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MATHEMATICAL MODELING OF THE SYNTHESIS OF ALIPHATIC ALCOHOLS ON THE BASIS OF THE REACTION OF TELOMERIZATION

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Abstract: In article results by investigation of telomerization of ethyl alcohol by etylene on the base high-based system and acetone. It was determined that in process of synthesis iso-butyl and iso-hexyl alcohols by telomerization of ethylene by has been investigated ethyl alcohol. Optimal parameters of investigated process were determined: influence of duration of reaction temperature and rate of feeding acetylene, nature of using catalysts and solvents on yield of forming products. Obtain results were treated wish using mathematical models and methods. Analysis of obtained experimental results of investigated chemical process has shown corresponding to theoretical data. Diagrams of results of activation energy and dynamics of changing of kinetic parameters have been elaborated and also graphs of analytical functions are also presented.

Keywords: ethylene, ethanol, hydrogen peroxide, benzoyl peroxide, synthesis at high pressure, optimal conditions, solvent, surfactants, telomerization, catalytic reactions. iso-butanol, iso-hexanol, acetone, monomer, telogen, surfactants.

1. Introdition. In the Republic methanol and ethanol are produced from aliphatic alcohols on an industrial scale. Other alcohols, including butyl, hexyl and iso-alcohols are used through imports. Establishing the synthesis of such alcohols on the base ethyl alcohol by the telomerization reaction is an urgent task [1-3].

In this work, synthesis of iso-butyl and iso-hexyl alcohols by telomerization of ethylene by has been invertigated ethyl alcohol [4-7]. Mathematical modeling of synthesis of these alcohols has been carried out and mathematical treatment of the results of experiments by the least squares method has been carried out [8]. As a result of the research, it was proved that the experimental results obtained in the laboratory coincide with those calculated using computer programs [9].

In general, the relationship between the results of the experiment in the formulation of the problem is presented in table 1.

Table 1

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

x - temperature, y - product yield

2.Materials and methods. In this case it is necessary to create an analytical dependence that most clearly illuminates the results of the experiment [10]. The this squares method $f(x, a_1, a_2, ..., a_k)$ is used to create such parameters. At this the function $f(x, a_1, a_2, ..., a_k)$ should be specified so that the squares of the results y, $f(x,$

a_1, a_2, ..., a_k) have shifts of unity $Y_i=f(x, a_1, a_2, ..., a_k)$ must be smaller than dimensions displacement [11-12] (Fig. 1).

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

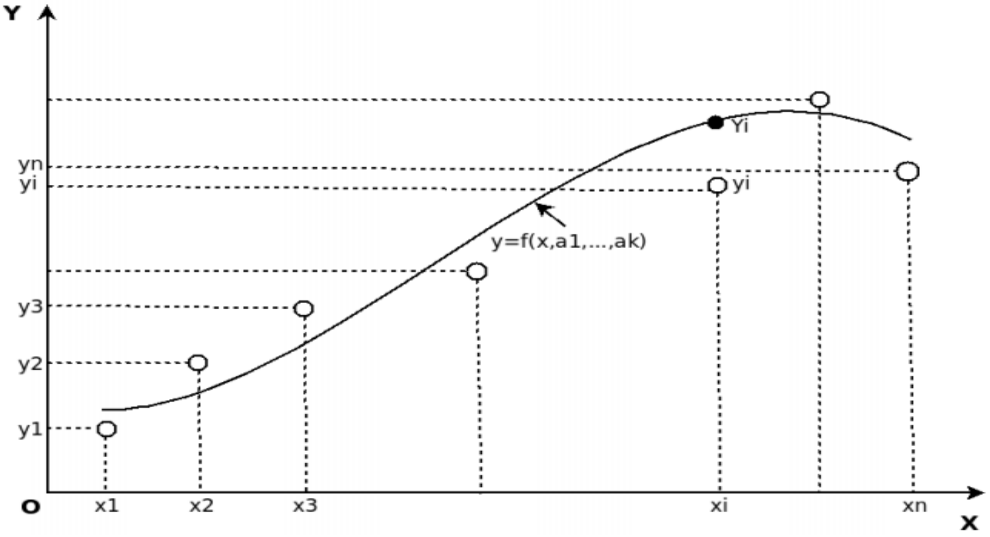


Fig 1. Analytical dependence of product yield on temperature

3.The results obtained and their discussion. Mathematical modelation and mathematical treatment of the results obtained by synthesis in the laboratory, consists of two stages:

1. Determination the external state of the selected dependence based on the results of the experiment.

2. The dependence coefficient in the function $Y=f(x, a_1, a_2, ..., a_k)$ is selected and this dependence is calculated by a_i in the first function.

The sufficient condition for the minimum of the function $S(a_1, a_2, ..., a_k)$ (1) is explained by the fact that all it's derivatives are equal to zero. Thus finding the minimum function is determined by solving of this algebraic equation:

$$\begin{cases} \frac{\partial S}{\partial a_1} = 0 \\ \frac{\partial S}{\partial a_2} = 0 \\ \dots \\ \frac{\partial S}{\partial a_k} = 0 \end{cases} \quad (2)$$

If the parameters a_i are linear with dependence in the function $Y=f(x, a_1, a_2, ..., a_k)$, then the following system (3) is obtained from k linear equations with k unknowns.

$$\begin{cases} \sum_{i=1}^{n} 2[y_i - f(x, a_1, a_2, \dots, a_k)] \frac{\partial f}{\partial a_1} = 0 \\ \sum_{i=1}^{n} 2[y_i - f(x, a_1, a_2, \dots, a_k)] \frac{\partial f}{\partial a_2} = 0 \\ \dots \\ \sum_{i=1}^{n} 2[y_i - f(x, a_1, a_2, \dots, a_k)] \frac{\partial f}{\partial a_k} = 0 \end{cases} \quad (3)$$

In the general case the system of equations for calculating the parameters ai is numerous and takes the form $Y = \sum_{i=1}^{k} a_i x^{i-1}$ to the degree k-1 and system (4) takes the following form (5):

$$\begin{cases} a_1 n + a_2 \sum_{i=1}^{n} x_i + a_3 \sum_{i=1}^{n} x_i^2 + \cdots + a_k \sum_{i=1}^{n} x_i^{k-1} = \sum_{i=1}^{n} y_i \\ a_1 \sum_{i=1}^{n} x_i + a_2 \sum_{i=1}^{n} x_i^2 + a_3 \sum_{i=1}^{n} x_i^3 + \cdots + a_k \sum_{i=1}^{n} x_i^k = \sum_{i=1}^{n} x_i y_i \\ \ldots \\ a_1 \sum_{i=1}^{n} x_i^k + a_2 \sum_{i=1}^{n} x_i^{k+1} + a_3 \sum_{i=1}^{n} x_i^{k+2} + \cdots + a_k \sum_{i=1}^{n} x_i^{2k-2} = \sum_{i=1}^{n} x_i^k y_i \end{cases} \quad (4)$$

and is written in matrix form:

$$Ca = g \qquad (5)$$

By this formula the elements of the matrix C and the vector g are calculated.

$$C_{i,j} = \sum_{k=1}^{n} x_k^{i+j-2}, i = 1, \ldots, k+1, j = 1, \ldots, k+1, \qquad (6)$$

$$g_i = \sum_{k=1}^{n} y_k x_k^{i-1}, i = 1, \ldots, k+1. \qquad (7)$$

On the base of system (4), with using these parameters of the dependence $Y=a_1+a_2x+a_3x^2+\ldots+a_{k+1}x^k$ mathematical modeling of the synthesis of iso-butyl and iso-hexyl alcohols based on ethylene and ethanol at high pressure and also mathematical treatment of the obtained results were carried out.

The results of the synthesis of iso-butyl alcohol in terms of it's yield were subjected to mathematical treatment (Table 2).

Table 2

Yield of iso-butyl alcohol at various temperatures

t[1] = 40	y[1] = 22,8
t[2] = 50	y[2] = 34,5
t[3] = 60	y[3] = 53,5
t[4] = 70	y[4] = 45,4

In an experiment on the synthesis of iso-butyl alcohol with at a reaction duration 3-6 hours, it was found that the product yield is higher at 6 hours. Therefore, the mathematical calculations of the process were carried out precisely at a duration of 6 hours (Table 3).

Table 3

The results obtained for mathematical treatment

Temperature, ^{0}C	Reaction time, h.	Product yield, %	Average reaction rate, %/h
40	3	22,8	7,33
50	4	34,5	8,5
60	5	53,5	10,6
70	6	45,4	7,5

Mathematical model for treatment the yield of iso-butyl alcohol based on ethylene and ethanol in the laboratory can be presented as:

Model 1

t_i	40	50	60	70
u_i	22,8	34,5	53,5	45,4

where: t_i – temperature, u_i – yield of isobutyl alcohol.

Using the experimental values and the function, the following system of linear equations is presented:

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

$$f(t_i, a_1, a_2, a_3, a_4) = a_1, a_2t_i + a_3t_i^2 + a_4t_i^3$$

Then the system of linear equations (A, B, C) is calculated by the matrix method.

$$A = \begin{pmatrix} 184026000000 & 2873200000 & 45780000 & 748000 \\ 2873200000 & 45780000 & 748000 & 12600 \\ 45780000 & 7480000 & 12600 & 220 \\ 748000 & 12600 & 220 & 4 \end{pmatrix}$$

$$B = \begin{pmatrix} 3.28999000 * 10^7 \\ 537790.0 \\ 9025.0 \\ 156.2 \end{pmatrix} C = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix}$$

$$A * C = B$$

And so, to determine the values (a_1,a_2,a_3,a_4) of the matrix C, A^{-1} is calculated, that is the reciprocal of A:

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

$C=A^{-1} * B$ has allowed to find the value of matrix C based on the formula and this matrix looks like this:

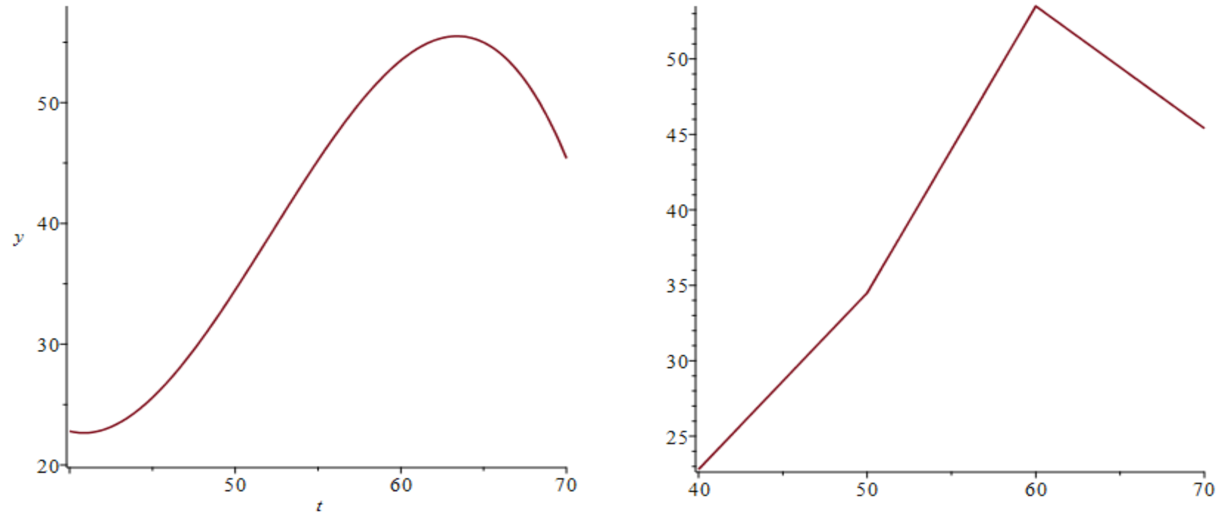
$$C = \begin{pmatrix} -0,0023668 \\ 9270 \\ -119,71 \\ 5173 \end{pmatrix}$$

and at this a_1=-0,0023668, a_2=9270, a_3=-119,71, a_4=5173.

Taking into account these values, based on the results obtained experimentally, the dependence of the formation of iso-butyl alcohol on the temperature and reaction rate was mathematically expressed by the following function:

$$f_1 = a_1 * 40^3 + a_2 * 40^2 + 40 * a_3 + a_4;\ \ f_1 = 22{,}798240$$
$$f_2 = a * 50^3 + b * 50^2 + 50 * c + d;\ \ f_2 = 34{,}497500$$
$$f_3 = a * 60^3 + b * 60^2 + 60 * c + d;\ \ f_3 = 53{,}496560$$
$$f_4 = a * 70^3 + b * 70^2 + 70 * c + d;\ \ f_4 = 45{,}395380$$

Based on the obtained results, a scheme for the formation of iso-butyl alcohol was elaborated using the Maple 2018 program. The function *f=a*t3+b*t2+c*t+d* at *t=40...70, f=20...58* in the formation of iso-butyl alcohol can be presented as follows (Fig. 2):



a) b)

Fig. 2. Graphs of the temperature dependence of the yield of iso-butyl alcohol: a) - according to experimental data, b) - based on mathematical modeling

It was determined that the results obtained on the basis of the experiment are coincided with the accuracy of 98% with the results obtained by mathematical treatment by the product yield.

$$u_1 - f_1 = 22{,}8 - 22 = 0{,}8;\ \ 96\%$$
$$u_2 - f_2 = 34{,}5 - 34 = 0{,}5;\ \ 98\%$$
$$u_3 - f_3 = 53{,}5 - 53 = 0{,}5;\ \ 99\%$$
$$u_4 - f_4 = 45{,}4 - 45 = 0{,}4;\ \ 99\%$$

The results obtained experimentally for the reaction rate were also presented by mathematical treatment. At the same time, based on the results of table 3 received was obtained model 2:

Model 2

t_i	40	50	60	70
v_i	7,6	8,62	10,7	7,56
u_i	22,8	34,5	53,8	45,4

where: t_i - temperature, v_i - reaction rate, u_i - yield of iso-butyl alcohol.

Based on these results, the following function is calculated:

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

$$f(t_i, v_i, a_1, a_2, a_3, a_4) = a_1 t_i, + a_2 t_i^2 + a_3 t_i v_i + a_4 t_i^2$$

Using the given values and the function, the following system of linear equations is obtained, which is simplified to the following form:

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

Based on linear systems, the process matrix *K* and *U* are calculated, which are reduced to the following value:

$$K = \begin{bmatrix} 12600 & 748000 & 109274.00 & 16895.7720 \\ 748000 & 45780000 & 6.46818000 * 10\text{^}6 & 970393.6400 \\ 109274.00 & 6.46818000 * 10\text{^}6 & 970393.6400 & 153332.5015 \\ 16895.7720 & 970393.6400 & 153332.5015 & 25231.85555 \end{bmatrix}$$

$$L = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} U = \begin{pmatrix} 9025.0 \\ 537790.0 \\ 80173.380 \\ 12600.41824 \end{pmatrix}$$

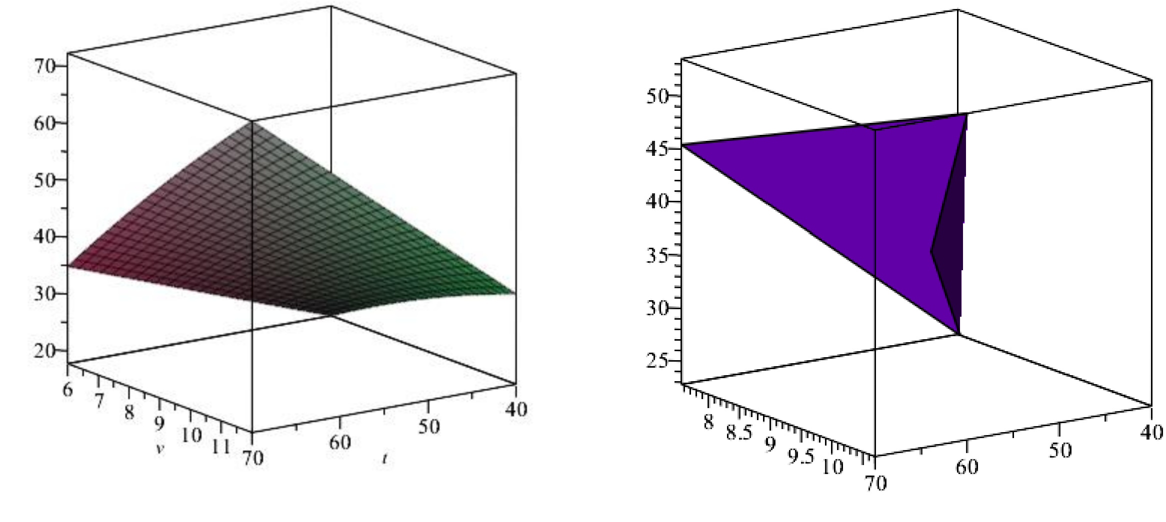
To find the (a_1, a_2, a_3, a_4) of matrix *L*, the formula *L=K-1*U* was used and the following results were obtained:

$$a_1 = -142979756350144$$
$$a_2 = 0{,}284994001094674e\text{-}2$$
$$a_3 = 0{,}0750329624543156$$
$$a_4 = 0{,}0364723829334253$$

On the base of the obtained experimental values, carried out in the laboratory using this function $f(t_i, v_i, a_1, a_2, a_3, a_4)$, it was shown that they were performed with an accuracy of 97%.

$$f_1 = a_1 * 40 + a_2 * 40^2 + 40 * 7{,}33 * a_3 + 7{,}33^2 * a_4;\ f_1 = 22{,}80000098$$
$$f_2 = a_1 * 50 + a_2 * 50^2 + 50 * 8{,}5 * a_3 + 8{,}13^2 * a_4;\ f_2 = 34{,}49999896$$
$$f_3 = a_1 * 60 + a_2 * 60^2 + 60 * 10{,}6 * a_3 + 10{,}6^2 * a_4;\ f_3 = 53{,}50000040$$
$$f_4 = a_1 * 70 + a_2 * 70^2 + 70 * 7{,}5 * a_3 + 7{,}5^2 * a_4;\ f_4 = 45{,}40000014$$

Based on the calculated and experimental results, iconograms of the temperature dependence of the yield of isobutyl alcohol were constructed (Fig. 3).



a) **b)**

Fig. 3. Iconograms of the temperature dependence of the synthesis of iso-butyl alcohol: a) - by experimental data, b) - obtained by mathematical modelation

Mathematical modelation of the process of iso-hexyl alcohol synthesis

It was found that at the telomerization of ethylene with ethyl alcohol along with iso-butyl alcohol, was formed iso-hexyl alcohol and the influence of various factors on the yield of the product was studied. At modelation this process, the results obtained at 40-90 °C were mainly used.

Taking into account that during telomerization of ethylene with ethyl alcohol, the duration of the reaction is 6 hours. Mathematical calculations of the process were carried on the base of the following data (Table 4).

Table 4

The results obtained for mathematical treatment

№	Pressure, atm.	Reaction time, h.	Temperature, °C	Yield, %
1	55	6	40	54,0
3			60	64,8
5			80	72,1
6			90	71,8

For mathematical treatment of the results by the yield of iso-hexyl alcohol synthesized by the method of telomerization of ethylene with ethyl alcohol, the following 3rd model was elaborated:

Model 3

t_i	40	60	80	90
u_i	54,0	64,8	72,1	71,8

where: t_i - temperature, u_i - yield of iso-hexyl alcohol.

At calculating the set values and functions using a computer program, the following system of linear equations is formed:

A=*Matrix*([[*sum*((*t*[*i*])^6, *i*=1..4), *sum*((*t*[*i*])^5, *i*=1..4), *sum*((*t*[*i*])^4, *i*=1..4), *sum*((*t*[*i*])^3, *i*=1..4)], [*sum*((*t*[*i*])^5, *i*=1..4), *sum*((*t*[*i*])^4, *i*=1..4), *sum*((*t*[*i*])^3, *i*=1..4), *sum*((*t*[*i*])^2, *i*=1..4)], [*sum*((*t*[*i*])^4, *i*=1..4), *sum*((*t*[*i*])^3, *i*=1..4), *sum*((*t*[*i*])^2, *i*=1..4), *sum*((*t*[*i*])^1, *i*=1..4)], [*sum*((*t*[*i*])^3, *i*=1..4), *sum*((*t*[*i*])^2, *i*=1..4), *sum*((*t*[*i*])^1, *i*=1..4)]]);

To simplify the system of linear equations and obtaining the corresponding values, the method of (*A*, *B*, *C*)-matrices was used.

$$A=\begin{bmatrix} 844337000000 & 10061700000 & 122090000 & 1521000 \\ 10061700000 & 122090000 & 1521000 & 19700 \\ 122090000 & 1521000 & 19700 & 270 \\ 1521000 & 19700 & 270 & 4 \end{bmatrix}$$

To find the values of the function (a_1, a_2, a_3, a_4) of the obtained matrix *C*, the inverse value of the matrix *A* was calculated, i.e. A^{-1}, and the following results are obtained:

$$A^{-1}=\begin{bmatrix} \frac{199}{7200000000} & -\frac{1289}{240000000} & \frac{187}{562500} & -\frac{3899}{600000} \\ -\frac{1289}{240000000} & \frac{8379}{8000000} & -\frac{39049}{600000} & \frac{25539}{20000} \\ \frac{187}{562500} & -\frac{39049}{600000} & \frac{731101}{180000} & -\frac{240143}{3000} \\ -\frac{3899}{600000} & \frac{25539}{20000} & -\frac{240143}{3000} & \frac{39637}{25} \end{bmatrix}$$

Since the process was carried out for 6 hours at various temperatures, matrix *B* was created:

B=*Matrix*([[*sum*(*y*[*i*]*(*t*[*i*])^3, *i*=1..4)], [*sum*(*y*[*i*]*(*t*[*i*])^2, *i*=1..4)], [*sum*(*y*[*i*]*t*[*i*], *i*=1..4)], [*sum*(*y*[*i*], *i*=1..4)]]), which had the following meanings:

$$B=\begin{bmatrix} 1.067102000\,10^{8} \\ 1.3627000\,10^{6} \\ 18278.0 \\ 262.7 \end{bmatrix}$$

$C=A^{-1} * B$ allows to find the value of the matrix *C* by the formula and it can be attached in the following form:

C=Matrix([[a], [b], [c], [d]]);

$$C=\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$$

At calculating matrix *C*, the results are written ($A^{-1}*B$);

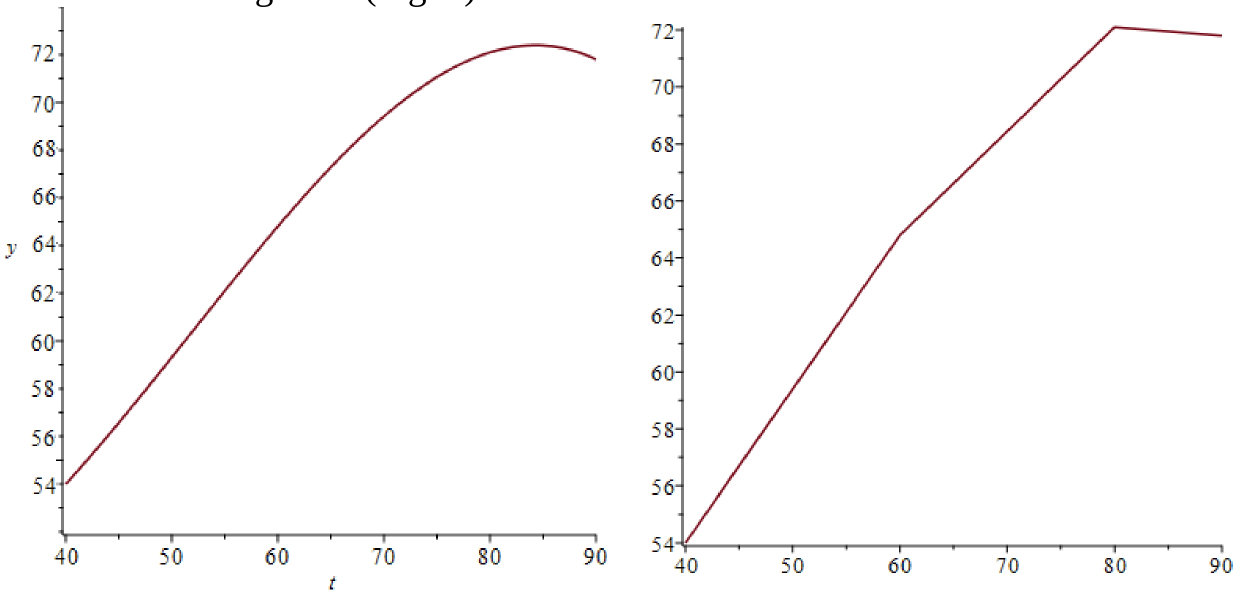
$$\begin{bmatrix} -0.000175834 \\ 0.0272748 \\ -0.85116 \\ 55.6600 \end{bmatrix}$$

and at this *a=-0,000175834; b=-0,0272748; c=-0,85116; d=55,6600.*

Taking into account these calculated values on the base of the dependence of the formation of iso-hexyl alcohol on the temperature and reaction rate, the results of mathematical calculation and experiment were expressed by the following functions:

$$y1=a\cdot 40^3+b\cdot 40^2+c\cdot 40^1+d; \quad y1=53{,}99990400$$
$$y2=a\cdot 60^3+b\cdot 60^2+c\cdot 60^1+d; \quad y2=64{,}79953600$$
$$y3=a\cdot 80^3+b\cdot 80^2+c\cdot 80^1+d; \quad y3=72{,}09891200$$
$$y4= a\cdot 90^3+b\cdot 90^2+c\cdot 90^1+d; \quad y4=71{,}7984940$$

$a\cdot t^3+b\cdot t^2+c\cdot t^1+d$ functions and iso-hexyl alcohol yield graph at *t=40..90, y=52..76* had the following form (Fig. 4).



a) **b)**

Fig. 4. Graphs of the dependence of the yield of iso-hexyl alcohol on temperature: a) - according to experimental data, b) - by mathematical modelation

By yield of iso-hexyl alcohol formed during the telomerization of ethylene with ethyl alcohol, the activation energy of the process and its rate were calculated. Based on the obtained results on the yield of the product and the reaction rate, mathematical treatment was carried out and their relationship was studied. First, the obtained results on the reaction rate were entered into the computer program, then the values of the product yield depending on were entered.

$$v[1]=9,0;\ v[2]=10,8;\ v[3]=12,01;\ v[4]=11,9;$$
$$u[1]=54;\ u[2]=64,8;\ u[3]=72,1;\ u[4]=71,8$$
$$t[1]=40;\ t[2]=60;\ t[3]=80;\ t[4]=90$$

Based on the obtained results, the K matrix was elaborated:
$K=Matrix([[sum((t[i])^2, i=1..4), sum((t[i])^3, i=1..4), sum(((t[i])^2\cdot v[i]), i=1..4), sum((t[i]\cdot(v[i])^2), i=1..4)], [sum((t[i])^3, i=1..4), sum((t[i])^4, i=1..4), sum(((t[i])^3 \cdot v[i], i=1..4), sum(((t[i])^2 \cdot (v[i])2), i=1..4)], [sum(((t[i])^2 \cdot v[i]), i=1..4), sum(((t[i])^3 \cdot v[i]), i=1..4), sum(((t[i])^2 \cdot (v[i])^2, i=1..4), sum(((t[i])^1 \cdot (v[i])^3), i=1..4)], [sum(((t[i])^1 \cdot (v[i])^2), i=1..4), sum(((t[i])^2 \cdot (v[i])^2), i=1..4), sum(((t[i])^1\cdot(v[i])^3), i=1..4), sum((v[i])^4, i=1..4)]]);$

The value of matrix K is as follows:

$$K=\begin{bmatrix} 19700 & 1521000 & 226534.00 & 34522.5080 \\ 1521000 & 122090000 & 1.773302000\,10^7 & 2.619681640\,10^6 \\ 226534.00 & 1.773302000\,10^7 & 2.619681640\,10^6 & 394992.9181 \\ 34522.5080 & 2.619681640\,10^6 & 394992.9181 & 61024.48815 \end{bmatrix}$$

To simplify the process, the values of L were determined and calculated as l,m,n and f.

$$L= Matrix([[l], [m], [n], [f]]);$$
$$l= 0,360196815370728$$
$$m= 0,0194829777191785$$
$$n= -0,301500165062407$$
$$f= 1,44394352862219$$

As a result, the values of L were obtained:

$$l = 0,360196815370728;$$
$$m = 0,0194829777191785,$$
$$n = -0,301500165062407;$$
$$f = 1,44394352862219;$$

For modelation and treatment of the temperature dependence of the yield of iso-hexyl alcohol formed during the telomerization of ethylene with ethyl alcohol, the function (u) was calculated:

$$u=l \cdot t + m \cdot t^2 + n \cdot t \cdot v + f \cdot v^2;$$
$$u=0,0194829777191785t^2 – 0,301500165062407tv + 1,44394352862219v^2 + 0,360196815370728t$$

Based on the temperature, reaction rate and yield of the product used in the process of mathematical modeling, the difference between the values of the experiment and mathematical processing was 0.8-1.4%.

$$u1 = l \cdot 40 + m \cdot 40^2 + n \cdot 40 \cdot 9,0 + f \cdot 9,0^2;\quad u1=54,00000337$$
$$u2 = l \cdot 60 + m \cdot 60^2 + n \cdot 60 \cdot 10,8 + f \cdot 10,8^2;\quad u2=64,7999949$$
$$u3 = l \cdot 80 + m \cdot 80^2 + n \cdot 80 \cdot 12,01 + f \cdot 12,01^2;\quad u3=72,1000030$$
$$u4 = l \cdot 90 + m \cdot 90^2 + n \cdot 90 \cdot 11,9 + f \cdot 11,9^2;\quad u4=71,7999992$$

At the same time the optimal conditions for telomerization of ethylene with ethyl alcohol were selected.

$$l \cdot t + m \cdot t^2 + n \cdot t \cdot v + f \cdot v^2,\ t=40..90,\ v=8..13$$

It is shown that the results of experiments and mathematical treatment on the yield of the product have an accuracy 99-100%:

u_1–f_1 = 54–54 = 0; 100 %
u_2–f_2 = 64,8–64,7 = 0,1; 99 %
u_3–f_3 = 72,1–72,1 = 0; 100 %
u_1–f_1 = 71,8–71,9 = -0,1; 99 %

Using the obtained experimental results, calculations were carried out on the reaction rate. In this process, model 4 was obtained from table 4:

Model 4

t_i	40	60	80	90
v_i	9	10,8	12,01	11,9
u_i	54	64,8	72,1	71,8

where: t_i - temperature, v_i - reaction rate, u_i - iso-hexyl alcohol yield.

Based on these results, the following functions are presented:

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

$$f(t_i, v_i, a_1, a_2, a_3, a_4) = a_1 t_i + a_2 t_i^2 + a_3 t_i v_i + a_4 v_i^2$$

Using the given values and the function, the following system of linear equations was elaborated, which was simplified to the following form:

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

On the basis of linear systems the matrices K and U of the process are calculated:

$$K=\begin{bmatrix} 19700 & 1521000 & 2.2653400\,10^5 & 34522.5080 \\ 1521000 & 122090000 & 1.773302000\,10^7 & 2.619681640\,10^6 \\ 2.2653400\,10^5 & 1.773302000\,10^7 & 2.619681640\,10^6 & 3.949929181\,10^5 \\ 34522.5080 & 2.619681640\,10^6 & 3.949929181\,10^5 & 61024.48815 \end{bmatrix}$$

U=*Matrix*([[*sum*(*u*[*i*] * *t*[*i*], *i*=1..4)], [*sum*(*u*[*i*] * $(t[i])^2$, *i*=1..4)], [*sum*(*u*[*i*] * *t*[*i*] * *v*[*i*], *i*=1..4)], [*sum*(*u*[*i*] * $(v[i])^2$, *i*=1..4)]])

$$U=\begin{bmatrix} 18278.0 \\ 1.3627000\,10^6 \\ 207601.880 \\ 32499.58121 \end{bmatrix}$$

$(K^{-1}*U)$;

$$\begin{bmatrix} 0.360196815370728 \\ 0.0194829777191785 \\ -0.301500165062407 \\ 1.44394352862219 \end{bmatrix}$$

l=0,360196815370728;

m=0,0194829777191785;

n=-0,301500165062407;

f=1,44394352862219

Based on the obtained values of the function $f(t_i, v_i, a_1, a_2, a_3, a_4)$ it follows that these experiments coincide with the data obtained by mathematical processing with an accuracy of 99%.

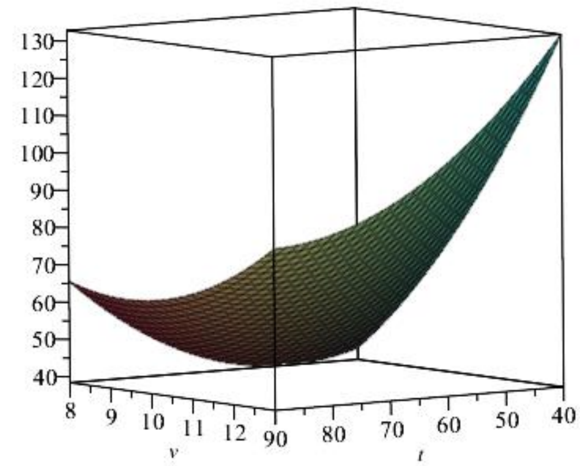
$f_1 = a_1 * 40 + a_2 * 40^2 + 40 * 9 * a_3 + 9^2 * a_4$; $f_1 = 54{,}00000337$

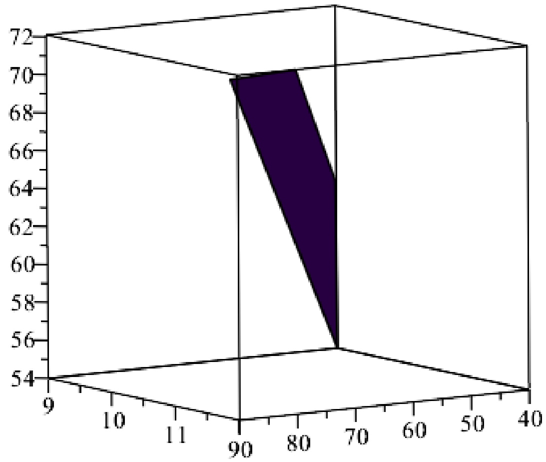
$f_2 = a_1 * 60 + a_2 * 60^2 + 60 * 10{,}8 * a_3 + 10{,}8^2 * a_4$; $f_2 = 64{,}79999949$

$f_3 = a_1 * 80 + a_2 * 80^2 + 80 * 12{,}1 * a_3 + 12{,}1^2 * a_4$; $f_3 = 72{,}10000030$

$f_4 = a_1 * 90 + a_2 * 90^2 + 90 * 11{,}9 * a_3 + 11{,}9^2 * a_4$; $f_4 = 71{,}99999992$

Iconograms were constructed based on the results of the temperature dependence of the synthesis of iso-hexyl alcohol according to its yield, obtained experimentally and by mathematical processing using computer programs (Fig. 5).





a) **b)**

Fig. 5. Iconograms of the temperature dependence of the synthesis of iso-hexyl alcohol according to its yield: a) - according to experimental data, b) - by mathematical modelation

Mathematical treatment of data by the synthesis of iso-butyl alcohol based on the values of its yield and reaction rate showed that the experiments were performed with an accuracy of 98 %.

CONCLUSION

After analyzation of kinetic parameters of the synthesis of iso-butyl and iso-hexyl alcohols, the average reaction rate was determined and it's activation energy was calculated. Using mathematical modeling, analysis of graphs of analytical functions and diagrams of kinetic parameters of synthesis it is possible to establishe that at a reaction time of 6 hours and a temperaturs of 60 and 80 °C the yields of alcohols have reached a maximum values: iso-butyl alcohol - 53,5 %, iso-hexyl alcohol - 72,1 %.

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