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THE RESULTS OF VERIFICATION OF THE CORRECT EXECUTION OF THE SEQUENCE OF EXPERIMENTS ON THE MATHEMATICAL OPTIMIZATION OF THE PROCESS OF OBTAINING MELAMINE FORMALDEHYDE RESIN

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Abstract

The degree of accuracy of experiments is important in studying the processes of synthesis of melamine formaldehyde resin. For this purpose, using the Maple computer program, the level of accuracy of the experiments was studied.

Keywords: chemical engineering, melamine, formaldehyde, mathematic planning, Box-Wilson, Maple.

Introduction

First of all, the correlation of the results of the experiment was formed. The results are shown in Table 1.

Table 1 Correlation of experimental results

x	x_1	x_2	x_3	$\cdots$	x_{n-1}	x_n
y	y_1	y_2	y_3	$\cdots$	y_{n-1}	y_n

In this case, it is necessary to develop an analytical relationship that illuminates the experimental results with a high degree of accuracy. In the development of such factors, it is appropriate to use the method of least squares $f(x, a_1, a_2, \dots, a_k)$, which has the following form. In this case, the function $f(x, a_1, a_2, \dots, a_k)$ should be placed in such a way that the squares of the obtained result are the displacements of the above y, $f(x, a_1, a_2, \dots, a_k)$ in size steps $Y_i = f(x, a_1, a_2, \dots, a_k)$ should be smaller than the values of the shifted dimensions (Fig. 1).

$$S(a_1, a_2, \dots, a_k) = \sum_{i=1}^{n}[y_i - Y_i]^2 = \sum_{i=1}^{n}[y_i - f(x, a_1, a_2, \dots, a_k)]^2 \to min$$

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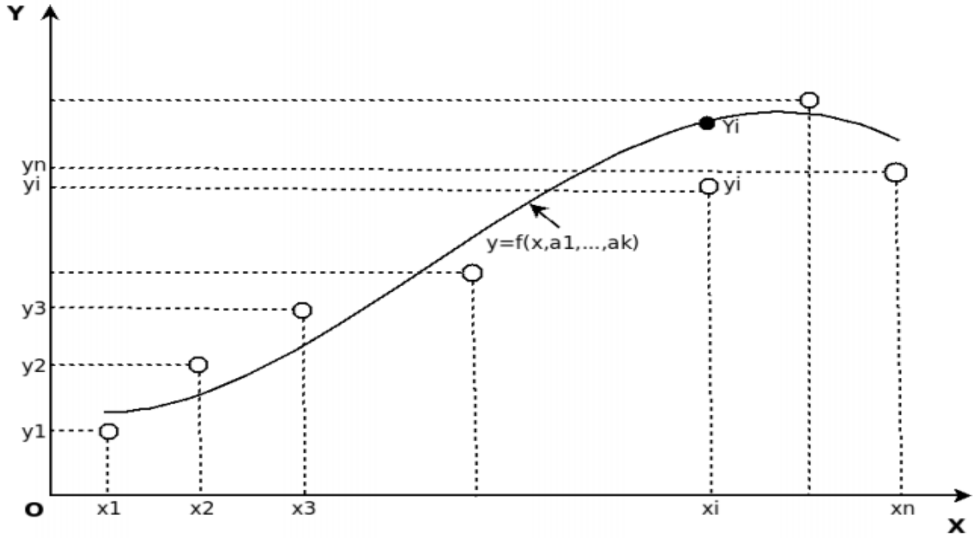

Fig.1. Temperature dependence curve of yield of melamine formaldehyde resin

This issue will consist of two stages:

1. Determination of the external expressive form of the selected connection according to the results obtained from the experiment;

2. choosing the static coefficient of dependence in the function $Y = f(x, a_1, a_2, \dots, a_k)$ and extracting this dependence through a_i in function 1.

The minimum condition satisfying the observer for the function $S(a_1, a_2, \dots, a_k)$ is that all its derivatives are equal to zero. As a result, to find the minimum of the function, it is necessary to solve the following algebraic equation.

$$\begin{cases} \frac{\partial S}{\partial a_1} = 0 \\ \frac{\partial S}{\partial a_2} = 0 \\ \dots \\ \frac{\partial S}{\partial a_k} = 0 \end{cases}$$

If the parameters a_i are determined to be linear with respect to each other by the dependence in the function $Y = f(x, a_1, a_2, \dots, a_k)$, using the unknown k from the k linear equation, we get the following system:

$$\begin{cases} \sum_{i=1}^{n} 2[y_i - f(x, a_1, a_2, \dots, a_k)] \frac{\partial f}{\partial a_1} = 0 \\ \sum_{i=1}^{n} 2[y_i - f(x, a_1, a_2, \dots, a_k)] \frac{\partial f}{\partial a_2} = 0 \\ \dots \\ \sum_{i=1}^{n} 2[y_i - f(x, a_1, a_2, \dots, a_k)] \frac{\partial f}{\partial a_k} = 0 \end{cases}$$

In this case, the value of a_i in the system of equations for calculating the necessary parameters is large, and at the specified level $k - 1 -$ takes the form $Y = \sum_{i=1}^{k} a_i x^{i-1}$ and the system looks as follows is caused:

$$\begin{cases} a_1 n + a_2 \sum_{i=1}^{n} x_i + a_3 \sum_{i=1}^{n} x_i^2 + \cdots + a_k \sum_{i=1}^{n} x_i^{k-1} = \sum_{i=1}^{n} y_i \\ a_1 \sum_{i=1}^{n} x_i + a_2 \sum_{i=1}^{n} x_i^2 + a_3 \sum_{i=1}^{n} x_i^3 + \cdots + a_k \sum_{i=1}^{n} x_i^k = \sum_{i=1}^{n} x_i y_i \\ \ldots \\ a_1 \sum_{i=1}^{n} x_i^k + a_2 \sum_{i=1}^{n} x_i^{k+1} + a_3 \sum_{i=1}^{n} x_i^{k+2} + \cdots + a_k \sum_{i=1}^{n} x_i^{2k-2} = \sum_{i=1}^{n} x_i^k y_i \end{cases}$$

Then this system of equations is opened and written in the form of a matrix.

$$Ca = g$$

The elements related to the matrix C and the vector g are calculated using the following formula:

$$C_{i,j} = \sum_{k=1}^{n} x_k^{i+j-2}, i = 1, \ldots, k+1, j = 1, \ldots, k+1$$

$$g_i = \sum_{k=1}^{n} y_k x_k^{i-1}, i = 1, \ldots, k+1$$

By solving the above system, $Y = a_1 + a_2 x + a_3 x^2 + \cdots + a_{k+1} x^k$ characteristic parameters of the dependence are determined.

Taking into account that the yield of melamine-formaldehyde resin is high when the duration of the reaction during the condensation of melamine and formaldehyde is 90-120 minutes, the accuracy of the experiments was checked based on the following values (Table 2).

Table 2 Results obtained for statistical processing of melamine formaldehyde resin extraction processes

Temperature, ºC	Duration of reaction, minutes	Product yield, %		
		Yield		The average speed of the reaction
		%	in grams	% / every 10 minutes
80	90	47,409	47	5,26
95	90	81,251	81	9,02
110	90	67,103	67	7,45

The mathematical model for processing the results of the reaction yield during the synthesis of the melamine-formaldehyde compound in the presence of melamine and formalin is presented in Table 3 below:

Table 3 Model 1 of the synthesis process of melamine-formaldehyde compound in the presence of melamine and formalin

t_i	80	95	110
u_i	47.4	81.2	67.1

Here: t_i– temperature, u_i – product of melamine formaldehyde resin. Result:

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$$S(a_1, a_2, \dots, a_k) = \sum_{i=1}^{4}[u_i - U_i]^2 = \sum_{i=1}^{4}[u_i - f(t_i, a_1, a_2, a_3, a_4)]^2 \to min$$

$$f(t_i, a_1, a_2, a_3, a_4) = a_1 + a_2 t_i + a_3 {t_i}^2 + a_4 {t_i}^3$$

A system of equations with the following form is created using the indicated values and the current:

$$\begin{cases} \sum_{i=1}^{4} 2[u_i - a_1 + a_2 t_i + a_3 {t_i}^2 + a_4 {t_i}^3]\, {t_i}^3 = 0 \\ \sum_{i=1}^{4} 2[u_i - a_1 - a_2 t_i - a_3 {t_i}^2 - a_4 {t_i}^3]\, {t_i}^2 = 0 \\ \sum_{i=1}^{4} 2[u_i - a_1 - a_2 t_i - a_3 {t_i}^2 - {t_i}^3]\, t_i = 0 \\ \sum_{i=1}^{4} 2[u_i - a_1 - a_2 t_i - a_3 {t_i}^2 - a_4 {t_i}^3] = 0 \end{cases}$$

By simplifying the above system of linear equations, the following system is obtained:

$$\begin{cases} a_1 \sum_{i=1}^{4} t_i^3 + a_2 \sum_{i=1}^{4} t_i^4 + a_3 \sum_{i=1}^{4} t_i^5 + a_{k+1} \sum_{i=1}^{4} t_i^6 = \sum_{i=1}^{n} t_i^3 u_i \\ a_1 \sum_{i=1}^{4} t_i^2 + a_2 \sum_{i=1}^{4} t_i^3 + a_3 \sum_{i=1}^{4} t_i^4 + a_4 \sum_{i=1}^{4} t_i^5 = \sum_{i=1}^{4} t_i^2 u_i \\ a_1 \sum_{i=1}^{4} t_i + a_2 \sum_{i=1}^{4} t_i^2 + a_3 \sum_{i=1}^{4} t_i^3 + a_4 \sum_{i=1}^{4} t_i^4 = \sum_{i=1}^{4} t_i u_i \\ 4a_1 + a_2 \sum_{i=1}^{4} t_i + a_3 \sum_{i=1}^{4} t_i^2 + a_4 \sum_{i=1}^{4} t_i^3 = \sum_{i=1}^{4} u_i \end{cases}$$

We find the solution of the system of simplified linear equations (A, B, C) shown above using the method of matrices (A, B, C):

$$A = \begin{pmatrix} 26732954000000 & 191732400000 & 1383380000 & 10044000 \\ 191732400000 & 1383380000 & 10044000 & 73400 \\ 1383380000 & 10044000 & 73400 & 540 \\ 10044000 & 73400 & 540 & 4 \end{pmatrix}$$

$$B = \begin{pmatrix} 8{,}404024000 * 10^8 \\ 6{,}0979000 * 10^6 \\ 44524{,}0 \\ 327{,}2 \end{pmatrix} C = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix}$$

$$A * C = B$$

It follows that in order to determine the values of the parameters (a_1, a_2, a_3, a_4) of the matrix C, A^{-1}, it is necessary to find the inverse value of A, and it is done in the following order:

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$$A^{-1} = \begin{pmatrix} \frac{1}{1800000} & -\frac{9}{40000} & \frac{5447}{180000} & -\frac{2703}{2000} \\ -\frac{9}{40000} & \frac{1823}{20000} & -\frac{-981}{80} & \frac{54781}{100} \\ \frac{5447}{180000} & -\frac{981}{80} & \frac{594053}{360} & -\frac{1474773}{20} \\ -\frac{-2703}{2000} & \frac{5478}{100} & -\frac{1474773}{20} & 3296021 \end{pmatrix}$$

relying on the formula $C = A^{-1} * B$, it is possible to find the value of the matrix C based on it, and this matrix will have the following form:

$$C = \begin{pmatrix} -0,00236 \\ 9270,02 \\ -119,711 \\ 5173,01 \end{pmatrix}$$

Based on the obtained results, taking into account the above values, the dependence of the formation of melamine-formaldehyde resin as a result of the chemical reaction on the temperature of the polycondensation process and the duration of the reaction is expressed as follows:

$$f_1 := a_1 * 80^3 + a_2 * 80^2 + 80 * a_3 + a_4; f_1 := 66,7$$
$$f_2 := a * 95^3 + b * 95^2 + 95 * c + d; f_2 := 77,1$$
$$f_3 := a * 110 + b * 110^2 + 110 * c + d; f_3 := 88,3$$

Function $f = a * t^3 + b * t^2 + c * t + d$ and $t = 80 \ldots 110$, $f = 66.7 \ldots 91$, the temperature dependence of the yield of melamine-formaldehyde resin in values is shown in the graphic form in the following pictures (Figure 2).

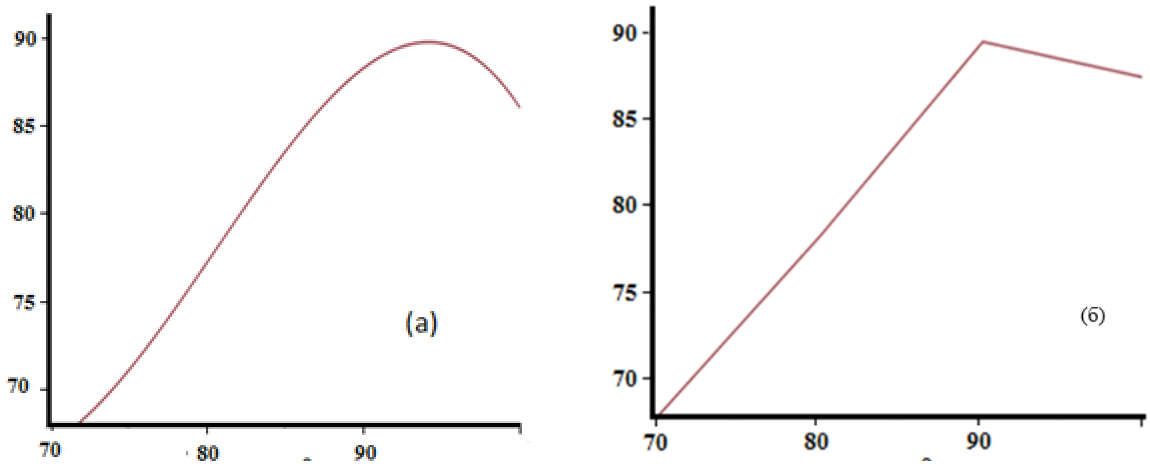

Fig.2. Temperature dependence of yield of melamine formaldehyde resin (a –experiment, b - mathematical model).

It can be seen from the graphs in Figure 2 that the results of the conducted experiments and the results obtained by mathematical modeling confirm and match each other. If the functional differences do not exceed 3%, the experiments are observed to be performed with an accuracy of 97% or higher and the condition is proved to be fulfilled:

$$u_1 - f_1 := 68,8 - 66,7 = 2,1; \quad \textit{precision higher than } 100 - 2.1 = 97\%$$
$$u_2 - f_2 := 79,3 - 77,1 = 2,2; \quad \textit{precision higher than } 100 - 2.1 = 97\%$$
$$u_3 - f_3 := 90,6 - 88,3 = 2,3; \quad \textit{precision higher than } 100 - 2.1 = 97\%$$

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As can be seen from the results of the above calculations, the experiments on the reaction of melamine with formalin were performed with an accuracy higher than 97%.

Conclusion. In order to achieve the level of accuracy of the experiments in the study of the processes of synthesis of melamine formaldehyde resin, the accuracy level of the experiments was studied using the Maple computer program, and the correlation of the experimental results was formed. The results of the experiments and the results obtained through mathematical modeling confirm each other and match each other. It was observed that the differences related to the function did not exceed 3%.

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