Original Article

MATHEMATICAL MODELING OF THE SYNTHESIS OF ACETYLENE HYDROXYACID AND PROCESSING OF EXPERIMENTAL RESULTS

Juraboev Fozil Mamasolievich

Doctor of Philosophy (PhD) in Chemical Sciences, Namangan Institute of Engineering and Technology, Republic of Uzbekistan, Namangan city.
E-mail: jfm-75@mail.ru

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Abstract

In this article, mathematical modeling of the synthesis of acetylene hydroxyacid by condensation of acetylene alcohol with monochloric acid in the presence of triethylamine is carried out. The results obtained were compared with the results of the synthesis of acetylene hydroxy acid by the method of the experiment.

Keywords: acetylene alcohol, monochloroacetic acid, triethylamine, acetylene hydroxyacid, mathematical modeling, product yields, reaction duration, mathematical processing.

Acetylene alcohols and their derivatives are widely used as biologically active substances in agriculture, medicine and industry. Increasing its reactive centers by introducing a carboxyl group in the acetylene alcohol molecule, thereby further increasing its biological activity is one of the urgent tasks. Mathematical modeling of the synthesis of acetylene hydroxyacids by cross-condensation of acetylene alcohol and hydrochloric acid with the participation of triethylamine makes it possible to determine the synthesis conditions and favorable technological parameters. Mathematical modeling allows you to optimize technological processes, develop modern, low-cost, minimal experiments [1-7].

In this paper, the method of a small number of squares was used in mathematical modeling based on the results of the experiment of the synthesis of acetylene hydroxyacid, the results of the experiment and the calculated results were close to each other. In general, the question can be formulated as follows. The state of dependence of the experimental results is shown in Table 1.

Table 1

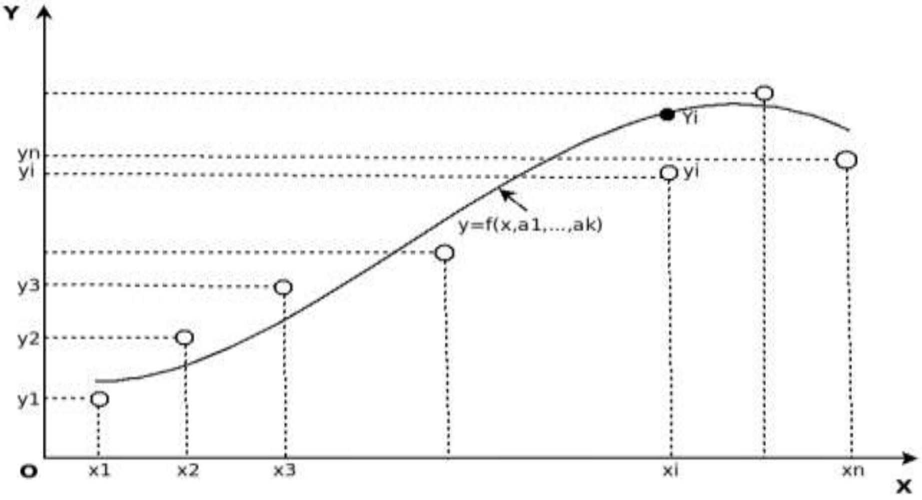
x	x_1	x_2	x_3	$\cdots$	x_{n-1}	x_n
y	y_1	y_2	y_3	$\cdots$	y_{n-1}	y_n

In this regard, there is a need to create an analytical link that will highlight the results of the experiment as accurately as possible. When creating such parameters, a small number of the following

$f(x,a_1,a_2,\dots,a_k)$ are used by the squares method. In this process, $f(x,a_1,a_2,\dots,a_k)$ the function a_k) should be set in such a way that in the squares of the result obtained by it, $f(x,a_1,a_2,\dots,a_k)$ is shifted by one size $Y_i=f(x,a_1,a_2,\dots,a_k)$, should be smaller than the size offsets in a_k (Figure 1).

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

Figure 1. Analytical dependence of product yield on temperature



Mathematical modeling and processing of synthesis results consists of two stages:

1. Determination of the appearance of the selected dependence based on the results of the experiment.

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

3. The sufficient condition for the minimum of the function $S(a_1,a_2,\dots,a_k)$ (1) is explained by the fact that it is zero in all its derivatives. Thus, finding the minimum function is determined by solving 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 $Y=f(x,a_1,a_2,\dots,a_k)$ are linear with the ratio in the function k from a linear equation K with an unknown, the following system (3) is obtained.

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

In general, in the system of equations for calculating the parameters a_i is in large numbers of $k - 1 -$level $Y = \sum_{i=1}^{k} a_i x^{i-1}$ takes the form and is reduced to the following (4) system form [5]:

$$\begin{cases} a_1 n + a_2 \sum_{i=1}^{n} x_i + a_3 \sum_{i=1}^{n} x_i^2 + \dots + a_k \sum_{i=1}^{n} x_i^{k-1} = \sum_{i=1}^{n} y_i \\ a_1 \sum_{i=1}^{n} x_i + a_2 \sum_{i=1}^{n} x_i^2 + a_3 \sum_{i=1}^{n} x_i^3 + \dots + a_k \sum_{i=1}^{n} x_i^k = \sum_{i=1}^{n} x_i y_i \\ \dots \\ a_1 \sum_{i=1}^{n} x_i^k + a_2 \sum_{i=1}^{n} x_i^{k+1} + a_3 \sum_{i=1}^{n} x_i^{k+2} + \dots + a_k \sum_{i=1}^{n} x_i^{2k-2} = \sum_{i=1}^{n} x_i^k y_i \end{cases} \tag{4}$$

Then (4) the system is written as a matrix.

$$Ca = g, \tag{5}$$

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

$$C_{i,j} = \sum_{k=1}^{n} x_k^{i+j-2}, i = 1, \dots, k+1, j = 1, \dots, k+1, \tag{6}$$

$$g_i = \sum_{k=1}^{n} y_k x_k^{i-1}, i = 1, \dots, k+1. \tag{7}$$

Based on the above system (4), these dependence parameters are determined $Y = a_1 + a_2 x + a_3 x^2 + \dots + a_{k+1} x^k$

In this paper, the results of the formation of acetylene hydroxyacid based on acetylene alcohol were mathematically modeled and processed (Table 2).

Table 2 Units of formation of acetylene hydroxyacid at different temperatures

t[1] := 80	y[1] := 39.7
t[2] := 90	y[2] := 61.9
t[3] := 95	y[3] :=64.4
t[4] := 100	y[4] := 65.6

Mathematical calculations were carried out on the basis of the following values, taking into account the fact that acetylene hydroxyacid is synthesized with high values when the reaction duration is carried out during the condensation of acetylene alcohol and monochloroacetic acid with the participation of triethylamine (Table 3). [7-11].

Table 3 Effect of temperature and reaction duration on the synthesis of acetylene hydroxyacid based on 2-methylbutyn-3-ol-2

Temperature, °C	Reaction time, hour	Product output, %	Average reaction speed, %/ hour
80	5	39.7	7,9
90	5	61.9	12.4
95	5	64.4	12.9
100	5	65.6	13.2

A model of mathematical processing of the results of a unit of product due to an increase in temperature during the synthesis of acetylene hydroxyacid based on acetylene alcohol:

Table 4 Model:

t_i	80	90	95	100
u_i	39,4	61,9	64,4	65,6

Where: t_i- is the temperature, u_i- is the unit of measurement of acetylene hydroxyacid.

Using the given values and the function, the following system of linear equations is formed.

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

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

We solve a system of linear equations (A, B, C) using the matrix method.

$$A = \begin{pmatrix} 2528676890625 & 26919509375 & 288020625 & 3098375 \\ 26919509375 & 288020625 & 3098375 & 33525 \\ 288020625 & 3098375 & 33525 & 365 \\ 3098375 & 33525 & 365 & 4 \end{pmatrix}$$

$$A^{-1} = \begin{pmatrix} \frac{11}{900000} & -\frac{199}{60000} & \frac{1681}{5625} & -\frac{8939}{1000} \\ -\frac{199}{60000} & \frac{18003}{20000} & -\frac{48671}{600} & \frac{485347}{200} \\ \frac{1681}{5625} & -\frac{48671}{6000} & \frac{2632001}{360} & -\frac{4374983}{20} \\ -\frac{8939}{1000} & \frac{485347}{200} & -\frac{4374983}{20} & 6545881 \end{pmatrix}$$

$$A * C = B$$

Therefore, the elements of the matrix C are equal to A^{-1} to find the values of (a_1, a_2, a_3, a_4), that is, the inverse value of A is found:

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

$C = A^{-1} * B$ allows you to find the value of the matrix C based on the formula, and this matrix will have

$$\begin{bmatrix} 0.004733 \\ -1.3755 \\ 13340 \\ -4252 \end{bmatrix}$$

views and the next value is a_1 = 0.004733, $a_1 = 0.004733$, $a_2 = -1.3755$, $a_3 = 133.40$, $a_4 = -4252$.

Table 5 Effect of temperature and reaction duration on the synthesis of acetylene hydroxyacid based on 2-methylbutyn-3-ol-2

Temperature, ºC	Reaction time, hour	Product output, %	Average reaction speed, %/ hour
80	1	17,4	17,4
	2	26,3	13,2
	3	32,1	10,7
	4	38,8	9,7

	5	39,7	7,9
90	1	27,3	27,3
	2	42,9	21,5
	3	54,6	18,2
	4	61,8	15,5
	5	61,9	12,4
95	1	32,2	32,2
	2	46,4	23,2
	3	58,6	19,5
	4	64,1	16,0
	5	64,4	12,9
100	1	34,1	34,1
	2	47,2	23,6
	3	59,4	19,8
	4	64,3	16,1
	5	65,6	13,1

The results obtained on the basis of the synthesis of acetylene hydroxy acid were modeled in the following order.

Initially, mathematical modeling was based on the highest product yield obtained during synthesis at various temperatures.

t[1] := 80; t[2] := 90; t[3] := 95; t[4] := 100

y[1] := 38.8; y[2] := 61.9; y[3] := 64.4; y[4] := 65.6;

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), 4]]);

$$A = \begin{pmatrix} 2528676890625 & 26919509375 & 288020625 & 3098375 \\ 26919509375 & 288020625 & 3098375 & 33525 \\ 288020625 & 3098375 & 33525 & 365 \\ 3098375 & 33525 & 365 & 4 \end{pmatrix}$$

$$A^{-1} = \begin{pmatrix} \frac{11}{900000} & -\frac{199}{60000} & \frac{1681}{5625} & -\frac{8939}{1000} \\ -\frac{199}{60000} & \frac{18003}{20000} & -\frac{48671}{600} & \frac{485347}{200} \\ \frac{1681}{5625} & -\frac{48671}{6000} & \frac{2632001}{360} & -\frac{4374983}{20} \\ -\frac{8939}{1000} & \frac{485347}{200} & -\frac{4374983}{20} & 6545881 \end{pmatrix}$$

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)]])

$$\mathrm{B} = \begin{bmatrix} 1.858056500 \cdot 10^{8} \\ 1.9869200 \cdot 10^{6} \\ 21353.0 \\ 230.7 \end{bmatrix} \qquad B = Matrix\ ([[\mathrm{a}], [b], [c], [d]]);$$

$$\mathrm{C} = \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} \qquad \begin{bmatrix} 0.004733 \\ -1.3455 \\ 133.40 \\ -4252. \end{bmatrix}$$

evalm(A^{-1}*&*B);*

$a := 0.004733; \quad b := -1.3755; \quad c := 133.40; \quad d := -4252;$

$y1 := a \cdot 80^3 + b \cdot 80^2 + c \cdot 80^1 + d; \quad y1 := 40.096000$

$y2 := a \cdot 90^3 + b \cdot 90^2 + c \cdot 90^1 + d; \quad y2 := 62.807000$

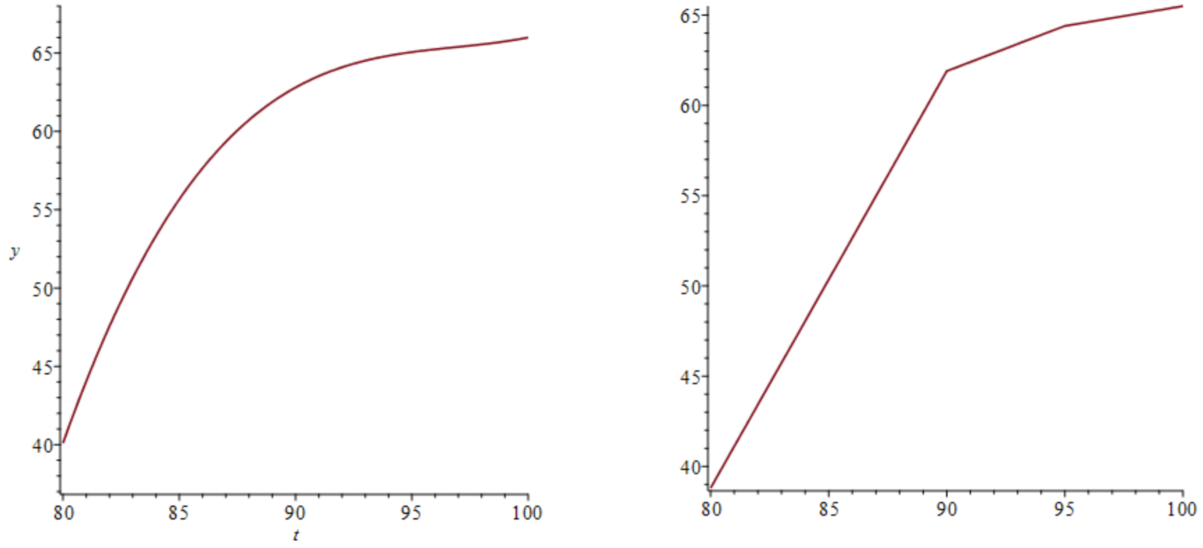
$y3 := a \cdot 95^3 + b \cdot 95^2 + c \cdot 95^1 + d; \quad y3 := 65.068375$

$y4 := a \cdot 100^3 + b \cdot 100^2 + c \cdot 100^1 + d; \quad y4 := 66.000000$

$plot(a \cdot t^3 + b \cdot t^2 + c \cdot t^1 + d; \quad t = 80..100, y = 37..68$

Figure 2. Effect of temperature at the outlet of acetylene hydroxyacid:

(a) - by experience; (b) - in mathematical modeling.



a) b)

$$plot\left(\begin{bmatrix}[80,39.7],[90,61.9a],\\ [95,64,4],[100,65.6]\end{bmatrix}\right)$$

$v_1 := 39.7;\ \ v_2 := 61.9;\ \ v_3 := 64.4;\ \ v_4 := 65.6;$

$u_1 := 7.94\ \ u_2 := 12.4;\ \ u_3 := 12.9;\ \ v_4 := 13.2;$

$t_1 := 80;\ \ t_2 := 90;\ \ t_3 := 95;\ \ t_4 := 100;$

$$K := Matrix([[sum(t[i])^2, i = 1..4), sum(t[i])^3, i = 1..4), sum\big((t[i])^2 \cdot v[i]), i = 1..4\big), sum\big((t[i] \cdot (v[i])^2), i = 1..4)\big], [sum((t[i])^3, i = 1..4), sum((t[i])^4, i = 1..4), sum((t[i])^3 \cdot v[i]), i = 1..4), sum((t[i])^2 \cdot v[i])^2), i = 1..4),\ sum(\ (t[i])^2 \cdot v[i]), i = 1..4), sum(\ (t[i])^3 \cdot v[i]), i = 1..4),\ \ sum((t[i])^2 \cdot v[i])^2), i = 1..4), sum((t[i])^1 \cdot v[i])^3), i = 1..4), sum((t[i])^1 \cdot v[i])^2), i = 1..4), sum((t[i])^2 \cdot v[i])^2), i = 1..4), sum((t[i])^1 \cdot v[i])^3), i = 1..4), sum\Big(\big((v[i])^4, i = 1..4)]\big]\Big);$$

$$K: = \begin{pmatrix} 33525 & 3098375 & 1.9869200\ 10^6 & 1.2896153010^6 \\ 3098375 & 288020625 & 1.858056500\ 10^8 & 1.211343810\ 10^8 \\ 1.9869200\ 10^6 & 1.858056500\ 10^8 & 1.211343810\ 10^8 & 7.962237515\ 10^7 \\ 1.2896153010^6 & 1.211343810\ 10^8 & 7.962237515\ 10^7 & 5.266708704\ 10^7 \end{pmatrix}$$

$$L := Matrix([[l],[m],[n],[f]]);$$

$$L := \begin{bmatrix} 0.732691129276645 \\ -0.0178480953891267 \\ 0.0428335753458668 \\ -0.0256024142145179 \end{bmatrix}$$

$$U := Matrix([[sum(u[i]\cdot t[i], i = 1\,..4], \left[sum(u[i]\cdot (t[i])^2, i = 1\,..4)\right], [sum(u[i]\cdot t[i]\cdot v[i], i = 1\,..4)], \left[sum(u[i]\cdot (v[i])^2, i = 1\,..4)\right]\right]);$$

$$U := \begin{bmatrix} 4296.70 \\ 399678.50 \\ 259240.360 \\ 169770.4536 \end{bmatrix}$$

*evalm(K^{-1}&*U);*

$$\begin{bmatrix} 0.157453224146593 \\ -0.00463584832777997 \\ 0.0119710721701267 \\ -0.00806743335942883 \end{bmatrix}$$

$$l := 0.157453224146593;\ \ m := -0.00463584832777997;$$

$$n := 0.0119710721701267;\ \ f := -0.00806743335942883;$$

$$u := l\cdot t + m\cdot t^2 + n\cdot t\cdot v + f\cdot v^2;$$

$$u := -0.00463584832777997t^2 + 0.0119710721701267tv - 0.00806743335942883v^2 + 0.157453224146593t$$

$$u := l\cdot 80 + m\cdot 80^2\cdot 39.7 + f\cdot 39.7^2;$$

$$u_1 := 7.9399977;\quad u_2 := 1\cdot 90 + m\cdot 90^2 + n\cdot 90\cdot 61.9 + f\cdot 61.9^2;$$

$$u_2 := 12.40000344;\quad u_3 := 1\cdot 95 + m\cdot 95^2 + n\cdot 95\cdot 61.9 + f\cdot 64.94^2;$$

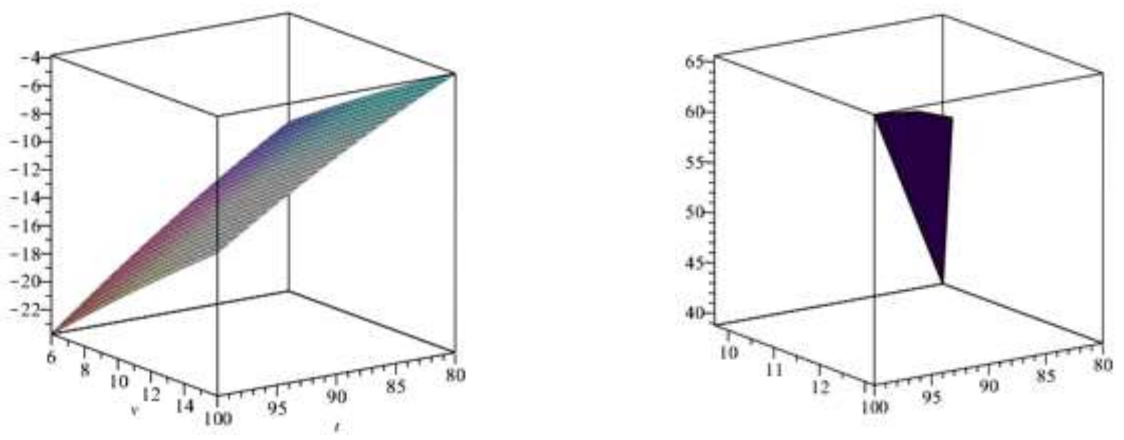
$$u_3 := 12.89999425;\quad u_4 := 1\cdot 100 + m\cdot 100^2 + n\cdot 100\cdot 65.6 + f\cdot 65.6^2;$$

$$u_4 := 13.20000255;\ plot3d(l\cdot t + m\cdot t^2 + n\cdot t\cdot v,\ t = 80\,..100, v = 6\,..16)$$

Based on the product yield and the average reaction rate, an iconogram of the results was compiled using the Maple18 program (Fig.3).

Figure 3. Ikonogram of the effect of temperature and reaction duration on the yield of acetylene hydroxyacid:

(a) - by experience; (b) - in mathematical modeling.


a) b)

```
With(plots) :
Polygonplot3d(Matrix ([[80,9.7,39,7], [90,12.4,61.9] [95,12.9,64.4],
        [100,13.2,65.6]],datatype = float),color = Indigo,axes
        = boxed)
```

The process of synthesis of acetylene hydroxyacid based on acetylene alcohol and chloroacetic acid was carried out at temperatures of 80-100 ^{O}C. In this process, the results obtained on the basis of mathematical processing with the amount of product obtained in the experiment can be viewed in the order indicated below.

Mathematical calculations were carried out taking into account the fact that during the synthesis of acetylene oxy acid, a product with relatively high yields was obtained when the reaction was carried out for 5 hours.

Taking into account these values, based on the results obtained, the dependence of the formation of acetylene hydroxyacid as a result of a chemical reaction on the temperature and duration of the reaction, the results of mathematical calculations and experiments were expressed by the following function.

$$f_1 := a_1 * 80^3 + a_2 * 80^2 + 80 * a_3 + a_4; f_1 := 40.096000$$

$$f_2 := a * 90^3 + b * 90^2 + 90 * c + d; f_2 := 62.807000$$

$$f_3 := a * 95^3 + b * 95^2 + 95 * c + d; f_3 := 65.068375$$

$$f_4 := a * 100^3 + b * 100^2 + 100 * c + d; f_4 := 66.000000$$

The functions $f = a * t^3 + b * t^2 + c * t + d$ and $\mathrm{t} = 80 \dots 100$, $\mathrm{f} = 40 \dots 68$ were studied on the basis of a graph of the formation of acetylene hydroxyacid in values and a graph of temperature dependence.

Conclusions

The calculations show that the yield of the product obtained in the experiment corresponds to the results obtained by mathematical processing by 96-98%.

$$u_1 - \mathrm{f}_1 := 40.096000 - 38.8 = 1.296; \quad 96\ \%$$

$$u_2 - \mathrm{f}_2 := 62.807000 - 61.9 = 0.907; \quad 97\ \%$$

$$u_3 - \mathrm{f}_3 := 65.068375 - 64.4 = 0{,}668; \quad 98\ \%$$

$$u_4 - \mathrm{f}_4 := 66.000000 - 65.6 = 0{,}4; \quad 98\ \%$$

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