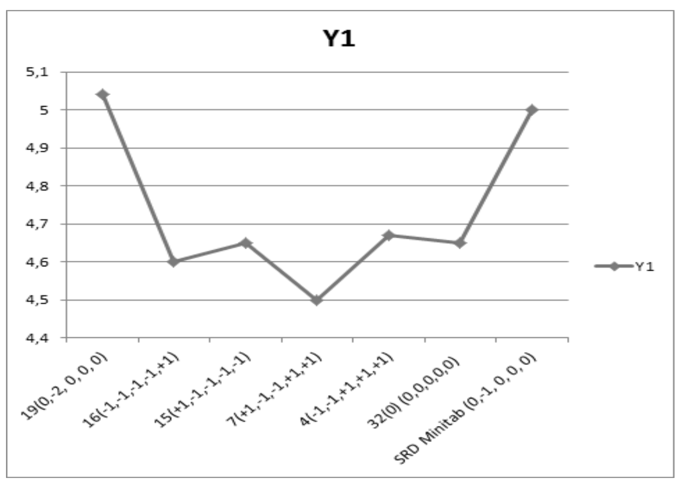

Fig. 7. The value of color strength Y1 at different optimal settings points for the following responses: Y1, Y2, Y3, Yn_gen

The highest desirability belongs to point **19** (0,-2, 0, 0, 0) in the case of NN and to RSD Minitab setting (0,-1, 0, 0, 0).

The result obtained using the neural network model shows slightly better color strength (5.04) than in the RSD model (5.00) reaching the highest possible desirability 1.000 in case of point **19** (0,-2,0,0,0) as well as for the result obtained using the RSD method (see Fig. 7).

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V. Conclusion

The goal of our study was to determine optimum operation conditions: factor levels of X1-X5 that produce the maximum responses Y1-Y3: color strength, tensile strength and elongation to break) in the process of pigment dyeing of high performance PABI fibers.

The feed forward bottle neck neural network (FFBN NN) provided 2D map of whole technological process with all optimums while response surface methodology (RSM) was based on second order polynomial regression.

We demonstrated the FFBN NN network method for finding optima in technological processes in comparison with the traditional RSD method. The visible projection of response in 2D map (in the FFBN method) enables to determine more numbers of optimal solutions than RSD method.

Both methods demonstrated closed results. Therefore, their integration provides double check and finding a more reliable solution.

The colour strength obtained using the FFBN NN method appeared to be slightly better (5,04) than by using RSD (5,00).

The FFBN NN algorithm was developed at the laboratory of chemometrics at the National Institute of Chemistry Ljubljana. This algorithm is easy to use, non-time consuming and provides the ability to obtain visualization of process parameters in a 2D map. Therefore, it can be recommended for finding optimum parameters in technological processes in different industry processes as well as in the Six Sigma (improvement phase).

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