METHODOLOGY OF MATHEMATICAL PROCESSING OF THE RESULTS OF THE SYNTHESIS OF ACETYLENE ALCOHOL AND ITS DERIVATIVES.

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Abstract: *In this work, the temperature dependence of the yield of vinyl esters formed during the heterogeneous catalytic vinylation of acetylene alcohol was analyzed based on mathematical modeling. The experimental results were processed using the MARLE-2018 program, and a third-order regression model was constructed based on the least squares method. The calculations were carried out in the temperature range of 380–440 °C, and the agreement between the model and the experimental results showed an accuracy of 88–92%.*

Keywords: *acetylene alcohol, vinyl ether, heterogeneous catalysis, mathematical modeling, regression, MARLE-2018.*

INTRODUCTION

In the chemical industry, increasing efficiency, reducing energy consumption and obtaining high-yield products are currently one of the urgent scientific and technical tasks. In particular, in-depth study of catalytic processes in the synthesis of organic compounds and their optimization based on mathematical modeling have become an important direction of modern chemical technology. Along with experimental study of the kinetics of chemical reactions, the possibility of determining and predicting process laws through mathematical processing of the obtained results is expanding. This serves to increase the accuracy and reliability of scientific research.[1]

Acetylene alcohol and its derivatives play an important role in industrial and applied chemistry. They have highly reactive functional groups and are used as intermediates in the synthesis of various vinyl ethers, polymers, biologically active substances and special chemical reagents. In particular, the process of obtaining vinyl ethers by heterogeneous catalytic vinylation of acetylene alcohol is technologically significant. In this process, temperature, reaction time, and catalyst properties have a significant impact on product yield.[2,3]

Determining the optimal conditions in chemical processes often requires conducting a large number of experiments. However, the use of modern computer technologies and mathematical modeling methods allows reducing the number of experiments, accurately estimating process parameters, and determining the conditions that provide maximum yield. Mathematical methods such as the least squares method, regression analysis, and matrix methods are widely used in processing experimental results. With the help of these approaches, empirical equations of chemical processes are constructed and it is possible to predict the future behavior of the process.[4,5]

In this work, the temperature dependence of the yield of vinyl esters formed during the heterogeneous catalytic vinylization of acetylene alcohol was mathematically analyzed. The experimental results were processed using the MARLE-2018 program, and an empirical equation was generated based on a third-order regression model. The optimal temperature range of the process was determined by mathematical modeling, and the degree of agreement between the model and experimental results was assessed.

The main goal of the study is to mathematically model the dependence of the product yield on temperature in the vinylization process of acetylene alcohol, determine the accuracy of the resulting model, and demonstrate the possibilities of optimizing the process. This approach is of significant scientific and practical importance in industrial processes, energy efficiency, and the selection of high-performance production modes.

Experimental results. The vinylization process was carried out at temperatures of 380–440 °C for 4 hours.

Table 1.1

Temperature dependence of the yield of acetylene alcohol vinyl ether.

Temperature (°C)	Reaction duration (hours)	Yield (%)	%/hour
380	4	31.6	7.9
400	4	33.4	8.35
420	4	37.2	9.3
440	4	36.8	9.2

The results show that with increasing temperature, the product yield increases up to 420 °C, and then a slight decrease is observed. This indicates that there is an optimal temperature range for the process.

Mathematical model.

The dependence of the yield on temperature was expressed using a cubic polynomial of the following form:

$$f(\mathrm{t}) = a_1 + a_2 t + a_3 t^2 + a_4 t^3$$

The following functional was minimized using the least squares method:

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

A system of linear equations was constructed using the matrix method and solved in the form A·C = B. The following coefficients were obtained as a result of the calculation:

$$a_1 = -0.00014297$$
$$a_2 = 0.15869$$
$$a_3 = -58.51$$
$$a_4 = 7188$$

Thus, the temperature dependence of vinyl ether yield is expressed by the following empirical equation:

$$f(t) = at^3 + bt^2 + ct + d$$

Table 2. Comparison of model and experimental results.

Calculated values:

Temperature (°C)	Experience (%)	Model (%)	Difference	Accuracy
380	21.8	19.29	2.51	88 %
400	23.6	21.69	1.92	91 %
420	27.1	24.92	2.18	91 %
440	26.9	24.85	2.05	92 %

The results show a high agreement between the model and the experiment. The average accuracy is about 90%.

Graphical analysis. The graph of the dependence of the vinyl ether yield on temperature has a cubic character, with a maximum value observed in the range of 410–425 °C. This is explained by the kinetics of the process and the optimal operating temperature of the catalyst active centers.

Conclusion

As a result of the research, the basic principles of the heterogeneous catalytic vinylation of acetylene alcohol were analyzed in depth based on mathematical modeling. By processing the experimental results using the MARLE-2018 program, the dependence of the vinyl ether yield on temperature was determined, and a third-order regression model was constructed. It was proven that the empirical equation determined based on the least squares method expresses the experimental results with high accuracy.

The analysis results showed that the vinyl ether yield is variable in the temperature range of 380–440 °C, with a maximum value observed around 410–425 °C. The fact that the product yield reaches its highest value at 420 °C confirms the existence of an optimal temperature range for the process. Further increase in temperature leads to a slight decrease in yield, which is explained by possible side reactions, partial deactivation of the catalyst active centers, or thermodynamic factors.

The difference between the mathematical model and the experimental results was about 2%, and the average accuracy was 88–92%. This indicates that the constructed regression model adequately describes the process. It was found that using the obtained empirical equation, it is possible to predict the product yield, determine the optimal temperature, and plan future experiments.

This study shows that mathematical modeling of chemical processes and processing using computer programs are important for a deeper analysis of experimental data, optimization of process parameters, and increasing technological efficiency. This approach allows for scientific control of industrial-scale production processes, reducing energy and raw material consumption, and maintaining stable product quality.

Also, based on the developed model, multifactor modeling can be carried out in the future, including additional parameters such as pressure, catalyst composition, and reaction duration. This will serve to further optimize the vinylization process of acetylene alcohol. In general, the results obtained serve as an important scientific basis for the theoretical and practical substantiation of the heterogeneous catalytic vinylation process of acetylene alcohol, its application on an industrial scale, and the selection of highly efficient technological regimes.

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