

Quadratic modeling of Al_2O_3 content during hydrochloric acid activation of Navbahor bentonite

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ABSTRACT

The present paper is concerned with mathematical modeling of the change in the Al_2O_3 content in the process of the acid activation of bentonite clay using hydrochloric acid (HCl). The objective of the research was to investigate the effect of the HCl concentration on the Al_2O_3 content in the bentonite and create a mathematical model that describes the relationship between these variables. To do this, bentonite samples were activated with HCl solutions of concentrations 5, 10, 15, and 20%. The acquired data were subjected to analysis by using the quadratic polynomial regression model based on the method of least squares in OriginPro 2026. The adequacy of the model was estimated using the coefficient of determination (R^2), the root means square error (RMSE), and the mean absolute error (MAE). The constructed model showed a very good fit to the experimental data ($R^2 = 0.9646$, RMSE = 0.2001, and MAE = 0.1790), but the relative error between calculated and experimental values varied from 0.73% to 2.60%. Thus, the results have shown that the suggested model could be successfully applied for the preliminary assessment of Al_2O_3 content at an intermediate concentration of HCl in the range of 5-20% and for the technological calculations. The suggested quadratic polynomial regression model is a valuable mathematical tool for the optimization of the acid activation process of bentonite, for the quantitative evaluation of the changes in Al_2O_3 content, and for the indirect assessment of the sorption properties of the clay.

Keywords: bentonite, hydrochloric acid, aluminum oxide, adsorption, mathematical modeling, quadratic regression model.

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Introduction

The research devoted to the development of methods of sorbent synthesis is progressing very fast within the framework of chemistry and food industry. It is especially worth mentioning that nowadays the issue of the utilization of the modified sorbents with high ion exchange capacity and developed porosity for separation of coloring matters along with other contaminants from food products and for processing of industrial wastewaters becomes one of the major lines of research [[1], [2], [3], [4]].

Also, the materials based on bentonite have great practical value in different areas such as construction, pharmaceutical, cosmetic and agricultural industries.

The vegetable oils consist of phospholipids, free fatty acids, chlorophylls, carotenoids and other accompanying components which need to be extracted during the refining process. The activated bentonite clays belong to the most efficient adsorbents for extraction of these impurities. However, the effectiveness of this process depends on the mineral composition, physicochemical properties and methods of the activated bentonite [[5], [6], [7], [8], [9], [10], [11], [12]].

Bentonite is a naturally occurring aluminosilicate clay that results from the diagenetic and hydrothermal modification of volcanic ash with the predominant mineral constituent being montmorillonite. Layered structure, ion-exchange capability, and the ability to absorb water of montmorillonite are the features of this mineral that make bentonite applicable in many areas of industry such as oil and gas, food, chemical, and environment.

Montmorillonite belongs to the 2:1 layered structure silicate minerals and is a member of the smectite group, which crystal structure contains two tetrahedral layers and one octahedral layer. Isomorphic replacements of the elements in the tetrahedral and octahedral layers result in the creation of permanent negative charges in the mineral crystal lattice. These charges are balanced by exchangeable interlayer cations (Na^+ , Ca^{2+} , and Mg^{2+}).

Interchange ability and hydration power of interlayer cations are main structural factors that control the cation exchange capacity, swelling, dispersion, and adsorption ability of montmorillonite. The abovementioned properties

have a great significance for determination of structural changes and sorption ability of bentonite in the course of acid activation treatment.

Thus, technological and sorption properties of bentonite and effectiveness of its acid activation are connected with the structure of bentonite [[13], [14], [15]].

In recent years, the broadening range of bentonite uses in different industrial areas has increased significantly the economical role of bentonite in the world market. According to statistics, in 2022, the global bentonite market size amounted to USD 7.45 billion, while over 20% of bentonite production in 2021 was used for drilling oil and gas wells [[16], [17], [18]]. Such numbers prove the high importance of bentonite as a universal industrial raw material due to the high adsorption ability and cation exchange capacity of bentonite. Thus, the scientific task of improving the physico-chemical and sorption properties of bentonite by its modification and acid activation is quite topical.

Although it has numerous applications, the natural bentonite has a fairly low specific surface area and low reactivity, limiting the adsorption and catalytic capabilities of the material to some extent. For this reason, several types of treatment, such as thermal, mechanical, organic, and acid treatment, are used to enhance the properties of bentonite.

The acid treatment stands out because of its high efficiency, technological simplicity, and economic rationality. The application of HCl or H_2SO_4 leads to the structural reorganization of montmorillonite, increasing the specific surface area, porosity, number of acidic active centers, and adsorptive and catalytic properties of the mineral [19].

In the course of the acid activation process, a number of physical and chemical processes take place due to the dissolution of cations in the layered structure of montmorillonite. The degree of such reactions is an important parameter that influences the characteristics of adsorption and catalytic capacity of bentonite.

The main effect on the acid-treated montmorillonite is caused by the partial dissolution of Al^{3+} , Fe^{3+} , and Mg^{2+} cations in the octahedral layer. Due to the removal of metals and aluminums, new pores are created in the clay, and the specific surface area, as well as the volume of micropores and mesopores increases.

The more aggressive the acidity and processing conditions are, the more active these transformations will be. But the presence of

excessively high concentration levels of acid along with extreme conditions of activation can cause considerable structural changes in montmorillonite clay. In this case, it is of particular scientific and practical interest to quantify structural transformations and identify the laws of their course during the activation process [[20], [21], [22], [23]].

It should be noted that during acid activation, not only the mineralogical but also the chemical composition of bentonite experiences significant alteration. Namely, the rise in the SiO_2 content and the drop in the Al_2O_3 , Fe_2O_3 , MgO , and CaO contents are due to the selective dissolution of the Al^{3+} , Fe^{3+} , and Mg^{2+} ions from the octahedral sheet of montmorillonite. In this way, the relatively acid-stable silica structure remains intact, whereas the content of amorphous silica in the solid phase rises.

Consequently, the efficiency of acid activation is mainly dependent on the extent to which octahedral layers are degraded and on the dissolution rate of metal cations into the solution. One of the important parameters that characterize this process is the change in the content of Al_2O_3 in bentonite. The reduction in Al_2O_3 content indicates the extent of dealumination and is directly related to the reorganization of bentonite structure and the physicochemical and sorption characteristics of the formed sorbent [[24], [25], [26]].

Mathematical modeling represents great scientific significance in terms of revealing the quantitative laws of physicochemical transformations that take place during the acid activation process. The use of regression models in the analysis of empirical data makes it possible to describe the parameters of the process, determine their dependence on each other, and calculate intermediate values. When experimental data indicate a nonlinear relationship between variables, quadratic polynomial regression can be used to describe this relationship quantitatively [[27], [28], [29], [30], [31], [32], [33]].

From the literature analysis, it follows that, while activating bentonite using HCl, the structural framework of montmorillonite remains intact; however, a reduction of the $\text{Al}_2\text{O}_3/\text{SiO}_2$ ratio is seen. Such a trend is due to the dealumination effect caused by the selective dissolution of aluminum ions from the octahedral layers. As a result, there is an increase in silica content, which creates prerequisites for pore formation.

Thus, changes in the content of Al_2O_3 can be regarded as one of the main criteria that describe

the properties of adsorption and catalysis of bentonite. It is important to establish the dependence of the Al_2O_3 content on the HCl concentration and to mathematically model this dependency in order to optimize the activation process using acids. In this way, the preliminary calculation of Al_2O_3 content and changes in sorption properties become possible [[34], [35]].

Therefore, from the literature review, it can be seen that mathematical modeling of the change in Al_2O_3 content during the acid activation of bentonite with HCl is significant in the quantitative description of the relations in the process, statistical processing of experimental data, and technological calculation. The majority of the existing researches are dedicated to the structural characterization and adsorption properties of the acid-activated bentonite. However, not enough attention has been paid to the quantitative description of the relation between the content of Al_2O_3 and HCl concentration in the form of a quadratic polynomial regression model.

In this study, the relationship between HCl concentration and Al_2O_3 content during the acid activation of Navbahor bentonite was analyzed using quadratic polynomial regression. The main contribution of this work is the development of a mathematical model describing changes in Al_2O_3 content as a function of HCl concentration within the investigated range of 5–20%. Model performance was evaluated by comparing the calculated values with the experimental data using statistical error metrics. A quadratic polynomial regression model was developed to describe the process and the adequacy of the model to experimental data was estimated by the coefficient of determination (R^2), root mean square error (RMSE) and mean absolute error (MAE).

Materials and Methods

Research material

Alkaline-earth bentonite (calcium bentonite), which was taken from the Navbahor ore deposit in Navoi region, Republic of Uzbekistan, was chosen as the object of study. SiO_2 and Al_2O_3 represent the main compounds in the natural bentonite in their shares 61.54% and 12.60%, correspondingly. Large share of silicon dioxide proves the presence of the silica framework of the mineral and provides stability of the silicate framework under the acidic activation. The shares of the other oxides are given in Table 1.

Table 1 - Chemical composition of natural Navbahor alkaline-earth bentonite

Sample	Content, %								
	SiO ₂	Al ₂ O ₃	Fe ₂ O ₃	TiO ₂	CaO	MgO	Na ₂ O	K ₂ O	LOI
Natural bentonite clay	61.54	12.60	6.23	0.56	0.75	3.98	0.82	2.11	11.41

On the basis of the results of analysis provided in Table 1, it can be stated that SiO₂ and Al₂O₃ oxides are dominant in bentonite. The presence of Fe₂O₃ and MgO implies the existence of these cations in octahedral layers of montmorillonite. The SiO₂/Al₂O₃ ratio is equal to 4.88, and this is the main initial characteristic which should be considered when analyzing dealumination process.

Acid activation process

A sample of bentonite weighing 100 g was treated with HCl solutions at concentrations of 5, 10, 15, and 20%, in which the solid-to-liquid ratio is 1:2.5. Acid activation was performed in the water bath at 373 K for 120 min with constant stirring.

After the acid treatment, the suspension obtained was washed with distilled water up to the value of pH equal to 4. Then, the samples were dried at 473 K, milled, and sieved into particles below 56 µm. The Al₂O₃ content in the natural and acid-activated bentonite samples was determined by a complexometric titration method. The procedure involved fusion of the sample at high temperature, dissolution of the resulting material, separation of iron ions, and back-titration of excess Trilon B (EDTA) solution with a zinc salt solution in the presence of an indicator [4].

Mathematical modeling

A quadratic polynomial regression model was constructed for mathematical description of the influence of HCl concentration on the Al₂O₃ content of bentonite within the acid activation process. The regression model was chosen to establish the functional dependence between the variables, evaluate the Al₂O₃ content within an interval of HCl concentrations, and make technological calculations.

The quadratic polynomial regression model is represented by the following general equation:

$$Y = a + bX + cX^2$$

where:

Y - Al₂O₃ content in bentonite (%);

X - HCl concentration (%);

a, b, and c - regression coefficients.

The regression parameters were calculated through the Polynomial Fit (Quadratic) routine of OriginPro 2026. The procedure employs the least-squares approach, according to which one has to minimize the sum of squared residuals between the observed values (Y_i) and the predicted ones ($\hat{Y}_i$):

$$S = \sum_{i=1}^n (Y_i - \hat{Y}_i)^2$$

The fitness of the model with the experimental data was assessed through the coefficient of determination (R^2), root mean square error (RMSE), and mean absolute error (MAE).

The coefficient of determination (R^2) was determined using the formula:

$$R^2 = 1 - \frac{\sum_{i=1}^n (Y_i - \hat{Y}_i)^2}{\sum_{i=1}^n (Y_i - \bar{Y})^2}$$

where:

Y_i - experimental value;

$\hat{Y}_i$ - value predicted by the model;

$\bar{Y}$ - arithmetic mean of the experimental values;

n - number of observations.

The root means square error (RMSE) of the model was calculated using the following equation:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2}$$

The mean absolute error (MAE) was calculated using the following equation:

where:

n - number of observations;

Y_i - experimental values;

$\hat{Y}_i$ - values predicted by the model.

In turn, the coefficient of determination (R^2) was applied to test the capabilities of the developed regression model to describe the experimental data, while RMSE and MAE served as criteria of its prediction accuracy. The obtained regression equation was utilized to describe the experimental data and to calculate the Al₂O₃ content at the intermediate values of HCl concentration, as well as to assess the possibility of using the equation to rapidly calculate the technological parameters of the acid activation process.

Results and Discussion

Effect of HCl concentration on the Al_2O_3 content of bentonite

Table 2 demonstrates the variation of Al_2O_3 composition in the acid treatment of bentonite clay by HCl, whereas the mathematical representation of the experimental results through the application of quadratic polynomial regression analysis is illustrated in Figure 1.

Table 2 - Changes in the Al_2O_3 content during the acid activation of bentonite with HCl

HCl concentration, %	Al_2O_3 content, %
5	12.26
10	11.81
15	10.34
20	9.64

As follows from the data in Table 2, increasing the HCl concentration from 5% to 20% reduced the Al_2O_3 content in bentonite from 12.26% to 9.64%, corresponding to a decrease of 2.62 percentage points. This trend is consistent with dealumination during acid activation, which involves the dissolution of aluminum from the octahedral layers of bentonite. However, the decrease was not uniform across the investigated concentration intervals: the Al_2O_3 content decreased by 0.45 percentage points between 5% and 10% HCl, by 1.47 percentage points between 10% and 15%, and by 0.70 percentage points between 15% and 20%. These differences indicate a nonlinear concentration-composition relationship rather than a constant decrease. Nevertheless, the four experimental concentration levels are insufficient to establish a change in the underlying dealumination mechanism.

Previous studies on acid-activated bentonites have also reported the dissolution of aluminum and other octahedral cations, with the extent of chemical and structural modification depending on the mineral composition and activation conditions [[24], [25], [35]]. Direct quantitative comparison with other bentonite deposits requires consideration of differences in acid concentration, temperature, treatment duration, and analytical methods.

A previous study by Boyjanov et al. [27] described the same experimental dataset using an exponential decay model, reporting $R^2 = 0.964$ and $\text{RMSE} = 0.231$. In the present study, quadratic

polynomial regression yielded $R^2 = 0.9646$ and $\text{RMSE} = 0.2001$. Both models describe the observed trend with similar goodness of fit, while the quadratic model produced a slightly lower RMSE for this dataset. However, this difference does not establish the superiority of either model, particularly because only four HCl concentration levels were investigated. Additional experimental data and independent validation are required to assess their relative predictive performance.

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The following quadratic polynomial regression model for Al_2O_3 estimation was constructed based on the obtained data (Figure 1).

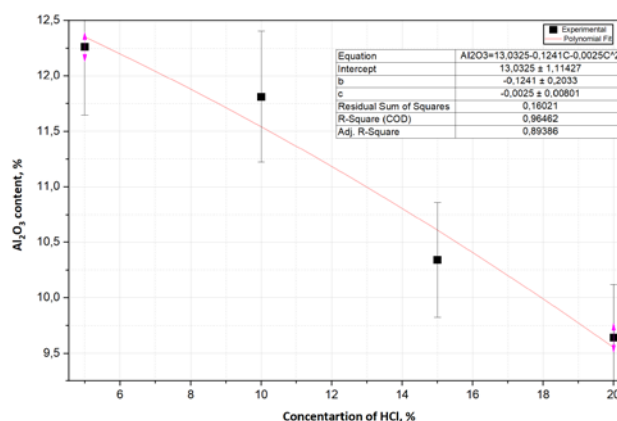


Figure 1 - Experimental Al_2O_3 content and the fitted quadratic polynomial regression model

The regression equation obtained using the Polynomial Fit (Quadratic) module in OriginPro 2026 is given as follows:

$$\text{Al}_2\text{O}_3 = 13.0325 - 0.1241C - 0.0025C^2$$

where:

C - hydrochloric acid (HCl) concentration (%);
 Al_2O_3 - aluminum oxide content in bentonite (%).

The coefficient of determination of the model was $R^2 = 0.9646$, meaning that the quadratic polynomial regression model accounts for 96.46% of the variance in the experimental data. Moreover, the adjusted $R^2 = 0.8939$ is consistent with the reliability of the parameters of the model on the basis of experimental data.

As one can see in Fig. 1 below, the curve of the quadratic polynomial regression model shows a strong correspondence with the experimental data points. The obtained results confirm that the developed quadratic polynomial regression model describes the relationship between the HCl concentration and the Al_2O_3 content in bentonite well and can be used to estimate the Al_2O_3 content at the intermediate HCl concentrations and to perform technological calculations.

First-order regression coefficient ($b = -0.1241$) is negative, which means that the quantity of Al_2O_3 in bentonite reduces while the concentration of HCl solution rises. This tendency is explained by the fact that the aluminum ions dissolve from the interlayer and octahedral structure due to acid treatment [[27], [35]].

Second-order coefficient ($c = -0.0025$) is also negative, which indicates that the change in Al_2O_3 content is not proportional to the increase in HCl concentration. In other words, the more concentrated HCl solution is used, the more aluminum oxide dissolves, thus, making the relationship nonlinear. So, we can conclude that the selected polynomial equation adequately describes the experimental relation.

The adequacy of the model was estimated on the basis of the comparison of the experimental data and calculated results. Specifically, the quantity of Al_2O_3 was estimated according to the quadratic polynomial regression equation and the experimental and calculated values were analyzed in terms of residuals and relative error (RE). The results of the calculation are provided in Table 3.

Table 3 - Comparison of the experimental and model-predicted Al_2O_3 values obtained using the quadratic polynomial regression model

HCl concentration, %	Al_2O_3 (experimental), %	Al_2O_3 (model-predicted), %	Residual ($\Delta = y - \hat{y}$)	Relative error (RE), %
5	12.26	12.3495	-0.0895	0.73
10	11.81	11.5415	0.2685	2.27
15	10.34	10.6085	-0.2685	2.60
20	9.64	9.5505	0.0895	0.93

The results shown in Table 3 indicate the presence of a high correlation between the calculated values

of Al_2O_3 and the results of experiments. All calculated values are close to experimental data with respect to different HCl concentrations. Residuals fluctuate in the range from -0.2685 to 0.2685 and relative errors (RE) are in the range from 0.73% to 2.60%. Minimum relative error of 0.73% was obtained at the HCl concentration equal to 5%, while maximum relative error of 2.60% was obtained at an HCl concentration of 15%. Relative error for all experimental data points was less than 3%. For the quadratic function, the coefficient of determination was found to be 0.9646, root mean square error is 0.2001, and the mean absolute error was 0.1790, showing that there is a good fit with the given experimental data points. But these are statistical measures and give information on the in-sample fit of the model and cannot determine its predictability separately. Thus, the developed model provides an accurate description of experimental data and allows us to estimate Al_2O_3 content at an HCl concentration of 5-20%. So, the developed quadratic polynomial regression model can be considered as a valid description of changes of Al_2O_3 content at the acid activation of bentonite with HCl.

Conclusions

For this research, a mathematical model of the dependence between HCl concentration and the Al_2O_3 content of bentonite in the process of its acid activation was created. The obtained quadratic polynomial regression model was built according to the results of the experiment and was shown to be able to describe adequately the dependence of the Al_2O_3 content of bentonite.

However, the obtained model does not only have the ability to describe the results of the experiment but also can provide preliminary evaluation of the Al_2O_3 content of bentonite at intermediate HCl concentrations, which will reduce the necessity to perform additional experiments and will allow the choice of the process parameters in a scientific way.

The present study focuses on modeling the relationship between HCl concentration and Al_2O_3 content in acid-activated Navbahor bentonite. Since both chemical composition and BET surface area have been determined for the same activated samples in our research, these data may provide a basis for investigating relationships between chemical composition and textural properties. Using such a model allows not only to numerically simulate and optimize the parameters of the acid

activation of bentonite but also to estimate the sorption properties of the mineral in advance. It is possible to conduct fewer experiments, which will lead to a reduction in the use of acid and water.

Since the proposed quadratic polynomial regression model describes well the change in the content of Al_2O_3 , it can also be used as a mathematical basis for indirect prediction of the change in the specific surface area (BET) of bentonite.

Conflicts of interest. On behalf of all authors, the corresponding author states that there is no conflict of interest.

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Навбахор бентонитін тұз қышқылымен белсендіру кезінде Al_2O_3 мөлшерін квадраттық модельдеу

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Мақала келді: 25 шілде 2026 Сараптамадан өтті: 9 қазан 2026 Қабылданды: 20 қазан 2026	ТҮЙІНДЕМЕ Бұл жұмыс бентонит сазын тұз қышқылымен (HCl) қышқылдық белсендіру процесі кезінде Al_2O_3 мөлшерінің өзгеруін математикалық модельдеуге арналған. Зерттеудің мақсаты бентонит құрамындағы Al_2O_3 мөлшеріне HCl концентрациясының әсерін зерттеу және осы тәуелділікті сипаттайтын математикалық модельді әзірлеу болып табылады. Осы мақсатта бентонит үлгілері 5, 10, 15 және 20% концентрациялы HCl ерітінділерімен белсендіріліп, Al_2O_3 мөлшері тәжірибелік жолмен анықталды. Алынған нәтижелер OriginPro 2026 бағдарламалық ең кіші квадраттар әдісін қолдану арқылы квадраттық полиномдық регрессия моделі бойынша талдаудан өткізілді. Модельдің сәйкестік дәрежесі детерминация коэффициенті (R^2), орташа квадраттық қате (RMSE) және орташа абсолюттік қате (MAE) көрсеткіштері арқылы бағаланды. Нәтижелер көрсеткендей, әзірленген модель тәжірибелік деректерді жоғары дәлдікпен сипаттады ($R^2 = 0.9646$, RMSE = 0.2001 және MAE = 0.1790), ал модель бойынша есептелген және тәжірибелік мәндер арасындағы салыстырмалы қателік 0.73-2.60% аралығында болды. Алынған нәтижелер модельді 5-20% HCl концентрациялары аралығындағы аралық нүктелерде Al_2O_3 мөлшерін алдын ала бағалау және технологиялық есептеулер жүргізу үшін тиімді пайдалануға болатынын көрсетті. Ұсынылған квадраттық полиномдық регрессиялық модель бентонитті қышқылмен белсендіру процесін оңтайландыруға, Al_2O_3 мөлшерінің өзгеруін сандық бағалау және саздың сорбциялық қасиеттерін жанама түрде бағалау үшін сенімді математикалық құрал болып табылады.
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Квадратичное моделирование содержания Al_2O_3 при солянокислотной активации Навбахорского бентонита

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Поступила: 25 июня 2026 Рецензирование: 9 октября 2026 Принята в печать: 20 октября 2026	АННОТАЦИЯ Настоящая работа посвящена математическому моделированию изменения содержания Al_2O_3 в процессе кислотной активации бентонитовой глины соляной кислотой (HCl). Целью исследования являлось изучение влияния концентрации HCl на содержание Al_2O_3 в бентоните и разработка математической модели, описывающей данную зависимость. Для этого образцы бентонита активировали растворами HCl с концентрацией 5, 10, 15 и 20 %. Полученные данные были проанализированы с использованием квадратичной полиномиальной регрессионной модели, основанной на методе наименьших квадратов в программе OriginPro 2026. Адекватность модели оценивали с помощью коэффициента детерминации (R^2), среднеквадратической ошибки (RMSE) и средней абсолютной ошибки (MAE). Разработанная модель продемонстрировала высокую степень соответствия экспериментальным данным ($R^2 = 0,9646$; RMSE = 0,2001; MAE = 0,1790), при этом относительная ошибка между расчетными и экспериментальными значениями находилась в диапазоне от 0,73 до 2,60 %. Полученные результаты показали, что предложенная модель может эффективно использоваться для предварительной оценки содержания Al_2O_3 при промежуточных концентрациях HCl в диапазоне 5-20%, а также для проведения технологических расчетов. Предложенная квадратичная полиномиальная регрессионная модель является надежным математическим инструментом для оптимизации процесса кислотной активации бентонита, количественной оценки изменений содержания Al_2O_3 и косвенной оценки сорбционных свойств глины. Ключевые слова: бентонит, соляная кислота, оксид алюминия, адсорбция, математическое моделирование, квадратичная полиномиальная регрессионная модель. Информация об авторах: Раджабов Мансур Фархадович Кандидат технических наук, заведующий кафедрой технологии пищевых продуктов Ургенчского государственного университета имени Абу Райхана Беруни, Ургенч, улица Х. Олимджона, 14, 220100, Узбекистан. Email: mansur.ra@urdu.uz; ORCID ID: https://orcid.org/0000-0003-2068-0595 Ниёзов Мамуржон Бобоназарович Докторант Каршинского государственного технического университета, пр-т Ханабад, 19, Узбекистан. E-mail: mamurniyozov43@gmail.com; ORCID ID: https://orcid.org/0009-0006-6488-0504
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