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Mathematical Modeling of the Processes of Synthesis of Vinyl Ether of Thymols

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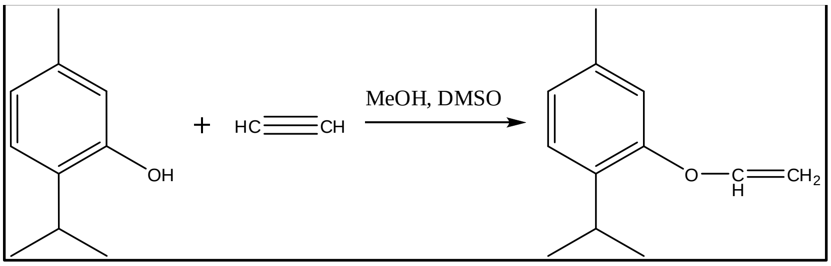
ABSTRACT: The influence of temperature in the reactions of vinylation of thymols with acetylenes, with experimental and theoretical paths, was compared. The optimum condition of the process is found.

KEY WORDS: thymol, acetylene, vinylation reaction, solvent, catalyst, vinyl ethers, highly basic system, dimethylsulfoxide (DMSO), dimethylformamide (DMF).

I. INTRODUCTION

Processes, including chemical processes, also go according to a particular rule. In-depth analysis of the essence of the process can be achieved with the help of experiments without the help of the experimental results. This requires a clear mathematical expression of the process, and the solution of this mathematical equation should correspond to the experimental results. This is called mathematical modeling in science [1].

Based on this, vinyl acetylene has been investigated with the participation of thymol in the presence of a homogeneous-catalytic high basis system (MeOH-DMCO, MeOH-DMFA) [2]. The vinyl ether of thymol is formed according to the following scheme:



there: Me – Li, Na, K.

Catalysts include Li, Na and K hydroxides. The choice of this system is caused by the fact that in the reaction of the reaction the volcanic environment is mainly required. DMSO, DMFA and other polar solvents make alkaline high-grade system, and the alkalinity of the alkali increases several times (up to 7 times) [3].

II. METHODS OF RESEARCH

At present, computer technology programs are widely used in mathematical modeling of chemical processes. We used the MathCad software for mathematical modeling of experimental processes.

The calculations were carried out on the basis of experimental-statistical modeling using linear regression method. The equation of the dependence of the regression curve was chosen and the "least squares method" was used to find the coefficient of equation [1].

By analyzing the results obtained from the vinylation process, the mathematical expression can be expressed as:

$$y = A{\cdot}t^3 + b{\cdot}t^2 + c{\cdot}t + d \quad (1)$$

Where: y - flour; t- temperature; a, b, c, d - identifying coefficients involved in the analytical relationship.

The equation is realized as follows;

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$$\begin{aligned}
&2\sum_{i=1}^{13}[y_i - at_i^3 - bt_i^2 - ct_i - d]x(-t_i^3) = 0\\
&2\sum_{i=1}^{13}[y_i - at_i^3 - bt_i^2 - ct_i - d]x(-t_i^2) = 0\\
&2\sum_{i=1}^{13}[y_i - at_i^3 - bt_i^2 - ct_i - d]x(-t_i) = 0\\
&2\sum_{i=1}^{13}[y_i - at_i^3 - bt_i^2 - ct_i - d]x(-1) = 0
\end{aligned} \quad (2)$$

The equation can be made more convenient;

$$\begin{aligned}
&\sum_{i=1}^{13} t_i^6 a + \sum_{i=1}^{13} t_i^5 b + \sum_{i=1}^{13} t_i^4 c + \sum_{i=1}^{13} t_i^3 d = \sum_{i=1}^{n} y_i t_i^3\\
&\sum_{i=1}^{13} t_i^5 a + \sum_{i=1}^{13} t_i^4 b + \sum_{i=1}^{13} t_i^3 c + \sum_{i=1}^{13} t_i^2 d = \sum_{i=1}^{n} y_i t_i^2\\
&\sum_{i=1}^{13} t_i^4 a + \sum_{i=1}^{13} t_i^3 b + \sum_{i=1}^{13} t_i^2 c + \sum_{i=1}^{13} t_i d = \sum_{i=1}^{n} y_i t_i\\
&\sum_{i=1}^{13} t_i^3 a + \sum_{i=1}^{13} t_i^2 b + \sum_{i=1}^{13} t_i c + nd = \sum_{i=1}^{13} y_i
\end{aligned} \quad (3)$$

There experiments of n performed here:

$$E(a,b,c,d) = \sum_{i=1}^{13}[y_i - at_i^3 - bt_i^2 - ct_i - d]^2 = \min \quad (4)$$

We make a special equation for E (a, b, c, d) by a, b, c, d;

$$\begin{aligned}
&\frac{\partial E(a,b,c,d)}{\partial a} = 2\sum_{i=1}^{13}[y_i - at_i^3 - bt_i^2 - ct_i - d]x(-t_i^3)\\
&\frac{\partial E(a,b,c,d)}{\partial b} = 2\sum_{i=1}^{13}[y_i - at_i^3 - bt_i^2 - ct_i - d]x(-t_i^2)\\
&\frac{\partial E(a,b,c,d)}{\partial c} = 2\sum_{i=1}^{13}[y_i - at_i^3 - bt_i^2 - ct_i - d]x(-t_i)\\
&\frac{\partial E(a,b,c,d)}{\partial d} = 2\sum_{i=1}^{13}[y_i - at_i^3 - bt_i^2 - ct_i - d]x(-1)
\end{aligned} \quad (5)$$

The function is characterized zero.

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$$\begin{cases} \frac{\partial E(a,b,c,d)}{\partial a} = 0 \\ \frac{\partial E(a,b,c,d)}{\partial b} = 0 \\ \frac{\partial E(a,b,c,d)}{\partial c} = 0 \\ \frac{\partial E(a,b,c,d)}{\partial d} = 0 \end{cases} \quad (6)$$

For convenience of calculations *i*- we bring the temperatures (t_i) corresponding to the number of experiments below;

For convenience of calculations, i - we bring the temperatures (ti) corresponding to the number of experiments below;

$$t^1{}_i = \frac{t_i}{10} \quad (7)$$

It follows from the equation (1) above;

$$y = at^3 + bt^2 + ct + d \quad (1)$$

Table-1
Temperature of the vinyl ether in Thymol
(4 hours)

Temperature, ^{0}C.	Product flavor%.
80	42,1
100	46,4
120	50,0
130	52,4
140	51,6

The temperature dependence of the unit is shown in the following figure (Fig. 1).

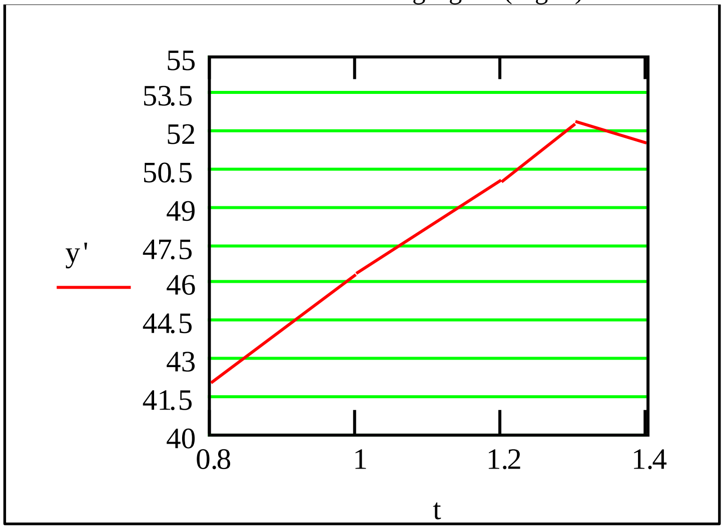

Fig.1. Temperature dependence of the product (experience).

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Process math, we write the steps in the following sequence in the MathCad workspace:

$$ORIGIN := 1 \qquad y(t) := A_1 \cdot t^3 + A_2 \cdot t^2 + A_3 \cdot t + A_4$$

Then we enter the values obtained in the experiments accordingly:

$$t := \begin{pmatrix} 8 \\ 10 \\ 12 \\ 13 \\ 14 \end{pmatrix} \qquad y := \begin{pmatrix} 42.1 \\ 46.4 \\ 50.0 \\ 52.4 \\ 51.6 \end{pmatrix}$$

Facilitate calculation, we divide temperature value by 10 :

$$t := \frac{t}{10} \qquad t = \begin{pmatrix} 0.8 \\ 1 \\ 1.2 \\ 1.3 \\ 1.4 \end{pmatrix}$$

After we will create the equation of this type in workspace:

$$u_{1,1} := \sum_{i=1}^{5} (t_i)^6 \quad u_{1,2} := \sum_{i=1}^{5} (t_i)^5 \quad u_{1,3} := \sum_{i=1}^{5} (t_i)^4 \quad u_{1,4} := \sum_{i=1}^{5} (t_i)^3$$

$$u_{2,1} := \sum_{i=1}^{5} (t_i)^5 \quad u_{2,2} := \sum_{i=1}^{5} (t_i)^4 \quad u_{2,3} := \sum_{i=1}^{5} (t_i)^3 \quad u_{2,4} := \sum_{i=1}^{5} (t_i)^2$$

$$u_{3,1} := \sum_{i=1}^{5} (t_i)^4 \quad u_{3,2} := \sum_{i=1}^{5} (t_i)^3 \quad u_{3,3} := \sum_{i=1}^{5} (t_i)^2 \quad u_{3,4} := \sum_{i=1}^{5} (t_i)^1$$

$$u_{4,1} := \sum_{i=1}^{5} (t_i)^3 \quad u_{4,2} := \sum_{i=1}^{5} (t_i)^2 \quad u_{4,3} := \sum_{i=1}^{5} (t_i)^1 \quad u_{4,4} := 5$$

$$v_1 := \sum_{i=1}^{5} y_i \cdot (t_i)^3 \quad v_2 := \sum_{i=1}^{5} y_i \cdot (t_i)^2 \quad v_3 := \sum_{i=1}^{5} y_i \cdot (t_i)^1 \quad v_4 := \sum_{i=1}^{5} y_i$$

Now the program automatically performs the calculation. To do this, use the "=" (equals) key on the keyboard and the following values:

$$v = \begin{pmatrix} 411.068 \\ 335.036 \\ 280.44 \\ 242.5 \end{pmatrix} \qquad u^T = \begin{pmatrix} 16.604 & 12.907 & 10.181 & 8.181 \\ 12.907 & 10.181 & 8.181 & 6.73 \\ 10.181 & 8.181 & 6.73 & 5.7 \\ 8.181 & 6.73 & 5.7 & 5 \end{pmatrix}$$

The values of A also include:

$$A := u^{-1} \cdot v \qquad y(t) := A_1 \cdot t^3 + A_2 \cdot t^2 + A_3 \cdot t + A_4 \qquad A = \begin{pmatrix} -71.601 \\ 218.454 \\ -198.156 \\ 97.512 \end{pmatrix}$$

The values of t_i corresponding to y_i the equations are as follows (Table 2):

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Table-2
Consumed product temperature at a suitable temperature %.

Temperature, ^{0}C	Calculated product flour%.
80	42,1
100	46,4
120	50,0
130	52,4
140	51,6

Table - 3
Results of the experiment and mathematical calculations

Temperature, 0C.	Product flour, %	
	At experience	calculated
80	42,1	42,1
100	46,4	46,4
120	50,0	50,0
130	52,4	52,4
140	51,6	51,6

The graphic looks like this (Fig.2)*:

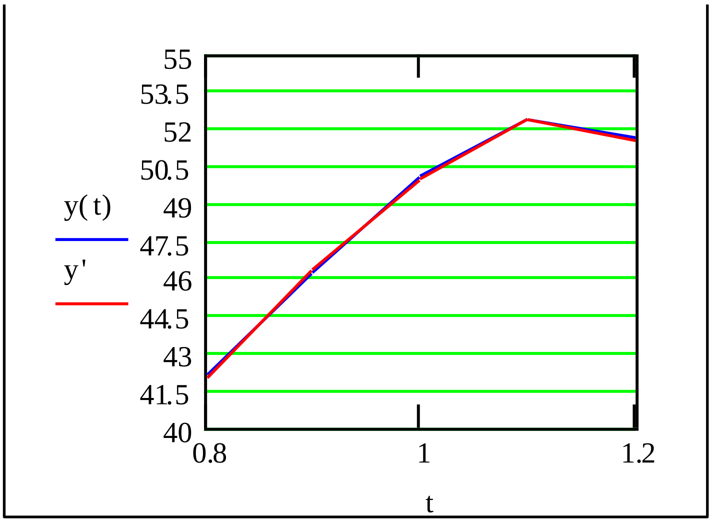

Fig. 2. Temperature dependence of the product:
red line - experiment; blue line - based on the calculation results.

III. CONCLUSION

As can be seen from the experiments and calculations, thymol and acetylene can be calculated reliably by means of mathematical modeling of the effect of the temperature on the reaction chamber in the process of ether synthesis.

Consequently, mathematical modeling allows to calculate the results even without a process.

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