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Building a Mathematical Model Synthesis of Methyl Ether 5-Acetyl-2- Pyrrolecarboxylic Acid

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Currently, mathematical modeling has become a common method of scientific knowledge and the creation of objects in many fields of science and technology. For chemical engineering simulation is the theoretical basis and method of solving the problems associated with the definition of the optimal conditions of catalytic processes and the creation of complex automation systems.

Mathematical modeling of catalytic processes allows, without resort to complicated and expensive natural experiments designed to explore the many features of the processes, use mathematical optimization techniques in order to find the optimum operating conditions. The general scheme of mathematical modeling was formulated by academician AA Samarskim [1].

Catalytic synthesis reaction of aromatic and heterocyclic compounds, such as synthesis of methyl ether 5-acetyl-2-pyrrolecarboxylic acid, possess a wide range of applications. Methyl ether 5-acetyl-2- pyrrolecarboxylic acid of great interest to obtain porphyrins and drugs. Pyrrolecarboxylic acid exhibit higher biological activity. Derivatives of 5-pyrrolecarboxylic acid possess an antiviral effect, in particular, they actively suppress classical fowl plague viruses [2] and the sodium salt of 2-aryl-5-pyrrolecarboxylic acid exhibit anticonvulsant activity [3].

The aim is the creation of physical-chemical model of synthesis of methyl 5-acetyl-2-pyrrolecarboxylic acid reacting 2-acetylpyrrolyl with carbon tetrachloride and methanol under the influence of iron catalysts and carrying out its formalization, t. E. Drawing up a mathematical model, which is a system of relations reflecting the basic conservation laws (mass, energy, momentum, etc.).

Based on the analysis of experimental data suggested the following

The mechanism of reaction formation synthesis of methyl ether 5-acetyl-2- pyrrolecarboxylic acid [4]:

1. $A_1 + A_2 \rightarrow A_3 + A_4$
2. $A_3 + A_5 \rightarrow A_6 + A_4$
3. $A_6 + A_5 \rightarrow A_7 + A_4$
4. $A_7 + A_5 \rightarrow A_8 + A_4$
5. $A_8 \rightarrow A_9 + A_{10}$

Here we have introduced the notation for the substances:

A_1 – 2-acetylpyrrole, A_2 – CCl_4 - carbon tetrachloride, A_3 – 2-acetyl-5-temarychlorinemethylpyrrol, A_4 – HCl, A_5 – Methanol, A_6 –2-acetyl-5- rhothanemethanepyrrol, A_7 – 2-acetyl-5- dimethoxymethanepyrrol, A_8 –2-acetyl-5-trimetoksimetanpirrol, A_9 – methyl ether 5-acetyl-2- pyrrolecarboxylic acid, A_{10} – CH_3OCH_3.

Matrix composition stoichiometric ratios of the chemical reaction. The matrix has the form:

$$\nu = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 0 & -1 & -1 & -1 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

where the i-th row corresponds to a substance, j-th column corresponds to the number of reaction. Speed of the j-th reaction is determined by the formula:

$$r = k^{+}\prod_{i=1}^{N_A} C_{A_i}^{\alpha_i} - k^{-}\prod_{i=1}^{N_B} C_{B_i}^{\beta_i}, \quad (1)$$

wherein N_A, N_B - the number of starting materials and reaction products, respectively, α_i and β_i - elements of stoichiometric ratios, ν, k^+ and k^- - a constant speed.[5] Then, in accordance with (1) reaction of synthesis of methyl ether 5-acetyl-2- pyrrolecarboxylic acid speed stages are (here and below refers to the C_i - concentration of the reactants A_i):

$r_1 = k_1 C_1 C_2$,
$r_2 = k_2 C_3 C_5$,
$r_3 = k_3 C_5 C_6$,
$r_4 = k_4 C_5 C_7$,
$r_5 = k_5 C_8$.

The rate constant of the reaction of i-th calculated through the selected reference temperature $T_r = 23^0 \tilde{N}$ ($T_r = 296\hat{E}$) by the formula:

$$K_i(T) = K_i(T_r)\exp\left(\frac{E_i}{RT_{\tilde{n}}}\left(1-\frac{T_r}{T}\right)\right),$$

where R- universal gas constant, R = 8,31 $\frac{J}{mol \cdot \hat{E}}$, Ej -activation energy of j-th reaction.

According to the law of mass action [6] the overall material balance $C = \sum_{i=1}^{m} C_i$ in the case where the total concentration varies over time, is:

$$\frac{dC_i}{dt} = \frac{d(Cx_i)}{dt} = \sum_{j=1}^{n} \nu_{ij} r_j, \ i = \overline{1,m} \quad (2)$$

with the initial conditions:

$$x_i(0) = x_i^0, \ x_i(0) = x_i^0. \quad (3)$$

In accordance with (2) and (3) we obtain the system of differential equations which a mathematical model synthesis of methyl ether 5-acetyl-2- pyrrolecarboxylic acid:

$$\begin{cases}
\frac{dC_1}{dt} = -k_1 C_1 C_2 \\
\frac{dC_2}{dt} = -k_1 C_1 C_2 \\
\frac{dC_3}{dt} = k_1 C_1 C_2 - k_2 C_3 C_5 \\
\frac{dC_4}{dt} = k_1 C_1 C_2 + k_2 C_3 C_5 + k_3 C_5 C_6 + k_4 C_5 C_7 \\
\frac{dC_5}{dt} = -k_3 C_5 C_6 - k_4 C_5 C_7 \\
\frac{dC_6}{dt} = k_2 C_3 C_5 - k_1 C_1 C_2 \\
\frac{dC_7}{dt} = k_3 C_5 C_6 - k_4 C_5 C_7 \\
\frac{dC_8}{dt} = k_4 C_5 C_7 - k_5 C_8 \\
\frac{dC_9}{dt} = k_5 C_8 \\
\frac{dC_{10}}{dt} = k_5 C_8
\end{cases}$$

With the initial conditions(3).

Since this system of differential equations containing 10 equations it is difficult to solve analytically. The solution is obtained approximately by numerical methods. Has been chosen classical Runge–Kutta method. The Runge–Kutta methods are an important family of implicit and explicit iterative methods, which are used in temporal discretization for the approximation of solutions of ordinary differential equations. These techniques were developed around 1900 by the German mathematicians C. Runge and M. W. Kutta.[7]

Building a mathematical model synthesis of methyl ether 5-acetyl-2- pyrrolecarboxylic acid provides information about the dynamics of the formation of substances and on the degree of influence of each substance in the course of the reaction.

Of reaction mechanism, it follows that first enters the reaction a substance

A_1 – 2-acetylpyrrole, A_2 – CCl_4 - carbon tetrachloride.

According to the results of numerical simulation we can talk about the good yield of the desired product.

Literature

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