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MATHEMATICAL MODELING OF DEVELOPED COMPOSITE POLYMER STABILIZERS

Abstract

This paper examines current mathematical modeling methods used for the development and optimization of composite polymer stabilizers. A review of key challenges related to the stability of polymer materials is provided, along with a discussion of modern computational approaches, including molecular dynamics, finite element analysis, thermodynamic modeling, and machine learning. The necessity of an interdisciplinary approach integrating chemistry, materials science, and computational technologies is justified. Perspectives on the further development of modeling methods to enhance the efficiency and stability of polymer stabilizers are presented.

Keywords: mathematical modeling, polymer stabilizers, molecular dynamics, machine learning, thermodynamic modeling.

Introduction. Mathematical modeling of drilling fluids is an effective method of scientific analysis and forecasting that allows their behavior to be studied and described in complex thermobaric conditions and under the influence of mineralized formation waters. The use of mathematical models makes it possible to calculate rheological and filtration parameters in advance, which contributes to a more informed selection of the fluid composition and reduces the amount of costly experimental research. Modeling is especially relevant in the development and application of new polymer stabilizers, as it allows for the evaluation of their effectiveness, the determination of optimal concentrations and conditions of use, and the identification of the limits of reagent performance in real drilling conditions. Thus, mathematical modeling serves not only as a tool for optimizing technological processes and improving the safety of drilling operations, but also as a theoretical basis for improving the chemical and technological systems of drilling fluids based on modified polymers [1-3].

The development of industries such as oil and gas, water treatment, and biomedicine requires the improvement of polymer materials with high stability and operational reliability. Composite polymer stabilizers help extend equipment lifespan, enhance process efficiency, and minimize environmental risks. One of the key methods for their development is mathematical modeling, which enables accurate prediction of material properties and optimization of their composition.

The aim of this study is to analyze modern approaches to mathematical modeling of polymer stabilizers and discuss their potential applications in predicting the thermal, chemical, and mechanical stability of materials.

Materials and methods. Regression analysis was performed to assess the relationship between the parameters under study. For this purpose, a design matrix was compiled, which made it possible to systematically analyze the influence of individual factors and their interactions. An important statistical indicator of this analysis is the coefficient of determination (R^2), which reflects the proportion of variance explained by the model and, therefore, the adequacy of the regression equation obtained. The methods and research presented were carried out as part of the Bolashak program at Constructor University.

Results and discussion. Mathematical processing of the experimental data consisted in constructing the answer in the form of z = f(x1, x2, x3). The investigated parameter z was the changes in physico-chemical properties during the copolymerization of acrylonitrile and vinylsulfonic acids, their hydrolysis and further modification [4-6].

Analyzing the data obtained during hydrolysis and modification of the copolymer using gossypol resin and fatty acids, graphs were constructed for comparison with trend dependence, and a regression ratio was determined for each factor. (Fig. 1, 2).

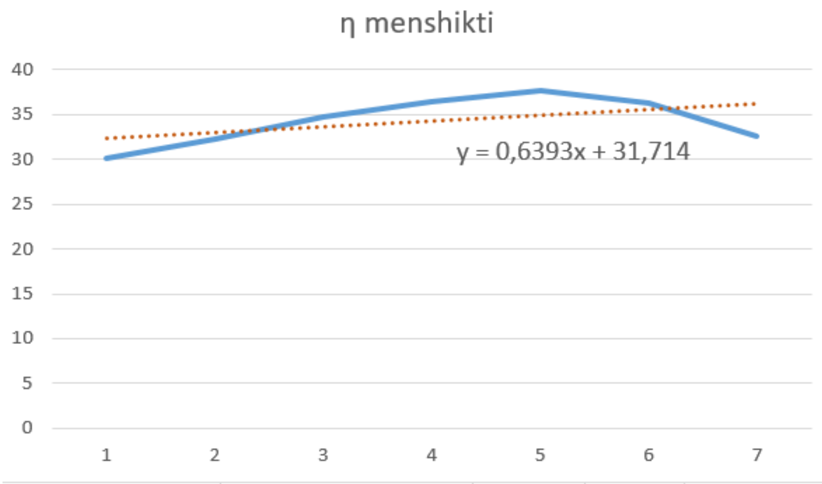

Fig. 1– Diagram for the eigenvalue factor η

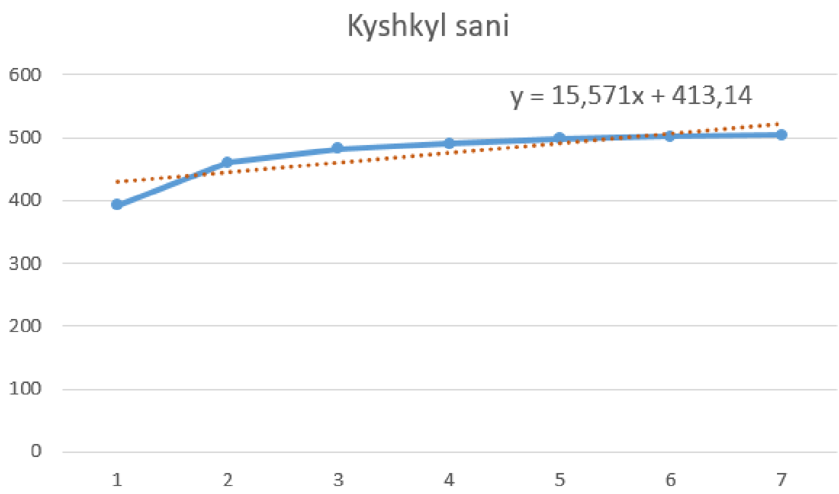

Fig. 2 – Diagram for acid number factor

Analysis was carried out according to the copolymerization data of acrylonitrile and vinylsulfonic acid (Fig. 3).

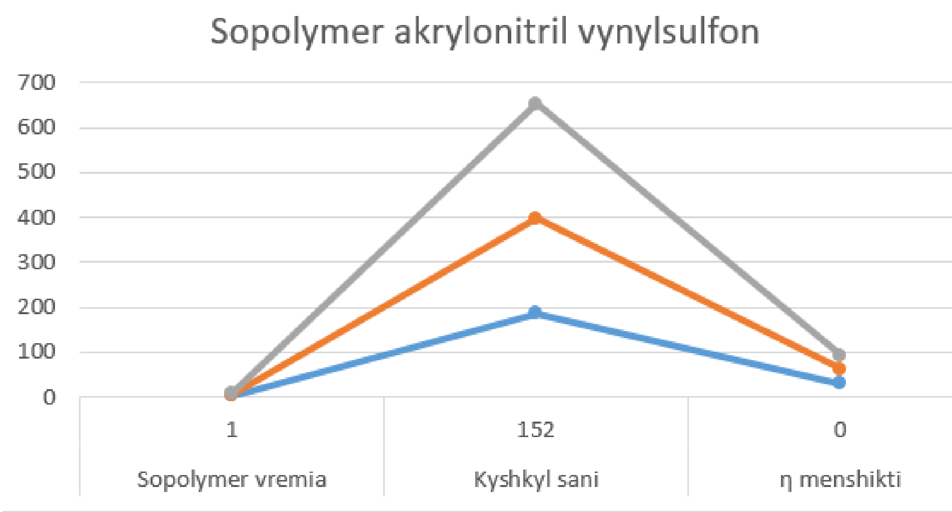

Fig. 3 – Acrylonitrile and vinylsulfonic acid copolymerization details

Regression analysis was performed according to the copolymerization data of acrylonitrile and vinylsulfonic acid (Table 1).

Table 1 – Regression analysis according to the copolymerization data of acrylonitrile and vinylsulfonic acid

	a11	a12	a13
a11	1		
a12	0,9956703	1	1
a13	0,7829549	0,758626294	

The design matrix is a statistical analysis tool that allows determining the degree of dependency between variables, evaluating their interrelationships, and using the obtained data for forecasting or decision-making. Each cell in the table shows the dependency between two specific variables.

The design matrix helps identify how changes in one variable can affect another, and based on this, make predictions, optimize processes, and make informed decisions.

The calculated coefficients of the design matrix indicate the strength of the relationship between the factors. The larger the absolute value of the coefficients, the closer the corresponding factor is to the result. The analysis of the matrix consists of two stages:

1. If there are elements in the first column of the calculated design matrix where $|r^{xy}| < 0.5$, the factors that meet this condition are removed from the model.
2. When considering the correlation of the calculated coefficients of the factors in the design matrix, it is necessary to assess their independence from each other. This is a required condition for regression analysis.

According to our calculations, the values of all parameters are at an adequate level, as shown in Table 2.

Table 2 – Regression Statistics

Multiple R	0,758626294
R-squared	0,575513853
Adjusted R-squared	0,36327078
Standard Error	34,76366004
Observations	4

Another important indicator is R-squared, also known as the coefficient of determination. It represents the proportion of the variance in the response variable that can be explained by the predictor variable.

The value of R-squared can range from 0 to 1. A value of 0 indicates that the response variable cannot be explained at all by the predictor variable. A value of 1 indicates that the response variable can be fully explained without error by the predictor variable.

One of the important indicators is the value located at the intersection of the "Y-intercept" row and the "coefficients" column. Here, the value of the "Y-intercept" is crucial. According to the calculations, this value is 151.43 (Table 3).

Table 3 – Coefficients

	Coefficients
Y-intercept	151,4289433
Variable X1	2,157608561

Additionally, the value at the intersection of the "Variable X1" row and the "Coefficients" column shows the level of dependency between Y and X. The coefficient of 2.158, obtained from the calculations, is considered a very high indicator of effect.

The calculations were performed using the "least squares method." The least squares method is a statistical procedure used to predict the behavior of dependent variables accurately. The essence of the least squares method is to find the closest approximation to reality among all linear functions. This can be done by searching for the function with the smallest deviation, or more precisely, by finding the minimal sum of squared deviations of the Y values from the regression equation obtained during the process.

The regression equation is written as follows:

$$Y=2.158x+151{,}429 \tag{1}$$

MatLab is a popular tool used for working with matrix data, virtualization, and mathematics. The MATLAB language is high-level and is used for modeling mechanical and chemical-technological processes. It includes an application package as well as an integrated development environment (IDE). MATLAB allows for efficient numerical computation, data visualization, and algorithm development, making it widely used in various fields such as engineering, science, and economics.

The regression equation results were obtained by solving through the values of the factors using programming code in the MatLab programming environment.

MatLab provides commands and functions for creating three-dimensional graphs. The values of elements in a numerical array are considered as points on a plane defined by the X and Y coordinates, with the Z coordinates representing the height above the plane. These functions and commands perform operations like connecting points in a cross-section (using the plot3 function) and creating mesh surfaces (using the mesh and surf functions). The surface drawn with the mesh function is a mesh surface, where its cells have a background color, and their boundaries can have a color defined by the EdgeColor property of the surface graphical object.

To graphically display the results of the regression equation, we use the functions of the MatLab programming environment. Using the mesh function, the following type of plot was obtained (Figures 4, 5, 6).

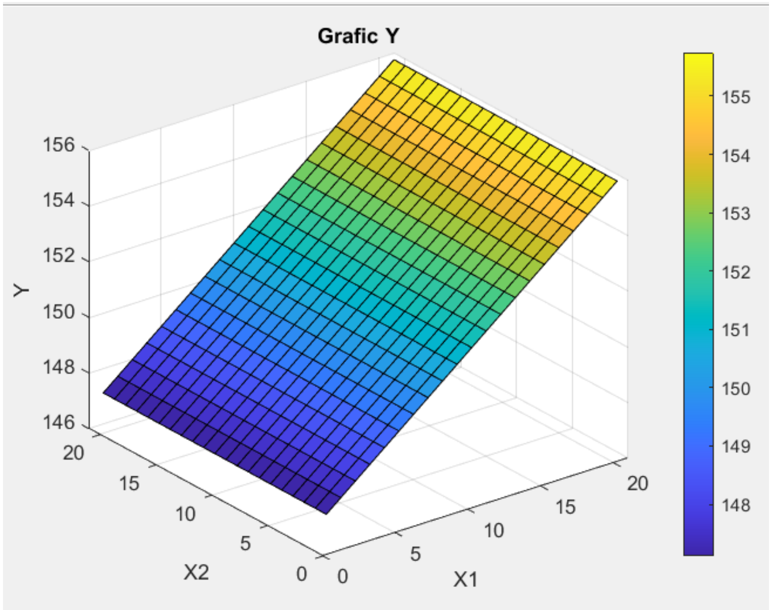

Fig. 4 – Results of the regression equation using the surf function

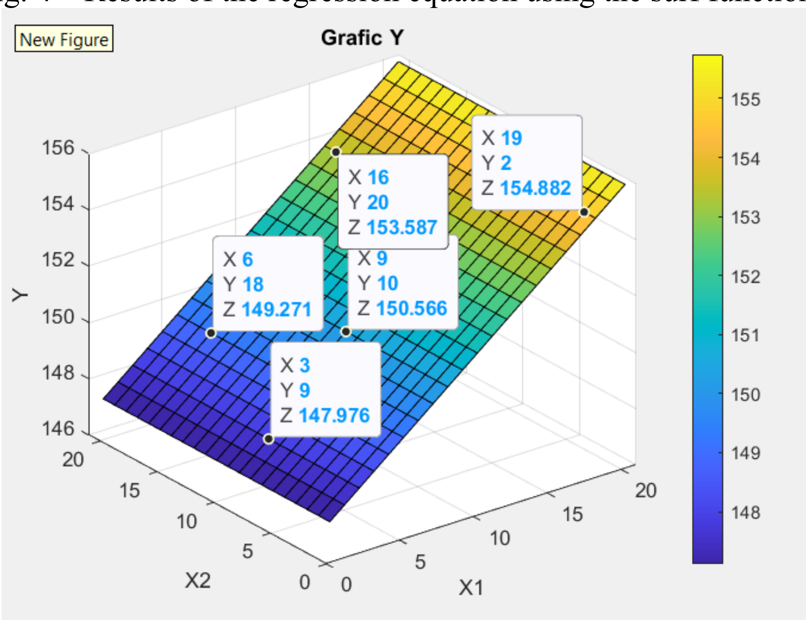

Fig. 5 – Results of the regression equation with the coordinates of the given point

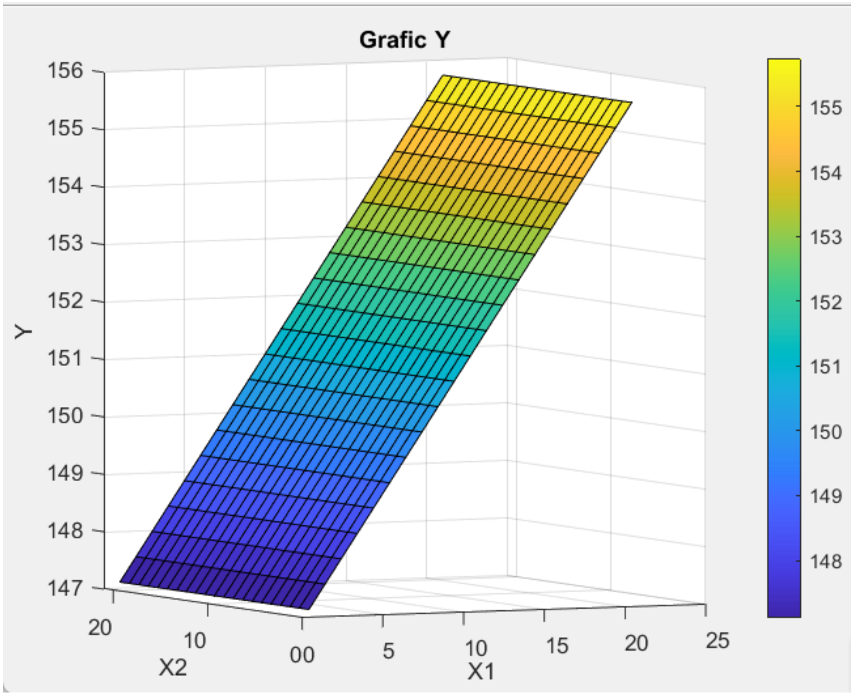

Fig. 6 – Visualization of the calculation results with step reduction

The residual values in the calculations are very small and satisfy all given conditions. We determine the standard errors, i.e., we calculate the deviations of the observed values from the regression line. These calculated values also satisfy the conditions [7-9].

During the data analysis, we calculate the following parameters:

df – degrees of freedom of the regression, which is equal to the number of regression coefficients.

$$df = \frac{\left(s_1^2/n_1 + s_2^2/n_2\right)^2}{\left(s_1^2/n_1\right)^2/(n_1-1) + \left(s_2^2/n_2\right)^2/(n_2-1)} \quad (2)$$

SS_l – the sum of the squared residuals is calculated using the following formula:

$$SS_l = \sum_{i=1}^{a}\sum_{j=1}^{n}(X_{ij} - \bar{X}_l)^2 = \sum_{i=1}^{a}(n_i - 1)s_i^2 = (n_1 - 1)s_1^2 + \dots + (n_i - 1)s_i^2 \quad (3)$$

MS_a – the mean squared residuals (also known as the mean squared error, MSE) are calculated using the following formulas:

$$MS_a = \frac{SS_a}{a-1} \quad (4)$$

$$MS_l = \frac{SS_l}{a-1} \quad (5)$$

The F-statistic is calculated as the ratio of the Mean Square of the regression (MS_regression) to the Mean Square of the residuals (MS_residual). This statistic shows how well the regression model fits the data compared to a model without independent variables. Essentially, it tests whether the regression model is generally useful.

The formula for the F-statistic is:

$$F = \frac{MS_a}{MS_l} \tag{6}$$

The calculation results are as follows (Table 4):

Table 4 – Calculation Results

	df	*SS*	*MS*	*F*	*F*
Regression	1	3276,075882	3276,975882	2,71157897	0,241373706
Residual	2	2417,024118	1208,512059		
Total	3	5694			

Each individual coefficient is interpreted as the average increase in the response variable for each unit increase of the corresponding predictor variable, assuming all other predictor variables remain constant. The accuracy of the regression analysis is checked according to Student's criteria.

Student's t-test is used to determine the statistical significance of the differences between means. To calculate this criterion, the mean value of the parameter from the first group is subtracted from the mean value of the parameter from the second group, and the result is divided by the sum of the squared errors. The latter is necessary to scale the t-criterion to the required measure.

Conditions for using the t-statistic:

– The data must be numerical;
– The data should follow a normal distribution;
– The Student's t-test can only be used to test the hypothesis of the difference between the means of two groups (if we are comparing multiple groups, then in most cases, we use analysis of variance (ANOVA));
– The variances of the two samples we are comparing should be approximately equal.

The data in the t-statistics column of the table represent the values of Student's t-test and are calculated using the following formula:

$$t = \frac{X_1 - X_2}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}} \tag{7}$$

Table 5 – Regression Analysis

	Coefficients	Standard Error	t- statistic	p-Value
Y Intercept	151,4289433	34,76131416	4,356249095	0,048865385
Variable X1	2,157608561	1,310272205	1,646687271	0,241373706

The calculated values of the t-criterion in the table are analyzed. For each group, the number of given pre-studied factors is taken into account. The value of the degrees of freedom f is determined using the following formula:

$$f = (n_1 + n_2) - 2 \tag{8}$$

After all the calculations, we concluded that the t-criterion's required significance level is appropriate. The calculated t-statistic is sufficiently large, exceeding the critical value. This allows us to conclude that the observed differences are statistically significant (significance level p<0.05) [10-12].

Conclusion. Mathematical modeling is a powerful tool for developing new polymer stabilizers, allowing their properties to be predicted and their composition to be optimized without the need for extensive experimental testing. Modern computational approaches, such as molecular dynamics, finite element analysis, and machine learning, open up new opportunities for creating materials with improved characteristics. Further development of hybrid models and interdisciplinary approaches will significantly increase the efficiency of polymer composition design. The calculated values of the t-criterion were analyzed, and after all calculations, we concluded that the required level of significance of the t-criterion meets the requirements. Statistics show how well the regression model fits the data compared to a model without independent variables.

References

1. Mahto V., Sharma V. Rheological study of a water based oil well drilling fluid // J. Pet. Sci. Eng. (2004) 123-128.
2. Rongxuan Hou; Patrick Matthew T. Chua; Kevin Cosing Tanet al. Trends in The Ongoing Research Regarding The Role of Xanthan Gum in Sustainable Geotechnical Engineering. Publication info Proceedings of International Exchange and Innovation Conference on Engineering & Sciences (IEICES). 11 (2024) 276 – 281.
3. Artykova, Zhadyra, Beisenbayev, Oral, Issa, Aziza and Kydyraliyeva, Aigul, Modification of polymers to synthesize thermo-salt-resistant stabilizers of drilling fluids. Open Engineering. 15(1) (2025) 20240097.
4. Artykova Zh.K., Beisenbayev O.K., Issa A.K., Kydyraliyeva A.Sh., Yegemberdieva S., The effect of polymer properties on the rheological behavior of Darbaza clay-Based Suspensions. A comparative experimental study on molecular weight, composition, and concentration effects. Engineering, Technology & Applied Science Research. 15(6) (2025) 29641-29646.
5. Alicia Lee Jia Wong; Anthony Nyangson Steven; Shamila Azmanet al. Effects of nutrients and photoperiod on production of polyhydroxyalkanoates (PHAs) by thermophilic cyanobacteria. Publication info Proceedings of International Exchange and Innovation Conference on Engineering & Sciences (IEICES). 11 (2023) 933 – 938.
6. Hamed S.B., Belhadri M. Rheological properties of biopolymers drilling fluids // J. Pet. Sci. Eng. (2009) 84-90.
7. Liu T., Leusheva E., Morenov V. et al. Influence of Polymer Reagents in the Drilling Fluids on the Efficiency of Deviated and Horizontal Wells Drilling // Energies. (2020) 4704-1-4704-16
8. Moradi S.S.T., Nikolaev N., Chudinova I. Geomechanical Analysis of Wellbore Stability in High-pressure, High-temperature Formations // In Proceed. of the Eage conf.& Exhibition.- Paris (2017) 1-3.
9. Myslyuk, M.A. On the interpretation of drilling fluids rotational viscometry data //Procced. Neft. Khozyaystvo Oil Ind. - Ivano-Frankivsk (2018) 50-53.
10. Adewale J., Lucky A.P., Abioye P. et al. Selecting the most appropriate model for rheological characterization of syntheticbased drilling mud // IJAER (2017) 7614-7629.
11. Dvoynikov M.V., Kuchin V.N., Mintzaev M.S. Development of viscoelastic systems and technologies for isolating water-bearing horizons with abnormal formation pressures during oil and gas wells drilling // J. Min. Inst. (2021) 57-65.
12. Reference to a chapter in an edited book:
13. Yu. Lazarev, Modeling Processes and Systems in MATLAB: Textbook, St. Petersburg, 2005, pp. 490–512.
14. A.M. Gumerov, Mathematical Modeling of Chemical and Technological Processes: Textbook. 2nd edition, revised. St. Petersburg: Lan, 2014, pp. 160-176.

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ӘЗІРЛЕНГЕН КОМПОЗИТТІК ПОЛИМЕРЛІ ТҰРАҚТАНДЫРҒЫШТАРДЫ МАТЕМАТИКАЛЫҚ МОДЕЛЬДЕУ

Түйін
Бұл жұмыста композиттік полимерлі тұрақтандырғыштарды жасау және оңтайландыру үшін қолданылатын математикалық модельдеудің қазіргі әдістері қарастырылған. Полимерлі материалдардың тұрақтылығына қатысты негізгі мәселелерге шолу, сонымен қатар молекулалық динамика, ақырлы элементтерді талдау, термодинамикалық модельдеу және машиналық оқытуды қоса алғанда, заманауи есептеу тәсілдерін талқылау қарастырылған. Химия, материалтану және есептеу технологияларын біріктіретін пәнаралық тәсілдің қажеттілігі негізделген. Полимерлі тұрақтандырғыштардың тиімділігі мен тұрақтылығын арттыру үшін модельдеу әдістерін одан әрі дамыту перспективалары ұсынылған.

Кілттік сөздер: математикалық модельдеу, полимерлі тұрақтандырғыштар, молекулалық динамика, машиналық оқыту, термодинамикалық модельдеу.

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МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ РАЗРАБОТАННЫХ КОМПОЗИТНЫХ ПОЛИМЕРНЫХ СТАБИЛИЗАТОРОВ

Аннотация
В данной статье рассматриваются современные методы математического моделирования, используемые для разработки и оптимизации композитных полимерных стабилизаторов. Дается обзор ключевых проблем, связанных со стабильностью полимерных материалов, а также обсуждаются современные вычислительные подходы, включая молекулярную динамику, конечно-элементный анализ, термодинамическое моделирование и машинное обучение. Обоснована необходимость междисциплинарного подхода, объединяющего химию, материаловедение и вычислительные технологии. Представлены перспективы дальнейшего развития методов моделирования для повышения эффективности и стабильности полимерных стабилизаторов.

Ключевые слова: математическое моделирование, полимерные стабилизаторы, молекулярная динамика, машинное обучение, термодинамическое моделирование.