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# Exponential modeling of $Al_2O_3$ reduction during activation of Navbahor alkaline-earth bentonite

[1*]Boyjanov N.I., [2]Otajonova G.M., [3]Kendjayev B.B., [1]Matyakubova M.X., [1]Sabirova N.K., [4]Masharipov A.T., [1]Boyjanov I.R., [5]Serkayev Q.P.

[1]Urgench State University named after Abu Rayhon Beruni, Urgench, Uzbekistan
[2]Mamun University, Khiva, Uzbekistan
[3]Urgench Innovation University, Urgench, Uzbekistan
[4]Academic Lyceum of Urgench State University, Urgench, Uzbekistan
[5]Tashkent Chemical-Technological Institute, Tashkent, Uzbekistan

*Corresponding author email: b.nodirbek@urdu.uz

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**ABSTRACT**
In this study, using mathematical modeling, the change in Al2O3 content as a function of acid concentration during hydrochloric acid activation of alkaline-earth bentonite from the Navbahor deposit is investigated. During the experiment, the HCl concentration varied from 5% to 20%, and the change in Al2O3 content was nonlinear. To describe the experimental data obtained during hydrochloric acid activation of alkaline-earth bentonite from the Navbahor deposit, an exponential decay model was proposed, and its parameters were estimated by regression analysis. The accuracy of this approach is supported by the coefficient of determination ($R^2$ = 0.964) and the root mean square error (RMSE = 0.231%), indicating high accuracy and stability. The results obtained show that the decrease in $Al_2O_3$ content under acid activation conditions exhibits a nonlinear dependence on hydrochloric acid concentration rather than on time, and they enable formulation of a mathematical expression for the quantitative description of the process and for evaluating the effect of concentration.

***Keywords:*** bentonite, acid, activation, relative area, modelling, exponential decay, coefficient of determination ($R^2$).

***Information about authors:***

| | |
|---|---|
| ***Boyjanov Nodirbek Ilxomovich*** | *Doctor of Philosophy in Technical Sciences, Associate Professor at the Faculty of Chemical Technology, Urgench State University named after Abu Rayhon Beruni, 220100, H. Olimjon Street 14, Urgench, Uzbekistan. Email: b.nodirbek@urdu.uz; ORCID ID: https://orcid.org/0009-0002-1454-9478* |
| ***Otajonova Gulkhayo Maqsud kizi*** | *Teacher at Mamun University, Khiva, Khorezm, Uzbekistan. Email: otajonovagulhayo1508@gmail.com; ORCID ID: https://orcid.org/0009-0008-7529-9656* |
| ***Kendjayev Bunyod Bahtiyor ugli*** | *Teacher, Urgench Innovation University, Khorezm region, Urgench, Uzbekistan. Email: bun0401kbb@gmail.com; ORCID ID: https://orcid.org/0009-0002-3235-5159* |
| ***Matyakubova Mavlyuda Xudayberganovna*** | *Doctor of Philosophy in Technical Sciences, Associate Professor at the Faculty of Chemical Technology, Urgench State University named after Abu Rayhon Beruni, 220100, H. Olimjon Street 14, Urgench, Uzbekistan. Email: matyaqubovamavluda2010@gmail.com; ORCID ID: https://orcid.org/0009-0000-2961-3626* |
| ***Sabirova Nadira Kamiljanovna*** | *Doctor of Philosophy in Technical Sciences, Associate Professor at the Faculty of Chemical Technology, Urgench State University named after Abu Rayhon Beruni, 220100, H. Olimjon Street 14, Urgench, Uzbekistan. Email: nodira.sob11@gmail.com; ORCID ID: https://orcid.org/0000-0001-9685-9861* |
| ***Masharipov Azamat Tursunboyevich*** | *Doctor of Philosophy in Chemical Sciences, Teacher Academic Lyceum of Urgench State University, Fayozov 27, Urgench, Uzbekistan. Email: yadrokimyo1@gmail.com; ORCID ID: https://orcid.org/0009-0003-3537-3130* |
| ***Boyjanov Islom Rajabboyevich*** | *Candidate of Technical Sciences, Associate Professor of the Faculty of Chemical Technology, Urgench State University named after Abu Rayhon Beruni, 220100, H. Olimjon Street 14, Urgench, Uzbekistan. Email: rajrajrajradju@gmail.com; ORCID ID: https://orcid.org/0000-0002-8416-5472* |
| ***Serkayev Qamar Pardayevich*** | *Professor at the Tashkent Institute of Chemical Technology, Navoi Street, 32, Tashkent, Uzbekistan. Email: serkayev@mail.ru; ORCID ID: https://orcid.org/0009-0009-8316-4994* |


## Introduction

At present, the development of adsorbents for the chemical and food industries, along with their technological enhancement, is recognized as one of the most pressing scientific and technical challenges. In this regard, a lot of research has been conducted to create modified adsorbents with micro-, meso-, and macroporous structures, along with their capacity to perform processes such as ion exchange and chemical bonding, to improve their technological efficiency under actual conditions [[1], [2], [3], [4]].

Activation methods for bentonite clays are applied under different conditions, depending on their mineral composition, structure, chemical composition, and intended use.

Acid activation is a chemical modification process wherein $H^+$ ions replace exchangeable metal ions, such as $K^+$, $Na^+$, $Ca^{2+}$, and $Mg^{2+}$. The removal of metal ions, located within the interlayer space, results in a silica-rich structure. At the same time, a variety of active sites are created during the process of acid activation, which increases the sorption potential of the clay material [5].

Natural pigments like chlorophyll, xanthophyll, carotenoids, gossypol, soapstock, and other soap-like compounds, free fatty acids, and peroxides, etc., present in vegetable oils, vary in nature due to their physicochemical properties. Depending upon the nature of the compounds present, the process of refining vegetable oils is carried out, either completely or partially, through processing cycles. The quality of the oil produced by various methods is evaluated based on the physicochemical properties of the oil produced by various methods. The properties include phospholipid, moisture, and volatile matter content, iodine value, color index, refractive index, and saponification value, etc. Improvement of these properties is not only related to the reagents used but is also associated with the application of advanced technology in the production process [[6], [7], [8], [9], [10], [11], [12]].

The mathematical modeling of any production process allows, in advance, the formulation of well-founded forecasts regarding the term of the technological process, the amount of consumed raw materials, and the quantity and quality of the obtained products. This allows the improvement of the stability and efficiency of the production process. Industrial and processing processes require the construction of mathematical models that allow the identification and quantification of the interaction between the technological parameters, such as moisture, temperature, concentration, pH, and others [[6], [7], [8], [9], [10]].

Mathematical modeling can also have an important methodological impact on the process of acid activation of bentonite clays, making it possible to describe changes in chemical composition during experiments in a unified and generalized form, which would allow us to speak of a controlled and predictable process. In particular, mathematical modeling can significantly inform the description of processes of interaction with mineral acids, including the specific leaching of $Al^{3+}$ ions from the mineral's octahedral layer and the formation of an amorphous $SiO_2$-rich phase [11].

The selection of exponential decay models is substantiated by the high accuracy that can be obtained with a small number of parameters and also by the robustness to errors in experiments. In these models, the rate constant serves as a universal criterion for kinetic analysis, enabling comparative studies of different raw materials and processes. Experimental evidence from a wide range of investigations published in the literature confirms that, for bentonite clays, an increase in acid concentration results in a substantial increase in leaching rate for $Al^{3+}$, $Mg^{2+}$, and other cations from the octahedral layer. The complex kinetic character of the process requires the use of non-linear regression models for adequate description [[12], [13]].

The mathematical modeling allows for a quantitative description of the overall kinetic trend detected during the process of acid activation of bentonite clays. It was detected that the decrease in $Al_2O_3$ content has a non-linear dependence on the acid concentration during the process, being rapid at the initial stages and slowing down with time, which can be described by a general kinetic pattern. An exponential decay model has been used as a simplified model from a statistical point of view. Its adequacy is checked based on the experiment [[14], [15]].

One of the key benefits of modeling is the possibility of a formal definition of product quality-oriented objective functions (such as the consistent decrease or stabilization of the $Al_2O_3$ content over a certain range), thereby creating the necessary basis for the calculation of the optimal acid concentration [16].

While the results of polynomial regression models can describe experimental points with a high degree of accuracy, they do not necessarily reflect real physicochemical processes. On the other hand, the exponential model naturally describes the process of $Al_2O_3$ depletion, the deceleration of which with increasing HCl concentration is quite logical, and yields stable results in prediction [[17], [18]].

The physical meaning of the selective leaching of $Al^{3+}$ ions while preserving the structural framework is logically consistent with the exponential decay-type kinetic law. In making a justified choice between two or more models, the coefficient of determination ($R^2$) value alone is not enough; rather, a detailed analysis including the root mean square error (RMSE) is needed [[19], [20], [21]].

The kinetic methods used in acid leaching processes provide a fundamental scientific tool for quantitative measurement and control of rate. They describe the rate of leaching with respect to time using mathematical expressions, which helps to determine the rate-controlling step of a chemical reaction [[22], [23]].

If, after such treatment by acid, there are no changes in the position of the peaks corresponding to the Si-O bonds, it is considered that these changes are mainly related to the selective leaching of Al, Mg, and Fe cations from the octahedral layer. It is then considered that the initial structure of tetrahedral Si-O bonds remains stable [[24], [25], [26], [27], [28], [29]]. Due to this process, the crystal lattice of clay minerals is preserved, and the main framework is kept intact. At the same time, the leaching of cations from the octahedral layer enhances the surface area and porosity of the material. Hence, this modified form of clay can be utilized effectively in adsorption and catalytic purposes [[30], [31], [32], [33], [34], [35]].

The mathematical way of understanding this activation process allows for the quantitative prediction of the sorption properties of the clay, which reduces the number of experiments and optimizes this process. With this approach, it is possible to plan the consumption of acid and water at a rational level, and it is possible to determine in advance the probable amount of additional reagents to be used. Thus, this activation process not only becomes scientifically understandable and controllable but also becomes an important tool for making efficient use of resources, for improving energy efficiency, and for reducing technological costs.

In this study, a new approach to summarizing experimental data was developed, which is based on a table, graph, and model sequence, thus facilitating the identification of a continuous governing relationship of the process from discrete experimental points. This new approach allows one to consider changes in $Al_2O_3$ content not only from a statistical point of view, but also in relation to the physicochemical nature of the acid activation process. Therefore, this study presents a new scientific and methodological basis for a deeper understanding of the acid activation of bentonites, the effective conditions of this process, and a predictive assessment of further stages of this process.

In this work, an exponential decay model is proposed for describing the variation of $Al_2O_3$ content as a function of hydrochloric acid concentration. Using this model, it is possible to represent quantitatively the non-linear and strictly decreasing trend of the experimental data.

## Materials and Methods

As the object of the study, the alkaline earth (calcium-type) bentonite from the Navbahor deposit was chosen. In the chemical composition of the natural bentonite clay, $Al_2O_3$ makes up 12.60% as the main exchangeable component. The $SiO_2$ content is 61.54%, which shows that this mineral has a silica-based structure. The high percentage of $SiO_2$ ensures the stability of the mineral layers and acts as a non-degradable framework during the acid activation process.

Additionally, the chemical composition of the bentonite clay contains small amounts of other oxides, and their composition is shown in Table 1. The chemical composition was not used as an initial parameter for the simulation of the kinetics of the reduction of $Al_2O_3$ during hydrochloric acid activation, as the simulation is based on the process that begins after the onset of acid activation.

**Table 1 -** Chemical composition of natural alkaline-earth bentonite from the Navbahor deposit

| Sample | Content, % | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | $SiO_2$ | $Al_2O_3$ | $Fe_2O_3$ | $TiO_2$ | CaO | MgO | $Na_2O$ | $K_2O$ |
| Natural bentonite clay | 61.54 | 12.60 | 6.23 | 0.56 | 0.75 | 3.98 | 0.82 | 2.11 |

Bentonite clay with a sample mass of 100 g was activated with different concentrations of HCl solution (5%, 10%, 15%, and 20%) with a ratio of 1:2.5 and a temperature of 373 K for 2 hours with continuous stirring in a water bath. After activation, the suspension was washed with distilled water until a pH value of 4 was reached. Then it was dried at 473 K and sieved through a 56 µm mesh sieve. The content of $Al_2O_3$ in clay was analyzed by a chemical method according to GOST 21216-2014.

Three experiments were carried out in parallel, and their average values were calculated. Based on the experimental results, the relationship between the increase in the hydrochloric acid content and the change in the $Al_2O_3$ content was investigated. A mathematical model for the decrease in the $Al_2O_3$ content as a function of increasing hydrochloric acid content was created based on the experimental results obtained.

The composition of the non-activated bentonite, as presented in the table, was described as the initial state; however, since the mathematical modeling is focused on the changes that occur during the acid activation in the concentration range of HCl from 5% to 20%, this value was not considered as a model parameter.

It was determined that the relationship between the decrease in Al2O3 content and hydrochloric acid concentration can be modeled by an exponential regression equation (1).

$$Al_2O_3 = A \cdot exp^{-k \cdot HCL} \quad (1)$$

where

$Al_2O_3$ - dependent variable, %

HCl - independent variable, %

A and k - determined parameters after regression analysis

To test the goodness of the model, the coefficient of determination ($R^2$) was calculated. The graphical analysis presented in Figure 1 was obtained by utilizing the Origin 2021 Pro software. This graphical representation demonstrates the agreement between the predictions and the experimentally obtained data.

The agreement between the data and the selected mathematical model was assessed using the coefficient of determination ($R^2$) and the root mean square error (RMSE). The RMSE was calculated with the help of the following formula (2).

$$RMSE = \sqrt{\frac{1}{n}} \sum_{i=1}^{n} (y_i - ýi)^2 \quad (2)$$

where

yi - $Al_2O_3$ content determined experimentally,

ŷi - value calculated by the model,

n - number of experimental data points.

To further validate the model's adequacy, a residual analysis was conducted. In this case, residuals were defined as differences between experimental and calculated values. Additionally, the absence of systematic deviations and a specific pattern in the residuals indicates that the chosen model adequately describes the experimental data.

## Results and Discussion

The changes in $Al_2O_3$ content in samples activated with HCl solutions of different concentrations (5, 10, 15, and 20%) at a solid-liquid ratio of 1:2.5 are shown in Table 2.

**Table 2 -** $Al_2O_3$ content % in clay samples activated at different concentrations of hydrochloric acid

| Acid concentration, % | $Al_2O_3$ content, % |
|---|---|
| 5 | 12.26 |
| 10 | 11.81 |
| 15 | 10.34 |
| 20 | 9.64 |

The experimental results, as represented in Table 2, show the decreasing trend of the parameter with increasing acid concentration. No abrupt changes were observed between the four measured data points. At the same time, the results represented in the table are not enough to show the exact nature of the relationship between the parameter and the acid concentration.

To achieve a more accurate interpretation of the dependence of the investigated parameter on the concentration of the acid, as well as to assess the mathematical nature of the observed dependence, the experimental points were represented in a graphical form. The graphical representation of the data revealed a nonlinear dependence, thereby supporting the use of an exponential model.

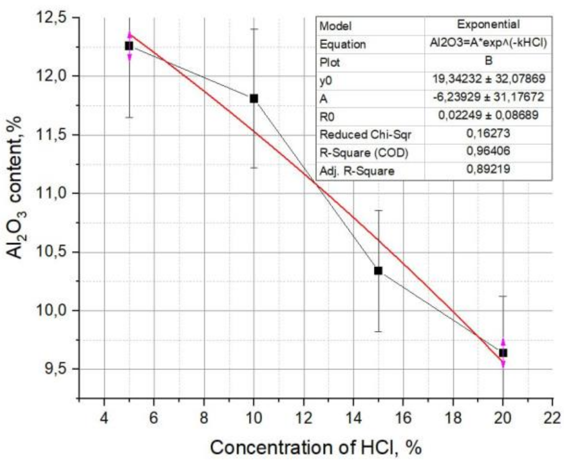


**Figure 1 -** Exponential decrease in $Al_2O_3$ content in clay with an increase in HCl concentration

As shown in the graph, the experimental data points follow an exponential curve, indicating that this mathematical model is appropriate for describing the phenomenon. There is no linear distribution of points, indicating that the decrease is not linear with increasing HCl concentration.

Based on the modeling results, the high coefficient of determination ($R^2$ = 0.964) indicates strong agreement with the experimental data.

To generalize the experimental data, the relationship was described by an exponential decay model. Thus, the dependence of the $Al_2O_3$ content on the HCl concentration was expressed by equation (3).

$$Al_2O_3 = 13.3 \cdot exp^{-0.01685 \cdot HCL} \quad (3)$$

This equation also demonstrates the fact that with an increase in the HCl solution concentration, the content of $Al_2O_3$ decreases rapidly and then slows down, which corresponds to the main physicochemical features of the selective leaching process.

The goodness of fit of the model is high, indicating a close and stable relationship between the experimental and calculated data, thereby demonstrating the high quality of the selected exponential method. The calculated value of the exponential coefficient k shows that the decrease in the content of $Al_2O_3$ does not occur at a constant rate but depends on the amount of the substance remaining in the system at a given time, which is typical for a kinetic process of selective leaching.

In the following sections, the mechanism of dissolution of $Al_2O_3$ during the acid activation of bentonite clay will be schematically illustrated step by step (Figure 2).

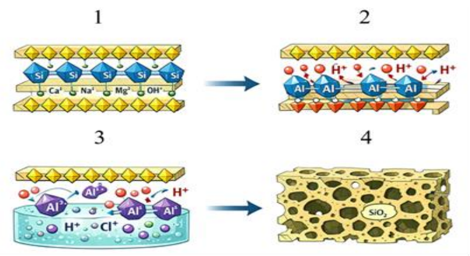


**Figure 2 -** Schematic illustration describing the selective dissolution of $Al_2O_3$ during activation of bentonite with HCl

It is possible to visualize the preservation of the $SiO_2$ network and the creation of porosity through this figure. In its natural state, this clay mineral is known as montmorillonite and is characterized by a layered-type crystalline structure. In this structure, aluminum ions are predominantly located in the octahedral layer. The interlayer space is occupied by exchangeable cations such as $Na^+$, $Ca^{2+}$, and $Mg^{2+}$, which maintain this structure in a relatively stable state. The removal of these ions leads to the creation of micropores and mesopores inside this clay structure. This increases the specific surface area of the clay and its adsorption properties.

In general, the exponential model captures the behavior of the change in Al2O3 content as a function of acid concentration in an appropriate mathematical form, thereby enabling accurate characterization of the process.

The following table facilitates a scientific analysis of the comparison between the experimentally obtained $Al_2O_3$ contents and those calculated using the exponential model as a function of HCl concentration (Table 3).

**Table 3 -** Experimental and modeled values of the decrease in $Al_2O_3$ content in the clay

| HCl concentration, % | $Al_2O_3$ (experimental), % | $Al_2O_3$ (model), % | Residual ($\Delta = y - \hat{y}$) | Relative error (RE), % |
|---|---|---|---|---|
| 5 | 12.26 | 12.46 | -0.20 | -1.63 |
| 10 | 11.81 | 11.46 | 0.35 | +2.96 |
| 15 | 10.34 | 10.55 | -0.21 | -2.03 |
| 20 | 9.64 | 9.72 | -0.08 | -0.83 |

The root mean square error (RMSE) between the experimental and model values is 0.231%.

The results obtained in Table 3 show that the $Al_2O_3$ content in the clay decreases with an increase in the concentration of hydrochloric acid in a non-linear manner. The differences between the experimental results and the results obtained by the model are low, with the maximum relative error not being more than 2.96%, thus confirming the high accuracy of the selected exponential model. The positive and negative residual values being distributed in a balanced manner confirm that there are no systematic errors in the model. The low value of the total root mean square error also confirms that the exponential model can be used with good accuracy to quantitatively define the relationship between the $Al_2O_3$ content and the concentration of HCl.

RMSE makes it possible to quantitatively estimate the average deviation between calculated and experimental $Al_2O_3$ values with the same unit (%). Although the coefficient of determination ($R^2$) is a measure of the quality of the model, RMSE was used because it directly represents the actual accuracy of the model.

These results confirm that the reduction of $Al_2O_3$ content occurs without destruction of the aluminosilicate framework of bentonite and that this process occurs under conditions of preservation of its structure. Thus, the suggested method of modeling can be considered a scientifically grounded tool for quantitative evaluation of $Al_2O_3$ content variation during the acid activation process, characterizing the process's intensity, optimizing the process conditions, and making a predictive assessment of this process.

In this study, structural methods such as FTIR and XRD were not used as research objectives. Still, they were employed as theoretical tools to substantiate the results of the kinetic research and the mathematical modeling. According to literature data, under low and moderate conditions of acid activation, the main aluminosilicate structure of bentonites, especially the Si-O bonds, is not destroyed. Therefore, the decrease in the $Al_2O_3$ content cannot be explained by the destruction of the structure under low and moderate conditions of acid activation. Thus, the main emphasis of this research has been on the mathematical and statistical substantiation of the results.

## Conclusions

The scientific contribution of this study lies in the quantitative description of the change in $Al_2O_3$ content as a function of hydrochloric acid concentration for bentonite from the Navbahor deposit using a mathematical model, as well as its analysis through graphical and statistical criteria.

The acid activation of bentonites in previous studies was often studied in relation to adsorption properties and an increase in specific surface area, and the change in aluminum oxide content in relation to acid concentration was not always analyzed from a mathematical point of view. The decrease in $Al_2O_3$ content in this study is analyzed as a selective leaching process that preserves the structural framework, and the nonlinear, continuously decreasing nature of this phenomenon is demonstrated through experimental and graphical analyses.

The model developed on the basis of experimental results clearly showed that the change in $Al_2O_3$ content has a regular, non-linear, and stable decreasing trend with an increase in acid concentration. The results of graphical analysis and statistical evaluation have proved that the selected model can adequately describe the general trend of experimental results with a high degree of accuracy.

As shown by the results of the modeling, a high adequacy of the model was attained. In particular, a large value of the coefficient of determination ($R^2$ = 0.964) suggests that a significant portion of the variation in the content of $Al_2O_3$ is explained by the variation of the hydrochloric acid concentration. The above results allow one to proceed from a set of discrete points of the experiment to a continuous description of the process, ensuring the quantitative reliability of the obtained relationship.

The scientific novelty of the research lies in the fact that the variation of the content of $Al_2O_3$ during the acid activation process has been mathematically and consistently substantiated as a selective chemical process under conditions of structural framework preservation.

The value of this approach is based on the possibility of calculating the increase in the specific surface area of the clay material during the activation process based on the decrease in the $Al_2O_3$ content using mathematical modeling. This, in turn, allows us to decrease the number of economically expensive analysis techniques, such as the BET method.

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

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# Навбахор кен орнының сілтілі жер бентонитін белсендіру кезінде $Al_2O_3$ мөлшерінің төмендеуін экспоненциалды модельдеу

**[1]Бойжанов Н.И., [2]Отажонова Г.М., [3]Кенжаев Б.Б., [1] Матяқубова М.Х,**
**[1]Сабирова Н.К., [4]Машарипов А.Т., [1]Бойжанов И.Р., [5]Серкаев К.П.**

*[1]Әбу Райхон Беруни атындағы Үргеніш мемлекеттік университеті, Үргеніш, Өзбекстан*
*[2]Мамун университеті, Хива, Өзбекстан*
*[3] Үргеніш инновациялық университеті, Үргеніш, Өзбекстан*
*[4]Үргеніш мемлекеттік университетінің академиялық лицейі, Үргеніш, Өзбекстан*
*[5]Ташкент химия-технология институты, Ташкент, Өзбекстан*

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Қабылданды: *16 наурыз 2026*

**ТҮЙІНДЕМЕ**
Осы зерттеуде математикалық модельдеу әдістерін қолдана отырып, тұз қышқылын пайдалана, Навбахор кен орнының сілтілі топырақ бентонитінің қышқыл белсенділігі процесіндегі қышқыл концентрациясына тәуелді өзгерісі зерттелді. Тәжірибе барысында HCl концентрациясы 5–20 % аралығында өзгерді, бұл ретте $Al_2O_3$ мөлшерінің өзгеруі сызықтық емес сипатқа ие екені анықталды. Көрсетілген бентониттің қышқылдық белсендіру кезінде алынған эксперименттік деректерді сипаттау үшін оның параметрлері регрессиялық талдау негізінде айқындалған экспоненциалдық кему моделі ұсынылған. Осы тәсілдің дәлдігі мен тиімділігі детерминация коэффициентінің ($R^2 \approx 0.964$) және орташа квадраттық қатенің (RMSE = 0.231 %) мәндерімен расталған, бұл модельдің жоғары дәлдігі мен тұрақтылығы дәлелденді. Алынған нәтижелер қышқылдық белсендіру жағдайында $Al_2O_3$ мөлшерінің төмендеуі уақыт факторына емес, тұз қышқылы концентрациясына сызықтық емес тәуелділік көрсететінін дәлелдейді және бұл процесті сандық тұрғыдан сипаттайтын математикалық өрнек құруға, сондай-ақ концентрацияның әсерін бағалауға мүмкіндік береді.

***Түйін сөздер:*** бентонит, қышқыл, белсендіру, салыстырмалы бет ауданы, модельдеу, экспоненциалдық азаю, детерминация коэффициенті ($R^2$).

***Авторлар туралы ақпарат:***

| | |
|---|---|
| ***Бойжанов Нодирбек Илхомович*** | *Техника ғылымдары бойынша философия докторы, Әбу Райхон Беруни атындағы Үргеніш мемлекеттік университетінің химиялық технология факультетінің қауымдастырылған профессоры, 220100, Х. Әлімжан көшесі, 14, Үргеніш, Өзбекстан. Email: b.nodirbek@urdu.uz; ORCID ID: https://orcid.org/0009-0002-1454-9478* |
| ***Отажонова Гулхайо Мақсудтың қызы*** | *Мамун университетінің оқытушысы, Хива, Хорезм, Өзбекстан. Email: otajonovagulhayo1508@gmail.com; ORCID ID: https://orcid.org/0009-0008-7529-9656* |
| ***Кенджаев Бунёд Бахтиёр угли*** | *Үргеніш инновациялық университетінің оқытушысы, Хорезм облысы, Үргеніш, Өзбекстан. Email: bun0401kbb@gmail.com; ORCID ID: https://orcid.org/0009-0002-3235-5159* |
| ***Матяқубова Мавлуда Худайбергановна*** | *Техника ғылымдарының кандидаты, Әбу Райхон Беруни атындағы Үргеніш мемлекеттік университетінің Тағам технологиясы кафедрасының меңгерушісі, 220100, Х. Әлімжан көшесі, 14, Үргеніш, Өзбекстан. Email: matyaqubovamavluda2010@gmail.com; ORCID ID: https://orcid.org/0009-0000-2961-3626* |
| ***Сабирова Надира Камилжановна*** | *Техника ғылымдары бойынша философия докторы, Әбу Райхон Беруни атындағы Үргеніш мемлекеттік университетінің химиялық технология факультетінің қауымдастырылған профессоры, 220100, Х. Әлімжан көшесі, 14, Үргеніш, Өзбекстан. Email: nodira.sob11@gmail.com; ORCID ID: https://orcid.org/0000-0001-9685-9861* |
| ***Машарипов Азамат Турсунбоевич*** | *Химия ғылымдарының философия докторы (PhD), Үргеніш мемлекеттік университеті академиялық лицейінің оқытушысы, Фаёзов к-сі, 27, Үргеніш, Өзбекстан. Email: yadrokimyo1@gmail.com; ORCID ID: https://orcid.org/0009-0003-3537-3130* |
| ***Бойжанов Ислом Ражаббоевич*** | *Техника ғылымдарының кандидаты, Әбу Райхон Беруни атындағы Үргеніш мемлекеттік университеті, Химия-технология факультетінің доценті, 220100, Х.Олимжон көшесі 14, Үргеніш, Өзбекстан. Email: rajrajrajradju@gmail.com; ORCID ID: https://orcid.org/0000-0002-8416-5472* |
| ***Серкаев Камар Пардаевич*** | *Ташкент химиялық технология институтының профессоры, Навои көшесі, 32, Ташкент, Өзбекстан. Email: serkayev@mail.ru; ORCID ID: https://orcid.org/0009-0009-8316-4994* |


# Экспоненциальное моделирование снижения содержания $Al_2O_3$ при активации щёлочноземельного бентонита Навбахорского месторождения

**[1]Бойжанов Н.И., [2]Отажонова Г.М., [3]Кенжаев Б.Б., [1]Матяқубова М.Х.,**
**[1]Сабирова Н.К., [4]Машарипов А.Т., [1]Бойжанов И.Р., [5]Серкаев К.П.**

*[1]Ургенчский государственный университет имени Абу Райхона Беруни, Ургенч, Узбекистан*
*[2]Университет Мамуна, Хива, Узбекистан*
*[3]Ургенчский инновационный университет, Ургенч, Узбекистан*
*[4]Академический лицей Ургенчского государственного университета, Ургенч, Узбекистан*
*[5]Ташкентский химико-технологический институт, Ташкент, Узбекистан*

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**АННОТАЦИЯ**
В настоящем исследовании с применением методов математического моделирования изучено изменение содержания $Al_2O_3$ в зависимости от концентрации кислоты в процессе кислотной активации щёлочноземельного бентонита Навбахорского месторождения с использованием соляной кислоты. В ходе эксперимента концентрация HCl изменялась в диапазоне 5–20 %, при этом установлено, что изменение содержания $Al_2O_3$ носит выраженный нелинейный характер. Для описания экспериментальных данных, полученных при кислотной активации указанного бентонита, предложена модель экспоненциального убывания, параметры которой определены на основе регрессионного анализа. Достоверность и эффективность данного подхода подтверждены значениями коэффициента детерминации ($R^2 \approx 0{,}964$) и среднеквадратичной ошибки (RMSE = 0,231 %), что свидетельствует о высокой точности и устойчивости модели. Полученные результаты показывают, что снижение содержания $Al_2O_3$ в условиях кислотной активации проявляет нелинейную зависимость от концентрации соляной кислоты, а не от временного фактора, и позволяют сформулировать математическое выражение для количественного описания процесса и оценки влияния концентрации.

***Ключевые слова:*** Бентонит, кислота, активация, удельная поверхность, моделирование, экспоненциальное убывание, коэффициент детерминации ($R^2$).

***Информация об авторах:***

***Бойжанов Нодирбек Илхомович*** — *Доктор технических наук, доцент факультета химической технологии Ургенчского государственного университета имени Абу Райхона Бируни, 220100, ул. Х. Олимжон, 14, Ургенч, Узбекистан. Email: b.nodirbek@urdu.uz; ORCID ID: https://orcid.org/0009-0002-1454-9478*

***Отажонова Гульхаё Максуд кизи*** — *Преподаватель университета Мамун, Хива, Хорезм, Узбекистан. Email: otajonovagulhayo1508@gmail.com; ORCID ID: https://orcid.org/0009-0008-7529-9656*

***Кенджаев Бунёд Бахтиёр угли*** — *Преподаватель Ургенчского инновационного университета, Хорезмская область, Ургенч, Узбекистан. Email: bun0401kbb@gmail.com; ORCID ID: https://orcid.org/0009-0002-3235-5159*

***Матякубова Мавлуда Худайбергановна*** — *Кандидат технических наук, заведующий кафедрой технологии пищевых продуктов Ургенчского государственного университета имени Абу Райхона Беруни, Ургенч, улица Х. Олимжона, 14, 220100, Узбекистан. Email: matyaqubovamavluda2010@gmail.com; ORCID ID: https://orcid.org/0009-0000-2961-3626*

***Сабирова Надира Камилжановна*** — *Доктор технических наук, доцент факультета химической технологии Ургенчского государственного университета имени Абу Райхона Бируни, 220100, ул. Х. Олимжон, 14, Ургенч, Узбекистан. Email: nodira.sob11@gmail.com; ORCID ID: https://orcid.org/0000-0001-9685-9861*

***Машарипов Азамат Турсунбоевич*** — *Доктор философии по химии, преподавательский академический лицей Ургенчского государственного университета, Фаёзов 27, Ургенч, Узбекистан. Email: yadrokimyo1@gmail.com; ORCID ID: https://orcid.org/0009-0003-3537-3130*

***Бойжанов Ислом Ражаббоевич*** — *Кандидат технических наук, доцент химико-технологического факультета Ургенчского государственного университета имени Абу Райхона Беруни, 220100, ул. Х. Олимжон, 14, Ургенч, Узбекистан. Email: rajrajrajradju@gmail.com; ORCID ID: https://orcid.org/0000-0002-8416-5472*

***Серкаев Камар Пардаевич*** — *Профессор Ташкентского института химической технологии, улица Навои, 32, Ташкент, Узбекистан. Email: serkayev@mail.ru; ORCID ID: https://orcid.org/0009-0009-8316-4994*

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