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Modeling of catalytic reforming process with fixed bed catalyst based on industrial data

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Abstract: This study presents the development of a kinetic model of the catalytic reforming process using data from a commercial fixed-bed catalyst plant. Model parameters were determined by minimizing discrepancies between calculated values and industrial data, ensuring high accuracy in predicting reformate composition. The proposed model combines the simplicity of generalized approaches with the benefits of more detailed models, enabling efficient prediction of reformate composition and accounting for key process variables (temperature, pressure, hydrogen/hydrocarbon ratio, and feed rate). Validation was conducted with both laboratory isothermal data and industrial data, confirming its practical applicability. The software developed from this model demonstrated high accuracy, with calculation errors under 3% and less than 1% error in determining aromatic hydrocarbon concentration. These results confirm the model's precision, making it suitable for real-time process control and optimization. The model's application in industry will not only increase the yield of target products and improve fuel quality but also reduce production costs by optimizing operating modes and extending catalyst life. Given tightening environmental regulations, the model is an important tool for ensuring sustainable development in oil refineries. Future research could enhance its integration with digital control systems and optimize energy efficiency in Kazakhstan's oil and gas enterprises.

Keywords: mathematical modeling, oil refining, optimization, resource efficiency, petrochemistry, catalytic reforming.

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1. Introduction

Catalytic reforming is a key process in the petrochemical industry, used to improve gasoline quality and produce high quality chemical products. This process plays an important role in increasing the octane rating of fuels, as well as in the production of aromatic hydrocarbons and hydrogen, making it indispensable in petroleum refining.

In the context of the global transition to sustainable development and tightening environmental regulations, the oil refining industry faces the need to introduce advanced technologies aimed at improving energy efficiency and reducing harmful emissions. One of the most important processes in the production of high-octane gasoline is catalytic reforming, which provides improvement of octane number and obtaining valuable aromatic hydrocarbons. However, this process is energy intensive and generates by-products such as carbon dioxide and other harmful emissions.

Development and use of mathematical models of reforming processes allow not only to optimize technological parameters, but also to significantly reduce energy consumption and emissions. The use of models contributes to:

reducing the time required to conduct pilot tests;

determination of optimal operating modes to maximize the yield of target products;

reduction of coke formation and prolongation of catalyst service life;

increase the safety of plant operation.

In the context of the transition to more environmentally friendly technologies, such models become an important tool for reducing the carbon footprint of production. Optimization of technological processes based on modeling helps to reduce the use of raw materials and energy, which is in line with the goals of sustainable development and global environmental requirements.

In Kazakhstan, the main oil refining is carried out by three large oil refineries (refineries). The total design capacity of these three refineries is 16.6 million tons of crude oil per year. However, actual refining volumes may differ from the design capacity due to various factors such as scheduled maintenance, modernization and market conditions.

In terms of global figures, as of January 2022, the total capacity of catalytic reforming processes was 14.6 million barrels per day, equivalent to about 730 million tons per year.

Thus, Kazakhstan's share in global reformate production is relatively small. Nevertheless, it is important for the country to optimize existing processes and introduce modern technologies to improve the efficiency and environmental safety of oil refining.

Given the strategic role of the oil refining industry for the economy of Kazakhstan, the development and implementation of mathematical models of catalytic reforming processes seem to be relevant and in demand. This will allow not only to improve the quality of produced fuel, but also to reduce the negative impact on the environment, meeting international environmental standards.

Mathematical modeling of catalytic reforming began to develop in the 1950s, when the first attempts were made to describe reactions in the catalyst using empirical data (Krane et al., 1959). In the 1970s and 1980s, models became more sophisticated, considering reactions such as isomerization, dehydrogenation, and other mechanisms, as well as hydrocarbon interactions. At this time, differential equations and numerical methods began to be used extensively to improve accuracy (Ramage et al., 1987, 1980; Zhorov et al., 1980).

In the 1990s, dynamic models became available that described real-time changes in concentrations and temperatures, including parameters such as temperature, pressure, and catalyst degradation, which improved the prediction of reactor performance (Rodríguez and Ancheyta, 2011; Stijepovic et al., 2009).

Since the early 2000s, molecular and machine learning approaches have been incorporated into modeling to optimize catalyst performance and predict product composition. These methods allowed a wide range of factors to be considered, thereby improving the accuracy of predictions and the economic efficiency of the process (Sotelo-Boyás and Froment, 2008; Wei et al., 2008a, 2008b).

Recent interest in the reforming process has been driven by two main factors: reformate has become a major source of aromatic hydrocarbons in gasoline, and new legislative restrictions address benzene and aromatic hydrocarbon content in commercial gasoline (Sapre and Katzer, 2020; Velázquez et al., 2023).

The main chemical reactions of catalytic reforming include (As Martínez et al., 2022; Rekoske et al., 2017):

1. Isomerization of normal alkanes into isoalkanes, which is a fast exothermic reaction and leads to a slight increase in octane number. The reaction itself does not depend on the number of carbon atoms in the molecule, and its thermodynamic equilibrium depends mainly on the temperature of the process. High temperature favors the acceleration of the reaction. Isomerization reactions take place on acidic catalyst centers.

$$n - C_6H_{14} \to C_6H_{14} \quad (1)$$

2. Dehydrocyclization of alkanes (aromatization), which involves dehydrogenation to form aromatic hydrocarbons and hydrogen. The reaction proceeds on metallic and acidic catalyst centers. Alkanes with higher molecular weight undergo this reaction most rapidly, but they are also the most susceptible to the side reaction of hydrocracking. The reaction is accelerated by high temperature and low pressure, but, in general, this rate is much lower than the rate of the cycloalkane dehydrogenation reaction.

$$C_6H_{14} \to C_6H_6 + 4H_2 \quad (2)$$

3. Dehydrogenation of naphthenes to aromatic hydrocarbons, which is an endothermic reaction requiring high temperatures and low pressures for efficient proceeding. The rate of these reactions is high compared to other reactions. Since dehydrogenation of naphthenes provides high-octane components, intensification of this reaction is the most desirable process.

$$C_6H_{12} \to C_6H_6 + 3H_2 \quad (3)$$

4. Isomerization of five-membered cycloalkanes into cyclohexane derivatives, an exothermic reaction with a relatively low rate.

$$C_5H_9 \to CH_3 + C_6H_{12} \quad (4)$$

5. Hydrocracking of alkanes has 2 stages and proceeds both on metal and acid catalyst centers. At the first stage, the dehydrogenation reaction takes place on metal centers, after which the resulting alkene molecule is broken on the acid center and the resulting short chain alkene is hydrogenated. The reaction rate increases with increasing temperature and pressure. It is an undesirable reaction, because due to hydrocracking the content of alkanes in reformate decreases, which leads to an increase in the concentration of aromatic hydrocarbons and a decrease in reformate yield.

$$n\text{–}\mathrm{C_9H_{20}} + \mathrm{H_2} \to i\text{–}\mathrm{C_4H_{10}} + i\text{–}\mathrm{C_5H_{12}} \quad (5)$$

Various kinetic models have been described in the literature to represent the catalytic reforming process. All these models take into account some or all of the reactions mentioned above, catalytic reforming, and simplify the complex mixture of naphthenes so that each of the three classes of hydrocarbons - paraffins, naphthenes and aromatic hydrocarbons – is represented by a single compound with the average properties of that class.

Mathematical modeling of the catalytic reforming process continues to develop. One of the popular models is the Jorge model (Arani et al., 2009), which includes 24 differential equations and 71 kinetic parameters, describing the behavior of paraffins, naphthenes, and aromatic hydrocarbons, as well as the effect of temperature and pressure on the kinetic constants. This model was validated using experimental data obtained from fixed bed catalyst plants. As a result, the deviation of calculated data from experimental data did not exceed 3%.

Other studies (Wei et al., 2017) focus on dynamic modeling of catalytic reforming of naphtha, examining changes in hydrocarbon concentrations as well as temperature and hydrogen profiles in the reactor to optimize conditions to produce high quality reformate. In recent years, much attention has been given to molecular models and grouping methods, which help simplify the calculation by combining feedstock components.

The authors (Elizalde and Ancheyta, 2015) focus on the construction of a molecular model of the catalytic reforming process of naphtha and its optimization considering molecular information. Reactions in the reactor are modeled using a reaction network including six classes of reactions. The process is then simulated using dynamic equations and kinetic constants to predict the molecular composition of the products.

Due to the large number of components in the feedstock, unaccounted reactions and high process temperature, the design and modeling of catalytic reforming reactors are accompanied by difficulties. To simplify modeling, the grouping method (lumping) is widely used, which allows combining feedstock components, which significantly reduces the complexity of calculations. We have considered several existing kinetic models of reforming, such as those proposed by (Arani et al., 2009). In this paper, the authors propose a model in which naphtha is represented by 17 hydrocarbon fractions with 15 reaction pathways and a simple catalyst deactivation model proposed by (Elizalde and Ancheyta, 2015; Jarullah et al., 2023). The model contains 17 "pseudo-components" connected by 15 reaction pathways. The kinetic and thermodynamic parameters of the model were obtained by optimization based on plant data. The authors also propose equations for calculating thermodynamic equilibrium constants between lumped hydrocarbons as a function of temperature.

Based on the above, there are several different kinetic models to describe the catalytic reforming process, each with its own advantages and limitations. The models simplify the complex mixture of hydrocarbons by dividing them into three main groups: paraffins, naphthenes and aromatic hydrocarbons. Some models, such as the Krane model (Krane et al., 1959), have shortcomings such as not accounting for isomerization or the effects of temperature and pressure on kinetic constants. In response to these limitations, newer models (Jarullah et al., 2023; Mokheimer et al., 2024), take into account more factors including temperature, pressure, and hydrocarbon domain expansion, resulting in a better fit to experimental data.

It is important to note that while simplified multi-group models may not perfectly capture all features of the process, the use of such models is often justified because they can effectively predict outcomes at a lower computational cost than more complex approaches.

2. Materials and methods

The main tool for numerical studies in this work is a mathematical model of the process of catalytic reforming of gasolines. The model is developed on the basis of a formalized scheme of hydrocarbon transformations, taking into account the main chemical reactions and the influence of technological parameters on the yield and quality of target products

The input data for model building was collected from the following sources:

- industrial data provided by operating catalytic reforming units at Kazakhstan refineries;
- laboratory analyses of component and group composition of feedstock and reformate;
- literature sources containing kinetic data and characterization of typical catalysts.

Gas chromatography to determine the individual composition of hydrocarbons; infrared spectrometry to assess the presence of functional groups; gravimetric method to measure the content of sulfur and other impurities (GOST 6370-83; GOST 31271-2012; GOST 13379-82) were used to analyze the composition of raw materials.

The data collected covered the characteristics of fractions such as: naphthenic hydrocarbons (cycloalkanes); paraffins (normal and isomeric); aromatic hydrocarbons (benzene, toluene, xylenes).

The model was developed using a sequential and multicomponent approach. At the first stage, a system of differential equations describing the dynamics of changes in component concentrations was determined. To describe the reaction rate, the Arrhenius equations were used, taking into account the influence of temperature and pressure. The equations of material and thermal balances were applied, taking into account the input of raw materials, reaction products and heat losses.

3. Results

3.1 Modeling and validation of the reforming process

The first stage of the study was to determine the key kinetic equations and parameters affecting the reforming process, as well as to build a mathematical model based on a software product. This stage included collection and analysis of data on chemical reactions occurring in the reforming process.

The mathematical model developed in the course of the study allows predicting the behavior of the plant under different conditions, which is the basis for process optimization.

The group and component composition of the oil was then determined. These oil samples were selected in accordance with the information provided by production, which allowed the oil that actually goes to the refinery to be examined.

The method of fractional composition determination was realized using a gas chromatograph ChromateK-5000 (Russia). The process of fractional composition determination was carried out according to the methods specified in (Russel et al., 2023; Sundari and Vaidya, 2012).

After analysis using a gas chromatograph, the chromatogram results were analyzed. Component analysis was performed on each of the oil samples to determine the group composition of the feedstock. This analysis is of key importance for further prediction of oil refining, as it allows not only to understand what hydrocarbons are present in the oil, but also how they can be used in various refining processes.

Oil components were categorized into 69 components, depending on the number of carbon atoms in the molecule. In addition, the contribution of each component to the process of octane number increase was taken into account during the analysis.

Next, process conditions identical to those of the actual operating plant were entered into the Reforming software we developed. This included parameters such as temperature, pressure, feedstock composition and other important factors that directly influence the efficiency of the reforming process. An example of input data such as catalyst temperature or feedstock composition was shown in Figure 1. This data allowed the accuracy of the mathematical model to be verified, as well as the prediction of plant performance under different conditions and with different feedstock types.

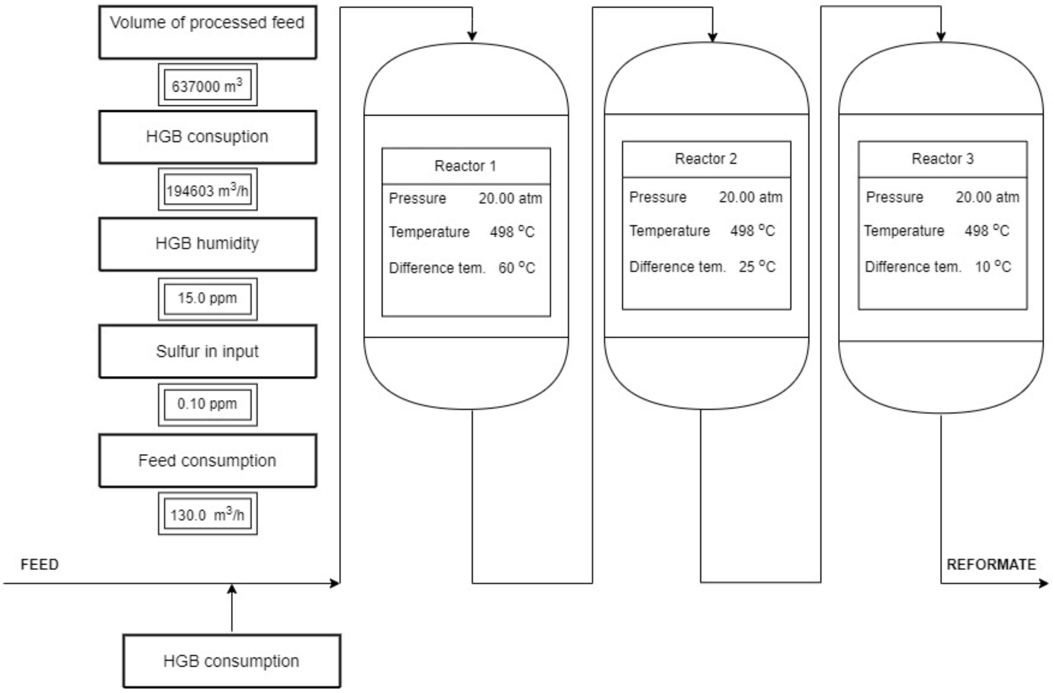


Figure 1. "Reforming" software product with process parameters

3.2 Kinetic and reactor equations

Formalization of the mechanism of hydrocarbons transformation in the reforming process together with aggregation of material flow compositions by homologous series and reactivity of components allows to simplify the model considerably, reduce the number of considered components to 69, while preserving its physicochemical essence.

Aggregation is performed at two levels: by contribution to the octane number increase and by the number of carbon atoms in the molecule, which is an undeniable advantage over numerous other techniques.

The scheme of transformations developed on the basis of the obtained experimental studies is presented in Figure 2.

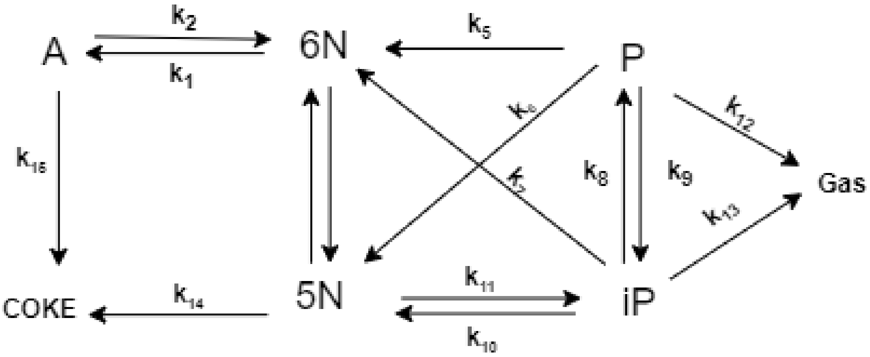


Figure 2. Scheme of hydrocarbon transformations in the catalytic reforming process with chemical reaction rate constants k_n

The catalyst is in a fixed bed through which the oil-gas mixture flows. The reaction kinetics in this case will be more stable and predictable because the reaction conditions in the catalyst bed will be more homogeneous.

The reaction rate will depend on the thickness of the catalyst layer, the intensity of heat exchange and the diffusion of reactants through the layer.

It is important to consider that due to the lack of catalyst movement in the reactor, localized overheating or accumulation of reaction products in the vicinity of the catalyst may occur, which can lead to reduced efficiency.

The catalyst efficiency may be lower than in the moving bed case due to possible diffusion and thermal issues.

The reaction order of each hydrocarbon reactant is one.

According to hypotheses (Chen, 2023; Pasandide and Rahmani, 2021; Yang et al., 2022) and reaction network, reaction rates are expressed by Equations (6–10).

Dehydrocyclization of n-paraffins (i=1–7)

$$r(i) = k_i\left(P(nP_s) - \frac{P(N_s)P(H_2)}{K_{eq,i}}\right), s = 6 - 12. \tag{6}$$

Dehydroaromatization of naphthenes (i=8-15)

$$r(i) = k_i]\left(P(N_s) - \frac{P(A_s)P(H_2)^3}{K_{eq,i}}\right), s = 6 - 12. \tag{7}$$

Isomerization of paraffins (i=16-24)

$$r(i) = k_i\left(P(nP_s) - \frac{P(iP_s)}{K_{eq,i}}\right., s = 4 - 12. \tag{8}$$

Transalkylation of aromatic compounds (i=25-32)

$$r(i) = k_i\left(P(A_s)^2 - \frac{P(A_{s-1})P(A_{s+1})}{K_{eq,i}}\right), s = 7 - 11. \tag{9}$$

Hydrocracking of n-paraffins (i=33–40)

$$r(i) = k_i P(nP_s)P(H_2), s = 5 - 12. \tag{10}$$

Hydrocracking of isoparaffins (i=41–48)

$$r(i) = k_i P(iP_s)P(H_2), s = 5 - 12. \tag{11}$$

Hydrodealkylation of aromatic compounds (i=49–67)

$$r(i) = k_i P(A_s)P(H_2), s = 7 - 12. \tag{12}$$

Reaction of addition of n-paraffins to $\mathrm{nP}_{11}(i = 68)$

$$r(i) = k_i P(nP_8) P(nP_3). \tag{13}$$

Reaction of addition of n-paraffins to $nP_{12} (i = 69 - 70)$

$$r(i) = k_i P(nP_s) P(nP_{12-s}), s = 7 - 8. \tag{14}$$

Reaction of addition of aromatic compounds to $A_{12} (i = 71 - 73)$

$$r(i) = k_i P(A_s) P(nP_{12-s}), s = 7 - 8. \tag{15}$$

In order to model the reforming kinetics taking into account the reversibility of the reactions, the equilibrium constants of the reactions of the aggregated components were first calculated by a procedure using the Want-Goff equation (Samad et al., 2023):

$$\mathrm{Ln}\, K_{pj} = \Delta S_j / R - \Delta H_j / RT. \tag{16}$$

Using standard algorithms of modeling of ideal displacement reactors and equations of material and heat balances, the following model of reforming reactor can be written down (17, 18):

$$\alpha \frac{dY_i}{d\xi} = \rho_k \frac{\tau}{c_0} (w_i - Y_i r_v), \ \frac{d\alpha}{d\xi} = \rho_k \frac{\tau}{c_0} r_v \tag{17}$$

$$\frac{dT}{d\xi} = \frac{\rho_k}{C_p} \frac{\tau}{c_0} \sum_j \ r_j \Delta H_j \tag{18}$$

The main technological parameters of the reforming process, in addition to temperature and pressure, are the volumetric feed rate of liquid feedstock and WSS circulation ratio.

Therefore, it is reasonable to write down the mathematical model of the reactor in the same terms.

$$V_L = \frac{v_L}{V_x^*} \ N_v = \frac{v_x}{v_L} \tag{19}$$

The equation for the temperature will, in this case, have the form:

$$\frac{dT}{d\xi} = \frac{\tau_B}{c_p} \sum \ r_j \Delta H_j. \tag{20}$$

It was found that the activation energies of reactions during the reforming process and for different feedstocks do not change, so their values are assumed constant. The variation of the reaction rate constant with temperature is described by the Arrhenius equation, so calculations are made using the following formula (Chen, 2023; Chen et al., 2023):

$$\mathrm{k_{T2}} = \mathrm{k_{T1}} \cdot \exp\left[-\frac{\mathrm{E_a}}{\mathrm{R}} \cdot \left(\frac{1}{\mathrm{T_2}} - \frac{1}{\mathrm{T_1}}\right)\right]. \tag{21}$$

4. Discussion

Table 1 presents the results of component analysis for 10 oil samples representing different types of hydrocarbon resources. For each sample, a comprehensive examination of the component composition, including determination of hydrocarbon content, was performed. These results facilitate comparative analysis and help identify compositional characteristics unique to each sample.

Table 1. Compositions of raw materials for catalytic reforming

Fraction	**Number of sample**									
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
n-paraffins, (%)	21.78	22.10	23.81	31.55	29.82	21.58	24.20	24.24	26.76	25.85
iso-paraffins, (%)	24.25	19.14	18.71	25.83	23.64	24.33	26.63	23.29	22.41	23.40
naphthenes, (%)	31.61	33.89	30.90	30.24	26.95	31.00	32.44	44.50	40.35	40.58
Aromatic hydrocarbons, (%)	22.34	24.90	26.60	12.39	19.58	23.07	16.73	7.11	9.62	8.88

Table 1 shows that the content of n-paraffins in the analyzed samples ranges from 21.58% to 31.55%. Higher concentration of n-paraffins increases the yield of high-octane products, as they are easily converted into aromatic hydrocarbons.

The share of isoparaffins varies from 18.71% to 26.63%. Despite their lower reactivity, their presence contributes to the increase of octane number in the final product due to isomerization and cyclization processes. The content of naphthenes ranges from 26.95% to 44.5%, which is advantageous for the reforming process, since naphthenes are easily transformed into aromatic compounds, which further increases the octane number.

The aromatic hydrocarbon content ranges from 7.11% to 26.6%, indicating that the feedstock already has some high-octane properties. Nevertheless, careful monitoring of coke formation is essential to maintain process efficiency. Among the analyzed feedstocks, materials with high naphthene content are considered to be the most valuable for the reforming process, since naphthenes are converted into aromatic hydrocarbons with higher selectivity than paraffinic hydrocarbons.

4.1 Simulation

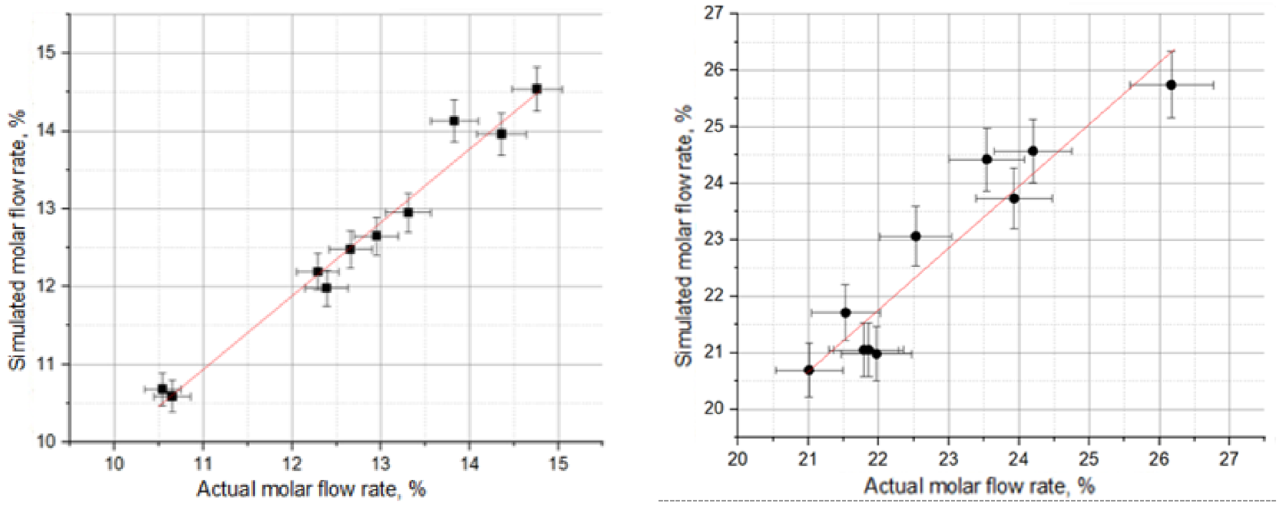
Based on the proposed mathematical model, a software tool for modeling and analysis of the reforming process was developed. The software functions as a database management system, providing efficient storage, management and quick access to source materials and process data.

The main component of the software is a digital block diagram that visualizes and simulates the entire processing sequence. This flowchart provides a comprehensive representation of material and energy flows at each process step, allowing detailed monitoring of changes in raw materials and reaction products. The system displays all inputs and outputs, as well as critical parameters such as temperature, pressure, feedstock flow rate and other key process characteristics needed for thorough analysis and optimization.

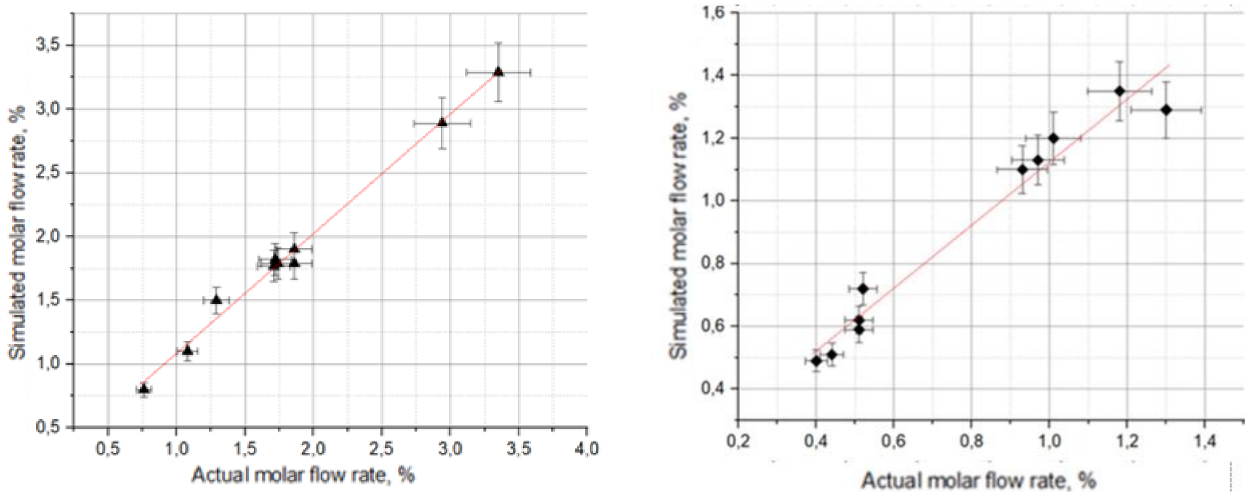
The software is implemented using the Python programming language for flexibility, scalability and easy integration with other analytical tools.

4.2 Model validation

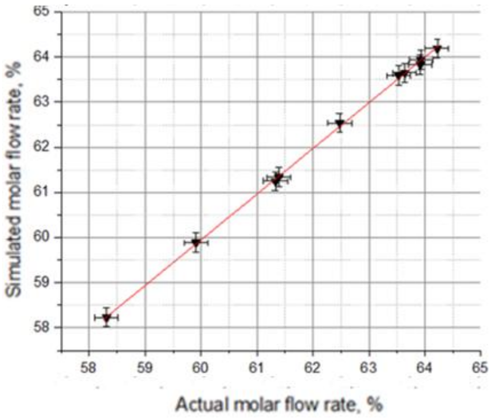
Figure 3 shows a comparison of actual plant data and model predictions, providing an assessment of the adequacy of the developed kinetic model. Ten data sets from the plant were analyzed to validate the model, with operating conditions and feedstock consumption set in accordance with the plant's technical regulations. This comparison allows us to evaluate the accuracy of the model in predicting the efficiency of the reforming process under real operating conditions, ensuring its reliability for further analysis and optimization of the process.



a) n-paraffins b) iso-paraffins



c) cycloalkanes – 5 d) cycloalkanes – 6



e) Aromatic hydrocarbons

Figure 3. Comparison of calculated and experimental values of catalytic parameters

To increase the reliability of the results of modeling and analysis of the catalytic reforming process, statistical processing of experimental and calculated data was carried out. The main statistical methods used were the estimation of standard deviation, coefficient of variation and correlation analysis between calculated and actual parameters.

Table 2. Results of statistical processing of data

Fraction	**Average error**	**Mean absolute error**	**Coefficient of determination (R^2)**
n-paraffins	-0.18	0.21	0.98
iso-paraffins	0.06	0.55	0.97
cycloalkanes-5	-0.03	0.06	0.99
cycloalkanes-6	-0.08	0.10	0.98
aromatic hydrocarbons	0.00	0.06	0.99

The coefficients of determination (R^2) for all fractions exceed 0.97, indicating a high degree of consistency of the calculated data with the industrial results.

The aromatics fraction showed the highest prediction accuracy ($R^2 = 0.99$) with the lowest average error. Iso-paraffins showed a slightly higher average absolute error (0.55), indicating the possible influence of compositional uncertainty or process variations.

It should be noted that rate constants in generalized kinetic models usually depend on feedstock and catalyst characteristics, and their use for modeling reforming reactors under other feed conditions may not be appropriate if they are determined for specific conditions. However, if the kinetic model is sufficiently detailed, the rate constants can be considered independent of the initial feedstock composition, allowing them to be used to model reactors at other feed conditions. The main problem with the use of more complex models is that the simplicity of the kinetic representations inherent in models with a small number of generalizations is partially lost. The use of models with a large number of generalizations requires much more experimental data.

The developed model can be used for operational control of the reforming process at operating plants. It allows predicting changes in product composition when varying process parameters, which contributes to increased production flexibility and adaptation to changing market conditions. In addition, the model can serve as a tool for personnel training and practicing various scenarios of plant operation without risk to real production.

Implementation of the developed mathematical model into industrial practice will improve the efficiency and environmental safety of the catalytic reforming process. Accounting for catalyst deactivation and optimization of process parameters on the basis of the model will ensure stable product quality and extension of catalyst service life, which has a significant economic effect for oil refining enterprises.

5. Conclusion

In the framework of this study, a kinetic model of the catalytic reforming process was developed based on data from a commercial fixed bed catalyst plant. The model parameters were determined using the method of minimization of discrepancies between calculated values and industrial data, which provided a high degree of accuracy in predicting the reformate composition.

The proposed model combines the simplicity of generalized approaches with the advantages of more detailed models to effectively predict reformate composition and account for key process variables (temperature, pressure, hydrogen/hydrocarbon ratio and feed rate). Validation of the model was performed on both laboratory isothermal data and industrial data from commercial plants, confirming its versatility and practical applicability.

The developed program product based on this mathematical model demonstrated a high degree of adequacy. The total error of calculations was less than 3%. The error in determining the concentration of aromatic hydrocarbons was less than 1%.

These results indicate the accuracy and high detail of the model, which allows using it for operational control of the reforming process and development of recommendations for optimization of the plant operation mode.

The application of the developed model in industry will allow not only to increase the yield of target products and improve fuel quality, but also to reduce production costs by optimizing operating modes and extending catalyst lifetime. In today's conditions of tightening environmental requirements, such a model is an important tool to ensure sustainable development of oil refineries.

Future research aimed at integrating the model with digital control systems and optimizing energy efficiency can significantly improve the competitiveness of Kazakhstan's oil and gas enterprises and ensure compliance with international quality and environmental safety standards.

Thus, the developed kinetic model is not only a scientific achievement, but also a practical solution to improve the efficiency of reforming processes under the conditions of modern requirements to fuel quality and sustainable development of the industry.

6. Supplementary Materials: No Supplementary Materials.

7. Author Contributions

R.D. – research concept, text writing; M.B. – data analysis; Y.S. – data collection and processing, illustrations; I.K. – data collection and processing.

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11. Conflicts of Interest: The authors declare no conflicts of interest.

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Өнеркәсіптік деректер негізінде бекітілген қабаттағы каталитикалық риформинг процесін модельдеу

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Аңдатпа: Бұл зерттеуде каталитикалық риформинг процесінің кинетикалық үлгісі коммерциялық тұрақты катализатор зауытының деректерін пайдалана отырып әзірленді. Модельдік параметрлер есептелген мәндер мен өнеркәсіптік деректер арасындағы сәйкессіздіктерді азайту арқылы, қайта пішімдеу құрамын болжауда жоғары дәлдікті қамтамасыз ету арқылы анықталды. Ұсынылған модель жалпыланған тәсілдердің қарапайымдылығын егжей-тегжейлі үлгілердің артықшылықтарымен біріктіреді, бұл қайта пішімдеу құрамын тиімді болжауға және негізгі технологиялық айнымалыларды (температура, қысым, сутегі/көмірсутек қатынасы және беру жылдамдығы) есепке алуға мүмкіндік береді. Валидация зертханалық изотермиялық деректермен де, оның практикалық қолдану мүмкіндігін растайтын өнеркәсіптік деректермен де жүргізілді. Осы үлгі бойынша әзірленген бағдарламалық қамтамасыз ету жоғары дәлдікті көрсетті, ароматты көмірсутек концентрациясын анықтауда 3%-дан аз және 1%-дан аз қателікпен есептеу қателері бар. Бұл нәтижелер модельдің дәлдігін растап, оны нақты уақыттағы процесті басқару және оңтайландыру үшін қолайлы етеді. Модельді өнеркәсіпте қолдану мақсатты өнімдердің шығымдылығын арттырып, отын сапасын жақсартып қана қоймайды, сонымен қатар жұмыс режимдерін оңтайландыру және катализатордың қызмет ету мерзімін ұзарту арқылы өндіріс шығындарын азайтады. Экологиялық ережелерді қатайтуды ескере отырып, модель мұнай өңдеу зауыттарында тұрақты дамуды қамтамасыз етудің маңызды құралы болып табылады. Болашақ зерттеулер оның цифрлық басқару жүйелерімен интеграциясын жақсартуға және Қазақстанның мұнай-газ кәсіпорындарында энергия тиімділігін оңтайландыруға мүмкіндік береді.

Түйін сөздер: математикалық модельдеу, мұнай өңдеу, оңтайландыру, ресурс тиімділігі, мұнай химиясы, каталитикалық риформинг

Моделирование процесса каталитического риформинга с неподвижным слоем катализатора на основе промышленных данных

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Аннотация: В данном исследовании была разработана кинетическая модель процесса каталитического риформинга с использованием данных с коммерческой установки с неподвижным слоем катализатора. Параметры модели были определены путем минимизации расхождений между расчетными значениями и промышленными данными, что обеспечивает высокую точность прогнозирования состава риформата. Предложенная модель сочетает в себе простоту обобщенных подходов с преимуществами более подробных моделей, что позволяет эффективно прогнозировать состав риформата и учитывать ключевые переменные процесса (температуру, давление, соотношение водорода и углеводородов и скорость подачи). Валидация была проведена как с лабораторными изотермическими данными, так и с промышленными данными, что подтвердило ее практическую применимость. Разработанное на основе этой модели программное обеспечение продемонстрировало высокую точность с погрешностью расчетов менее 3% и погрешностью определения концентрации ароматических углеводородов менее 1%. Эти результаты подтверждают точность модели, что делает ее пригодной для управления процессом в реальном времени и его оптимизации.

Применение модели в промышленности позволит не только увеличить выход целевых продуктов и улучшить качество топлива, но и снизить себестоимость продукции за счет оптимизации режимов работы и продления срока службы катализатора. Учитывая ужесточение экологических норм, модель является важным инструментом для обеспечения устойчивого развития нефтеперерабатывающих заводов. Дальнейшие исследования могут улучшить интеграцию с цифровыми системами управления и оптимизировать энергоэффективность на нефтегазовых предприятиях Казахстана.

Ключевые слова: математическое моделирование, нефтепереработка, оптимизация, ресурсоэффективность, нефтехимия, каталитический риформинг