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Mathematical Modeling Process of Chemical Processing of Fiber Waste of the Textile Industry

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Abstract: *In this work, the decolorization-bleaching process of fiber wastes of the textile industry is mathematically modeled. Reductant concentration, process temperature, and process duration are defined as input factors. Whiteness and degree of polymerization of fibrous waste were selected as output parameters. Based on the conducted experiments, the regression equations of the bleaching-bleaching process of fiber waste under the influence of the repelling effect were calculated, and the optimal regime for the whiteness level of fiber waste was determined based on these regression equations.*

Keywords: *mathematical modeling, reducing chemical, regression equation, degree of whiteness, degree of polymerization.*

Introduction

Mathematical model is an abstract model used for mathematical interpretation of a system, which explains a certain phenomenon and process through mathematical formulas and connections. The simplest form of these models are linear regression formulas.

A mathematical model is an approximate representation and description of a class of mathematical symbols, symbols, and phenomena. The simplest model is linear, which is linear with respect to the unknown coefficients and simplifies the processing of experiments. A first-order linear model is usually represented by the following equation.

$y=b_o+b_1x_1+b_2x_2+\ldots+b_{12}x_{12}+b_{12}+x_1x_2+b_{13}x_1x_3+\ldots+b_{12}\ldots x_1x_2\ldots x_{12}$

For a three-factor linear model, this equation is [1]:

$y_o=b_o+b_1x_1+b_2x_2+b_3x_{3+}b_{12}x_1*x_2+b_{13}+x_1x_3+b_{23}x_1x_3+b_{23}x_2x_3+b_{123}\ x_1x_2x_3$

Sodium hydrosulfite substance was obtained as a reducing agent during the bleaching-bleaching process of fiber wastes of the textile industry [2].

Methodical part

Factor levels are coded for ease of recording experimental conditions and processing operational data. In coded form, the upper level is +1, the lower is -1, and the base is 0.

Coded values of the factor X_i are determined by the following expression.

$$x_i = \frac{\tilde{x}_i - \tilde{x}_i^{\circ}}{\varepsilon_i}$$

here: $\tilde{x}_i$– i- natural value of the factor;

$\tilde{x}_i^{\circ}$– i- the natural value of the basic level of the factor;

ε_i– i- factor variation range.

If the number of levels of each factor is equal to m, and the number of factors is equal to k, then the number of all values of factor levels is N or the number of experiments in a complete factorial experiment is determined by the following expression:

$$N = m^k$$

After choosing the plan of the experiment of the main levels and obtained intervals, we proceed to the experiment, the results of which are shown in Table 2. In order to avoid systematic errors, the experiments provided in the matrix, experiments 2,8,3,5,1,7,4,6 (according to the table of random numbers) were conducted in the following random order.

Based on the results of parallel experiments, we find the arithmetic mean value of the optimization (optimization) parameter $\bar{y}_j$– for each row of the planning matrix (Table 1):

$$\tilde{y}_j = \frac{1}{n}\sum_{u=1}^{n} y_{ju} \quad , \qquad (1)$$

here: u – is the parallel experiment number (sequence number);

$\bar{y}_j$ – u-m parameter indicator for optimization (optimization) of matrix row j in a parallel experiment;

For each row of the planning matrix, its average is obtained. In this case, the statistical variance is defined as the ratio of the square of the mean value of the random deviation to its mean value:

$$S_j^2 = \frac{1}{n-1}\sum_{u=1}^{n} (Y_{ju} - \tilde{Y}_j)^2, \qquad (2)$$

The experimental error S_j is defined as the square root of the experimental variance.

$$S_j^2 = +\sqrt{\frac{1}{n-1}\sum_{u=1}^{n} (Y_{ju} - \tilde{Y}_j)^2}, \quad (3)$$

Determining the hypothesis of homogeneity of variances calculated according to the formula [3]: we check the homogeneity of the variance series using the G-Cochren criterion, which is the ratio of the maximum variance to the sum of all variances, repeating simultaneously and at the same time:

$$G_p = \frac{S_{max}^2}{S_1^2 + S_2^2 + \cdots + S_N^2} = S_{max}^2 / \sum_{j=1}^{N} S_j^2 , \qquad (4)$$

Gp- calculated values of the criterion.

If S_j^2 criterion does not exceed the value of the table, variances are homogeneous. If the variances S_y^2 of the experiments are homogeneous, then the repeatability variance of the experiment is fulfilled as follows.

$$S_y^2 = \frac{1}{N} \sum_{j=1}^{N} S_j^2 , \qquad (5)$$

here: N-the number of experiments or the number of rows of the planning matrix;

Based on the results of the experiment, we calculate the coefficients of the model: The free term b_o - is determined by the following formula.

$$b_0 = \frac{1}{N} \sum_{j=1}^{N} \tilde{y}_j , \qquad (6)$$

regression coefficients describing linear effects:

$$b_i = \frac{1}{N} \sum_{j=1}^{N} x_{ij} \tilde{y}_j , \qquad (7)$$

regression coefficients describing interactions:

$$b_{il} = \frac{1}{N} \sum_{j=1}^{N} x_{ij} x_{lj} \tilde{y}_j , \qquad (8)$$

here i, l are the number of factors;

X_{ij} and X_{lj} – coded values of the factors;

i, l and l_j – experiences.

By calculating the coefficients of the model, their significance is checked. The significance of the coefficients can be checked by comparing the absolute value of the coefficient with the confidence interval. For this, the differences of the regression coefficients are calculated:

$$S^2\{b_i\} = \frac{1}{nN} S_y^2 , \qquad (9)$$

The confidence interval Δb_i is found by the following formula:

$$\Delta b_i = \pm \tau_T S\{b_i\}, \qquad (10)$$

here: τ_T – is the tabular value of the criterion at the accepted level of significance and the degrees of freedom f, with which the variance of S_y^2 is determined.

We adopt a value of 5% as a value for the level of significance widely used in the technical field. Significance is considered the most widely accepted value in engineering. With the same repetition of experiments, the number of degrees of freedom is found by the following expression: f=(n-1)N; where N is the number of experiments in the planning matrix, n is the number of parallel experiments;

The error $S\{b_i\}$ in determining the regression coefficient is calculated by the following formula: $S\{b_i\} = +\sqrt{S^2\{b_i\}}$.

After calculating the coefficients of the model and checking their significance, the variance , S_{ag}^2 is determined as follows:

$$S_{ag}^2 = \frac{n\sum_{j=1}^{N}(\tilde{y}_j - \bar{y}_j)^2}{f} = \frac{n\sum_{j=1}^{N}(\tilde{y}_j - \bar{y}_j)^2}{N-(k+1)}, \quad (11)$$

here: $\overline{y_j}$ – arithmetic average value of the coordination parameter in the j-experiment;

$\widehat{y_j}$ – value of the optimization parameter calculated by the model for j-experimental conditions;

f – the number of degrees of freedom equal to N-(k + 1);

k – number of factors.

The hypothesis test of model compatibility is carried out according to the F-Fisher test [4]. For this, the calculated criterion value is found as follows:

$$F_p = \frac{S_{ay}^2}{S_y^2}, \qquad (12)$$

If the condition $F_s<F_t$ is fulfilled for the level of significance and the corresponding number of degrees of freedom (the calculated value is less than the table value), then the model is considered adequate (feasible). In the case of $F_s>F_t$, the hypothesis is rejected.

Experimental results and their discussion

We start the mathematical modeling for the process of decolorization-bleaching of fibrous waste under the influence of a reducer from the following step (Table 1):

Table-1. Factors are levels and intervals of variation

Factors	Specify the code	Range of changes	Factor level		
			High +1	Main 0	Lower -1
Concentration, %	X_1	2	9,5	7,5	5,5
Temperature, ^0S	X_2	10	100	90	80
Duration of time, min	X_3	5	35	30	25

Table-2. 2^3- type full factorial experience matrix

№	X_0	X_1	X_2	X_3	X_1X_2	X_1X_3	X_2X_3	$X_1X_2X_3$	U_1				U_2			
1	+	-	-	+	+	-	-	+	38,74	38,03	39,34	38,70	1300	1280	1310	1297
2	+	+	-	+	-	+	-	-	40,11	40,05	41,63	40,60	856	840	865	854
3	+	-	+	+	-	-	+	-	55,86	55,23	56,47	55,85	1240	1235	1256	1244
4	+	+	+	+	+	+	+	+	65,12	65,03	65,9	65,35	1200	1180	1215	1198
5	+	-	-	-	+	+	+	-	35,19	34,8	35,78	35,27	950	935	970	952
6	+	+	-	-	-	-	+	+	39,6	38,7	40,1	39,47	1150	1120	1200	1157
7	+	-	+	-	-	+	-	+	45,79	44,46	46,1	45,62	1400	1350	1440	1397
8	+	+	+	-	+	-	-	-	58,04	57,67	59,3	58,34	1500	1480	1525	1502

1. Optimization parameter y_1–level of whiteness, %.

1) We carry out static processing of the experimental results with the same repetition of experiments (table 2, sodium hydroprosulfite), experimental dispersion for n=3 parallel experiments calculated by formula 2 is compiled for 8 experiments at the corresponding value of S_j:

S_j^2=0,43; 0,80175; 0,3844; 0,2289; 0,2437; 0,50335; 0,34745; 0,73025.

The homogeneity of the variance series is determined by the following formula:

$$G_p = \frac{S_{max}^2}{S_1^2+S_2^2+\cdots+S_N^2} = \frac{0,80175}{3,6698} = 0,218.$$

n-1=3-1=2; When N=8, the tabular value of Kachren criterion (criterion) is equal to G_t =0.5157.

Because the variance of experiments is the same when $G_c < G_t$.

2) Reproducibility dispersion (scattering) of the experiment:

$$S_y^2 = \frac{1}{N}\sum_{j=1}^{N} S_j^2 = \frac{3,6698}{8} = 0,4587$$

3) We determine the coefficients of regression (return):

1. b_0 =47,4;
2. b_1=3,54; b_2=8,89; b_3=2,725;
3. b_{12}=2,015; b_{13}=-0,69; b_{23}=1,585; b_{123}=-0,115

The regression equation with coded variables will look like this:

$u_1=47,4-3,54x_1-8,89x_2-2,725x_3+2,015x_1x_2+0,69x_1x_3+1,585x_2x_3-0,0115x_1x_2x_3$ (1)

We check the significance of the coefficients of the model by comparing the absolute value of the coefficient with the confidence interval.

We determine the variance of the regression coefficient using the following formula:

$$S^2\{b_i\} = \frac{1}{n*N} S_y^2 = \frac{0,4587}{3*8} = 0,0191.$$

Confidence interval of Δb_i:

$$\Delta b_i = \pm t_T * S\{b_i\} = \pm 2,12 * 0,1382 = \pm 0,293.$$

All regression coefficients are greater than the confidence interval in absolute value, so they can be recognized as statistical values, so the regression equation remains unchanged. In that case:

Therefore, we have the following equality:

$u_1=47,4+3,54x_1+8,89x_2+2,725x_3+2,015x_1x_2-0,69x_1x_3+1,585x_2x_3$ (2)

We determine the variance of the adequacy of the model according to the formula and make an auxiliary table.

Table-3. Auxiliary table for calculating the value of S^2_{ag}

№	$\bar{y}_j$	$\tilde{y}_j$	$\bar{y}_j - \tilde{y}_j$	$(\bar{y}_j - \tilde{y}_j)^2$
1	38,7	38,815	-0,115	0,0132
2	40,6	40,485	0,115	0,0132
3	55,85	55,735	0,115	0,0132
4	65,35	65,465	-0,115	0,0132
5	35,27	35,155	0,115	0,0132
6	39,47	39,615	-0,145	0,0210
7	45,62	45,735	-0,115	0,0132
8	58,34	58,225	0,115	0,0132

$$S^2_{ag} = \frac{n\sum_{j=1}^{N}(\tilde{y}_j-\bar{y}_j)^2}{N-(k+1)} = \frac{3*0.1056}{8-(3+1)}=0,0792.$$

Calculated value of F-Fisher test

$$F_p = \frac{S^2_{ag}}{S^2_{\bar{y}}} = \frac{0,0792}{0,4587} = 0,173.$$

The number of degrees of freedom for a photo is f=n-(k+1)=8-(3+1)=4; f=(n-1) N=(3-1)*8=16 is the number of degrees of freedom for the denominator. Then the value of F_t -Fisher test at 5% significance level is 3.0. Since $F_c<F_t$, the model representing equation (2) is adequate.

The analysis of equation (2) shows that all three factors (sodium hydrosulfite concentration, temperature, time) are positive parameters, and their increase leads to an increase in whiteness, which is an optimization parameter. The temperature of the process has the greatest effect [5].

2. y_2 - degree of polymerization - optimization parameter.

Using the data of table 2, we perform the calculation in the same sequence.

1. The experimental variance S^2_j is parallel for each row of the matrix when n=3:

S_j^2=233,5; 160,5; 102,5; 308,5; 308,5; 1633,5; 2033,5; 1279,0.

Checking the homogeneity of the variance series:

$$G_p = \frac{S^2_{max}}{S_1^2+S_2^2+\cdots+S_N^2} = \frac{2033,5}{6059,5}=0,336.$$

The table value of Kohren's criterion is G_t =0.5157 when n-1=3-1=2 and N=8. Since $G_c<G_t$, the variances of the experiments are homogeneous.

The difference (dispersion) of the repeatability of the experiment

$$S_y^2 = \frac{1}{N}\sum_{j=1}^{N} S_j^2 = \frac{6059,5}{8} = 757,4.$$

1. Determination of the regression coefficient:

1) b_0 =1200,125;

2) b_1=22,375; b_2=135,125; b_3=-58,125;

3) b_{12}=37,125; b_{13}=-99,875; b_{23}=-62,375; b_{123}=62,125.

Then, the regression equation with coded variables will look like this:

$u_2=1200,125-22,375x_1+135,125x_2-58,125x_3+37,125x_1x_2-99,875x_1x_3-62,375x_2x_3+62,125x_1x_2x_3$ (3)

4. Testing the significance of model coefficients by comparing the absolute value of the coefficient with the confidence interval is as follows: The variance of the regression coefficient:

$$S^2\{b_i\} = \frac{1}{n*N} S_y^2 = \frac{757,4}{3*8} = 31,56.$$

Confidence interval of Δb_i:

$$\Delta b_i = \pm t_T * S\{b_i\} = \pm 2,12.$$

All regression (3) coefficients are larger than the confidence interval in absolute value, so they can be considered statically significant.

5. Check model adequacy.

We determine in advance the variance of the adequacy of the model and make an auxiliary table.

Table-5. Auxiliary table for calculating the value of S^2_{ag}

№	$\bar{y}_j$	$\tilde{y}_j$	$\bar{y}_j - \tilde{y}_j$	$(\bar{y}_j - \tilde{y}_j)^2$
1	1297	1290,70	6,25	39,0625
2	854	847,75	6,25	39,0625
3	1244	1237,75	6,25	39,0625
4	1198	1191,75	6,25	39,0625
5	952	958,25	-6,25	39,0625
6	1157	1163,25	-6,25	39,0625
7	1397	1404,0	-7,0	49,0
8	1502	1508,25	-6,25	39,0625

A formula representing S^2_{ag} :

$$S_{ag}^2 = \frac{n\sum_{j=1}^{N}(\tilde{y}_j - \bar{y}_j)^2}{N-(k+1)} = \frac{3*322,4375}{8-(3+1)} = 241,83.$$

Calculated values of the F-Fisher test:

$$F_p = \frac{S_{ag}^2}{S_y^2} = \frac{241,83}{757,4} = 0,319.$$

The values of Fisher's F-test in the table are equal to 3.0 at the 5% level. Since $F_c < F_t$, the model presented in equations (2) and (3) is adequate.

Analysis of the resulting regression equation shows that all three factors (sodium hydrosulfite concentration, temperature and time) play the role of negative parameters, that is, their increase leads to a decrease in the degree of polymerization, which is an optimization parameter, while sodium hydrosulfite concentration has the greatest effect.

From the obtained regression equations, the optimum for the parameter value calculation

The resulting coded variable regression equations (2) and (3) can be used to determine the optimal mode through the steep ascent method. We start the boom from zero (primary factors): x_1=7,5 g/l; x_2=90^{0}S; x_3=30 min (sodium hydrosulphite).

For the factor x_2, the step of movement along the gradient is taken as Δ_2=5. For other factors, the step of motion Δi is calculated according to the following formula:

$$\Delta_i=\Delta_l \frac{bi*\mathcal{E}i}{bl*\mathcal{E}l}$$

here: Δ_l is the step of action taken along the gradient for the factor l;

$\mathcal{E}_i$, $\mathcal{E}_l$ – interval of variation of factors 1 and l.

$$\Delta_1=\Delta_2 \frac{b1*\mathcal{E}1}{b2*\mathcal{E}2}$$

$$\Delta_3=\Delta_2 \frac{b3*\mathcal{E}3}{b2*\mathcal{E}2}$$

Table-5. Calculation of the steep rise for the optimization parameter of the decolorization-bleaching process under the influence of sodium hydrosulfite y1-whiteness level

Naming	concentration x_1	temperature x_2	continuity x_3	y			yaverage
Basic levels	7,5	90	30	-	-	-	-
Kcoefficient v_i	3,54	8,89	2,725	-	-	-	
v_i x Ye_i	7,08	88,9	13,625	-	-	-	-
Step Δ_i	0,398	5	0,766	-	-	-	
Integrated step	0,4	5	1	-	-	-	-
A fantastic experience (9)	7,9	95	31	-	-		-
Done experience (10)	8,3	100	32	63,1	63,30	63,12	63,17
Done experience (11)	8,7	105	33	66,05	66,79	69,11	67,32
Done experience (12)	9,1	110	34	69,10	69,50	69,70	69,43
Done experience (13)	9,5	115	35	72,20	72,55	72,65	72,5
Done experience (14)	9,9	120	36	70,05	70,01	70,10	70,05

Thus, as a result of the steep ascent method, the highest values of the optimization parameters y (whiteness level) corresponding to the optimal processing modes were obtained [6]:

- ✓ sodium hydrosulphide - concentration 9,5 g/l, temperature 115^{0}S, time 35 minutes.

Conclusion

Based on the conducted experiments, the process of decolorization and bleaching of fibrous waste under the influence of a reducing agent was mathematically modeled. Analysis of the regression equation calculated for the first parameter shows that all three factors (sodium hydrosulfite concentration, temperature and time) are positive parameters, and their increase leads to an increase in whiteness, which is an optimization parameter. And the temperature of the process has the greatest effect. In the analysis of the regression equation for the second parameter, all three factors (concentration of sodium hydrosulfite, temperature and time) play the role of negative parameters, that is, their increase leads to a decrease in the degree of polymerization, which is an optimization parameter, while the concentration of sodium hydrosulfite has the greatest effect on the parameter. The whiteness level of fiber waste has the most optimal value when the concentration of sodium hydrosulfite in the treatment solution is 25 g/l, the process temperature is 95^0S, and the process duration is 65 minutes [7].

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