International Journal of Innovative Research and Scientific Studies, 8(2) 2025, pages: 3403-3413

ISSN: 2617-6548

URL: www.ijirss.com

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

Yekaterina Zhakmanova[1], Rizagul Dyussova[2], Gaini Seitenova[1*], Moldir Borashova[3]

[1]*Department of Chemistry, L.N. Gumilyov Eurasian National University, Astana 010000, Kazakhstan.*
[2]*Department of Mechanics and Oil and Gas Business Institution Toraigyrov University, Astana, 010000, Kazakhstan.*
[3]*Department of Oil and Gas Engineering and Ecology Institution Atyrau University of Oil and Gas, Atyrau, 060000, Kazakhstan.*

Corresponding author: Gaini Seitenova (*Email: gainiseitenova@gmail.com*)

Abstract

This study presents the development of a mathematical model for the simulation and analysis of the catalytic reforming process using a Python-based software tool. The model captures the kinetics of hydrocarbon feedstock processing within a fixed catalyst bed, ensuring a balance between accuracy and computational efficiency. A key feature of the software is a digital flow diagram that visualizes material and energy flows at each stage of the process while displaying critical parameters such as temperature, pressure, and flow rate. To validate the model's accuracy, the calculated data were compared with experimental values obtained from commercial fixed-bed reforming units. The results showed an absolute calculation error of no more than 3%, confirming the model’s reliability in accurately describing reforming processes. Furthermore, the study investigates the effects of temperature and pressure variations on the final product yield to enhance process efficiency and optimize operating conditions.

Keywords: Catalytic reforming, chemical engineering, fuel, mathematical modeling, process simulation.

DOI: 10.53894/ijirss.v8i2.6015
Funding: This research was funded by the Committee of Science of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP23487495 «Improving resource efficiency and energy conservation in the technology of petroleum processing product preparation through hybrid modeling»).
History: Received: 7 March 2025 / **Revised:** 3 April 2025 / **Accepted:** 5 April 2025 / **Published:** 8 April 2025

Competing Interests: The authors declare that they have no competing interests.
Authors’ Contributions: All authors contributed equally to the conception and design of the study. All authors have read and agreed to the published version of the manuscript.
Transparency: The authors confirm that the manuscript is an honest, accurate, and transparent account of the study; that no vital features of the study have been omitted; and that any discrepancies from the study as planned have been explained. This study followed all ethical practices during writing.
Publisher: Innovative Research Publishing

1. Introduction

Catalytic reforming is an important process in the petrochemical industry to improve petrol quality and produce high-quality chemical products. It plays a key role in increasing the octane rating of fuels and the production of aromatic hydrocarbons and hydrogen, making it an indispensable process in petroleum refining. Mathematical modeling of the catalytic reforming process began to develop in the 1950s when the first attempts to describe the reactions in the catalyst using empirical data appeared. In the 1970s and 1980s, the models became more complex, considering isomerization, dehydrogenation, and other reaction mechanisms, as well as hydrocarbon interactions. Since then, differential equations and numerical methods have begun to be used to improve accuracy [1-4]. In the 1990s, dynamic models describing real-time changes in concentrations and temperature became available. The inclusion of parameters such as temperature, pressure, and catalyst degradation improved the prediction of reactor performance. Grouping methods have also become popular for simplifying modeling [5-7]. Since the 2000s, molecular models and new techniques such as machine learning have been used to optimize catalyst performance and predict product composition. The models have taken into account a wider range of parameters, which has improved the accuracy of predictions and the economic efficiency of the process [8-10].

Recently, there has been renewed interest in the reforming process, firstly because reformate is the main source of aromatic hydrocarbons in petrol, and secondly because of new legislation concerning benzene and aromatic hydrocarbon content in commercial petrol [11, 12].

Below are the basic chemical reactions of the reforming process [13]:

Equation 1 shows the isomerization of normal alkanes into azoalkanes. It is a fast-running exothermic reaction with negligible heat release and a small 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 temperatures favor the acceleration of the reaction. Isomerization reactions take place on acidic catalyst centers.

$$\text{n-}C_6H_{14} \rightarrow C_6H_{14} \tag{1}$$

Equation 2 shows the dehydrocyclization (aromatization) of alkanes, which proceeds in several stages, the main one being dehydrogenation with the release of 1 mole of H2 and subsequent rearrangement of the molecule, formation of a cycloalkane, and subsequent dehydrogenation of this cycloalkane. The reaction proceeds on the metallic and acidic centers of the catalyst. Alkanes with higher molecular weights 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; however, in general, this rate is much lower than the rate of the cycloalkane dehydrogenation reaction.

$$C_6H_{14} \rightarrow C_6H_6 + 4H_2 \tag{2}$$

The dehydrogenation of naphthenes to arenes, shown in Equation 3, proceeds on metal catalyst centers. These are endothermic reactions favored by high temperature and low pressure. The rate of these reactions is high compared to other reactions. Since the dehydrogenation of naphthenes provides high-octane components, the intensification of this reaction is the most desirable process.

$$C_6H_{12} \rightarrow C_6H_6 + 3H_2 \tag{3}$$

Equation 4 shows the isomerization of five-membered cycloalkanes into cyclohexane derivatives. An exothermic reaction proceeds at a relatively low rate, increasing with increasing number of carbon atoms in the molecule.

$$C_5H_9\text{-}CH_3 \rightarrow C_6H_{12} \tag{4}$$

Equation 5 shows the hydrocracking of alkanes: the reaction, which has two stages and proceeds on both metal and acid catalyst centres. In the first stage, the dehydrogenation reaction takes place on the metal centres, followed by the rupture of the resulting alkene molecule on the acid centre and hydrogenation of the resulting short-chain alkene. 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.

$$\text{n-}C_9H_{20} + H_2 \rightarrow \text{i-}C_4H_{10} + \text{i-}C_5H_{12} \tag{5}$$

Equation 6 shows the conversion of naphthenes to alkanes: an exothermic side reaction, shown in Equation 6, accelerating with increasing temperature and pressure.

$$C_6H_{12} + H_2 \rightarrow C_6H_{14} \tag{6}$$

Various kinetic models have been described in the literature to represent the catalytic reforming process. All these models consider 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.

Arani et al. [14] presented a new kinetic model that accounts for the most important reforming reactions for paraffins, naphthenes, and aromatic hydrocarbons, and extends the hydrocarbon region to 11 carbon atoms. The effect of temperature and pressure on the kinetic constants is modeled through an Arrhenius-type variation. The proposed model includes 24 differential equations and 71 kinetic parameters, which were estimated using experimental data from a fixed-bed catalyst plant. The results of the reformate composition calculations agree well with the experimental data, with a deviation of less than 3%. Wei et al. [15] devoted themselves to the dynamic modeling of the catalytic reforming of naphtha to study the behavior of hydrocarbon components such as paraffin, naphthene, and aromatic hydrocarbons in the reactor under different operating conditions. The study focuses on modeling changes in hydrocarbon concentrations during the reforming process, as well as analyzing temperature and hydrogen profiles along the reactor. Using mathematical modeling, the authors demonstrate how different behaviors arise in the reactor at various stages of the process, and how reactor temperature and hydrogen concentration evolve. Additionally, the effect of variations in naphtha feed temperature on process dynamics and output product concentration is investigated, resulting in conclusions on optimizing reactor operation to achieve optimal results in high-octane reformation production.

Researchers Mokheimer et al. [16] showed the construction of a molecular model of the catalytic reforming process of naphtha and its optimization taking into account 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. Additionally, other researchers [14] devoted themselves to modeling the catalytic reforming process of naphtha, which is important for the production of high-octane gasoline. 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 the combining of feedstock components, which significantly reduces the complexity of calculations. Researchers Elizalde and Ancheyta [17] and Jarullah et al. [18] derived several kinetic models of reforming - which are used in this study - and proposed a model in which naphtha is represented by 17 hydrocarbon fractions with 15 reaction pathways and a simple catalyst deactivation model proposed in Mokheimer et al. [16]. The model contains 17 "pseudo-components" connected by 15 reaction pathways. The kinetic and thermodynamic parameters of the model were obtained by optimization using plant data. Additionally, the authors propose equations for calculating thermodynamic constants of equilibrium 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 advantages and limitations Some models, such as the model [19], have disadvantages such as not accounting for isomerization or the effect of temperature and pressure on the kinetic constants. In response to these limitations, new models [16] take into account more factors including temperature, pressure, and hydrocarbon domain expansion, resulting in a better fit to the experimental data.

In addition, dynamic modeling proposed in other works helps to study the behavior of hydrocarbons in the reactor as well as the influence of operating conditions, such as temperature and hydrogen concentration, on the reforming process. Some studies focus on optimizing reactor operation to produce high-quality reformate, as well as improving the accuracy of predicting product composition through molecular and grouping models [20, 21]. The method of lumping (grouping) components greatly simplifies modeling, making it more manageable.

In general, current approaches to catalytic reforming modeling aim to enhance accuracy and optimize the process by considering multiple factors, thereby improving the efficiency of high-quality fuel production.

It is important to note that, although a simple multi-lump model may not perfectly align with existing scenarios, the use of compact models is not always justified. This is because a significant volume of experimental data must be collected to determine the parameters, which is both time-consuming and costly. Therefore, the most appropriate model is one that, despite its simplicity, can accurately predict the outcomes.

2. Materials and Methods

The main tool for numerical studies in this work is a mathematical model of the catalytic reforming of petrol. This model is based on a formalized scheme of hydrocarbon transformations, in which all components of naphtha and reformate are divided into groups: naphthenic (cyclohexanes and cyclopentanes), normal and isomeric paraffins, and aromatic hydrocarbons:

A sequential and multi-component approach was implemented during the study. In the first stages, data on dynamic reactions and conditions affecting the reforming process were collected. This is an analysis of the composition and characterization of the initial result, as well as a study of the reactions occurring during the reforming process.

The component and group composition of the studied feedstock was determined. Based on the collected information, a mathematical model reflecting the key processes of reforming was developed. Specialized software was utilized to integrate key process parameters (temperature, pressure, flow composition) to create a model capable of predicting plant performance under varying conditions. This model served as the foundation for further process simulations, enabling analysis of the system’s behavior under different scenarios.

2.1. Process and Commercial Plant Description

The modeling was conducted for a semi-regenerative reforming unit processing straight-run gasoline (fraction 85–140°C). The rate constants and activation energies for individual reactions were previously determined by researchers based on laboratory and semi-industrial installations and were refined in this study using chromatographic data to achieve a more accurate representation of the feedstock and reaction product composition. Figure 1 illustrates the technological scheme of the semi-regenerative reforming unit, highlighting the key process stages and flow configuration. This includes the catalytic reforming of hydrocarbons facilitated by the Pt-Sn catalyst.

The feedstock, a stable hydrogenated product obtained from the unit where gasoline fraction hydrofining takes place, is first directed to the raw material pumps, which transport it to a mixing tee for blending with the circulating hydrogen-bearing gas (HGB). The resulting mixture is preheated in heat exchanger 1 by the gas-product flow from reactor 3, then further heated in the first section of heater 2 before entering reactor 1. Subsequently, it undergoes additional heating in the second section of heater 3, passes through reactor 2, and finally flows through the third section of heater 1 before reaching reactor 3.

The gas-product mixture from reactor 3 transfers part of its heat to the gas-feed flow in heat exchanger 2, then undergoes cooling in air cooler 1 and water cooler 2 before entering gas separator 1. In the separator, hydrogen-containing gas is separated from the liquid product, known as the unstable catalyst. The separated hydrogen-containing gas is sent for excess moisture removal and subsequently directed to the intake of the circulation compressor, which recycles it for mixing with the feedstock. Excess HBG is either directed to the gasoline fraction hydrofining unit or to the plant's hydrogen network.

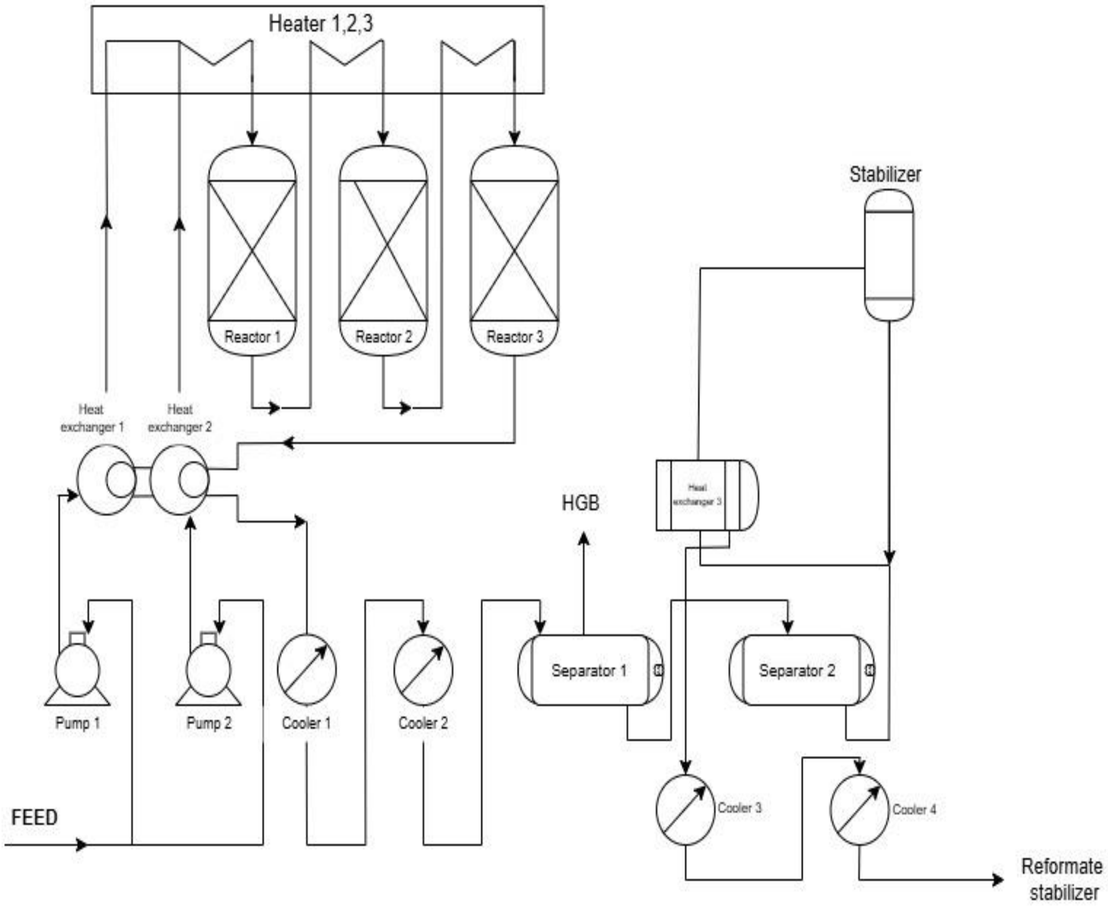

Figure 1.
Basic process flow diagram of a reforming unit with a fixed catalyst bed.

The unstable product from separator 1 is preheated in heat exchanger 3 by the stable catalyst flow and then enters the middle section of stabilizer column 1 for stabilization, where dissolved gaseous hydrocarbons are separated. Light hydrocarbons, including butanes, are removed from the top of the stabilizer. The stable reforming catalyst is withdrawn from the bottom of stabilizer column 1, passes through heat exchanger 3, is cooled in air cooler 3 and water cooler 4, and is subsequently sent to the storage park as a finished product.

2.2 Modeling and Validation of the Reforming Process

The initial stage of this study involved identifying key kinetic equations and parameters influencing the reforming process, followed by the development of a mathematical model using specialised software. This phase encompassed data collection and analysis of the chemical reactions occurring during reforming. The resulting mathematical model facilitates the prediction of plant behaviour under various conditions, serving as a foundation for process optimisation.

Subsequently, the group and component composition of the oil was determined. Oil samples were selected based on production data to ensure an accurate representation of the refinery's feedstock. The fractional composition of the oil was analysed using a ChromateK-5000 gas chromatograph (Russia), per established methodologies [22, 23].

The chromatographic data was then examined to determine the group composition of the feedstock, which is critical for predicting refining performance. This analysis provides insights into the hydrocarbon content and its potential utilisation in various refining processes.

Oil components were categorised into 69 groups based on the number of carbon atoms in their molecules, with their contributions to octane number enhancement carefully considered during the analysis.

Process conditions replicating those of the actual operating plant were then integrated into the custom-developed software "Reforming". These conditions included parameters such as temperature, pressure, and feedstock composition - key factors influencing reforming efficiency. Figure 2 presents an example of input data, including catalyst temperature and feedstock composition. These inputs enabled the verification of the model's accuracy and facilitated performance predictions under varying conditions and different feedstocks.

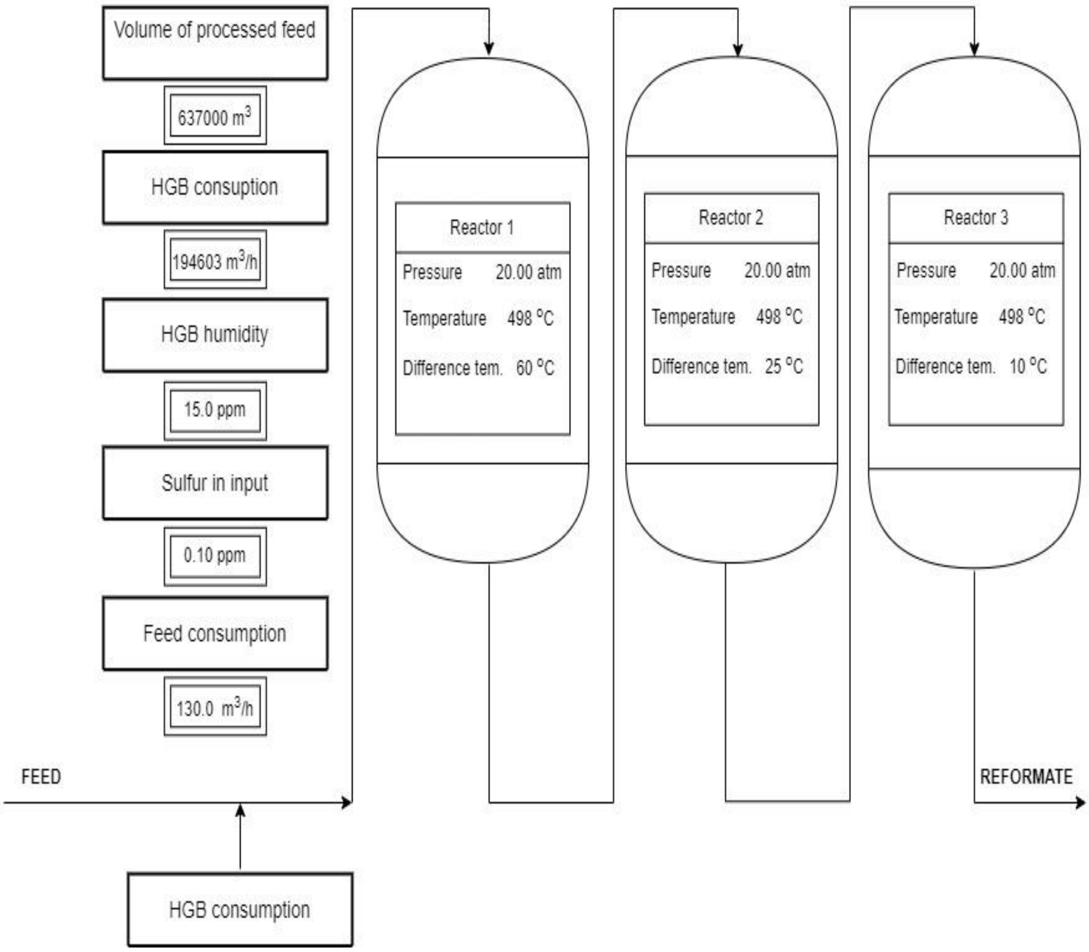

Figure 2.
Reforming" software product with entered technological modes.

2.3. Kinetic and Reactor Equations

The formalization of the hydrocarbon transformation mechanism in the reforming process, combined with the aggregation of material flow compositions by homologous series and component reactivity, significantly simplifies the model. This approach reduces the number of considered components to 69 while preserving the fundamental physicochemical properties of the process.

Aggregation is carried out on two levels: based on the contribution to octane number improvement and the number of carbon atoms in the molecule. This dual-level aggregation provides a distinct advantage over many existing methods by enhancing model accuracy and computational efficiency.

Figure 3 illustrates the transformation scheme, developed based on the experimental findings.

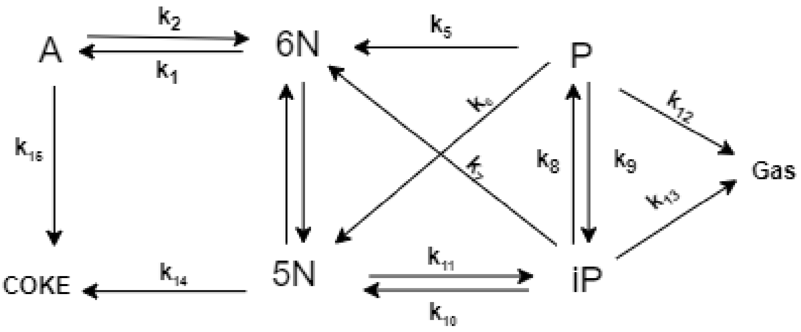

Figure 3.
Scheme of hydrocarbon transformations in the catalytic reforming process with chemical reaction rate constants (k_n).

The rate constants of chemical reactions (k_n), corresponding to the chosen formalised mechanism of the process, are determined from the available experimental information, measured with some error, as well as according to references in the literature [24, 25].

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 since the reaction conditions in the catalyst bed will be more homogeneous [26].

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, localised 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 problems and thermal phenomena [27].

The reaction order of each hydrocarbon reactant is one.

According to the hypotheses [28-31] and the reaction network, the reaction rates are expressed by equations (7-16)
Dehydrocyclization of n-paraffins ($i = 1 - 7$)

$$r(i) = k_i \left(P(nP_s) - \frac{P(N_S)P(H_2)}{K_{eq,i}} \right), s = 6 - 12 \tag{7}$$

Dehydroaromatisation of naphthenes ($i = 8 - 15$)

$$r(i) = k_i \left(P(N_s) - \frac{P(A_S)P(H_2)^3}{K_{eq,i}} \right) s = 6 - 12 \tag{8}$$

Isomerisation of paraffins ($i = 16 - 24$)

$$r(i) = k_i \left(P(nP_s) - \frac{P(iP_S)}{K_{eq,i}} \right), s = 4 - 12 \tag{9}$$

Transalkylation of aromatics ($i = 25 - 32$)

$$r(i) = k_i \left(P(A_s)^2 - \frac{P(A_{S-1})P(A_{S+1})}{K_{eq,i}} \right), s = 7 - 11 \tag{10}$$

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

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

Hydrocracking of iso-paraffins ($i = 41 - 48$)

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

Hydrodealkylation of aromatics ($i = 49 - 67$)

$$r(i) = k_i P(A_s)P(H_2), s = 7 - 12 \tag{13}$$

Addition reaction of n -paraffins to nP_{11}($i = 68$)

$$r(i) = k_i P(nP_8)P(nP_3) \tag{14}$$

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

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

Addition reaction of aromatics to A_{12}($i = 71 - 73$)

$$r(i) = k_i P(A_s)P(nP_{12-s}), s = 7 - 8 \tag{16}$$

To model the kinetics of reforming while accounting for the reversibility of reactions, the equilibrium constants for the reactions of aggregated components were initially calculated using the Van't Hoff equation (17) [30]:

$$\ln K_{pj} = \Delta S_j / R - \Delta H_j / RT \tag{17}$$

By applying standard algorithms for modeling ideal plug flow reactors, along with material and heat balance equations, the reforming reactor model can be formulated as follows (18,19) [24]:

$$\alpha \frac{dY_i}{d\xi} = \rho_k \frac{\tau}{c_0}(w_i - Y_i r_v),\ \frac{d\alpha}{d\xi} = \rho_k \frac{\tau}{c_0} r_v \tag{18}$$

$$\frac{dT}{d\xi} = \frac{\rho_k}{C_p}\frac{\tau}{c_0}\sum_j r_j \Delta H_j \tag{19}$$

Aside from temperature and pressure, the primary technological parameters of the reforming process include the liquid feedstock's volumetric feed rate and the hydrogen-bearing gas (HGB) circulation ratio. Accordingly, it is appropriate to formulate the mathematical model of the reactor using these parameters.

$$V_L = \frac{v_L}{V_x^*}\ N_v = \frac{v_x}{v_L} \tag{20}$$

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

$$\frac{dT}{d\xi} = \frac{\tau_B}{c_p}\sum r_j \Delta H_j \tag{21}$$

It has been established that the activation energies of reactions during the reforming process remain constant across different feedstocks; therefore, their values are assumed to be invariant. The Arrhenius equation describes the temperature dependence of the reaction rate constant, and the calculations are performed using the following formula [31]:

$$\mathrm{K_{T2}} = \mathrm{k_{T1}} \cdot \exp\left[-\frac{\mathrm{E_a}}{\mathrm{R}} \cdot \left(\frac{1}{\mathrm{T_2}} - \frac{1}{\mathrm{T_1}}\right)\right] \tag{22}$$

3. Results

This section may be divided by subheadings. It should provide a concise and precise description of the experimental results, their interpretation, as well as the experimental conclusions that can be drawn. Table 1 presents the results of the component analysis for 10 different oil samples, representing various types of hydrocarbon resources. A comprehensive examination of the component composition was conducted for each sample, including the determination of hydrocarbon content. These results facilitate comparative analysis and help identify the compositional characteristics unique to each sample.

Table 1 shows that the content of n-paraffins in the analyzed samples ranges from 21.58% to 31.55%. A higher concentration of n-paraffins enhances the yield of high-octane products, as they readily convert into aromatic hydrocarbons.

Table 1.
Compositions of raw materials for catalytic reforming.

Fraction	Number of samples									
	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

The proportion of iso-paraffins varies between 18.71% and 26.63%. Although less reactive, their presence contributes to an improved octane number in the final product through isomerization and cyclization processes.

Naphthene content ranges from 26.95% to 44.5%, which is advantageous for the reforming process, as naphthenes are easily transformed into aromatics, further enhancing the octane number.

The aromatic hydrocarbon content varies between 7.11% and 26.6%, indicating that the feedstock already possesses some high-octane properties. However, careful monitoring of coke formation is essential to maintain process efficiency.

Among the analyzed feedstocks, those with a high naphthene content are considered the most valuable for the reforming process, as naphthenes convert to aromatic hydrocarbons with higher selectivity compared to paraffin hydrocarbons.

3.1. Simulation

A software tool was developed based on the proposed mathematical model to simulate and analyse the reforming process. The software functions as a relational database management system, ensuring efficient storage, management, and rapid access to feedstock and process data.

The core component of the software is a digital flow chart that visualizes and simulates the entire processing sequence. This flow chart provides a comprehensive representation of material and energy flows at each stage of the process, enabling detailed tracking of changes in raw materials and reaction products. The system displays all inputs and outputs, along with critical parameters such as temperature, pressure, feedstock flow rate, and other key process characteristics essential for thorough analysis and optimization.

The software is implemented using Python programming language, ensuring flexibility, scalability, and ease of integration with other analytical tools.

3.2. Model Validation

Figure 4 presents the comparison between actual plant data and model predictions, providing an assessment of the adequacy of the developed kinetic model. To validate the model, ten datasets from the plant were analyzed, with operating conditions and raw material flow rates set according to the plant's technical regulations. This comparison enables the evaluation of the model's accuracy in predicting the reforming process performance under real operating conditions, ensuring its reliability for further process analysis and optimization.

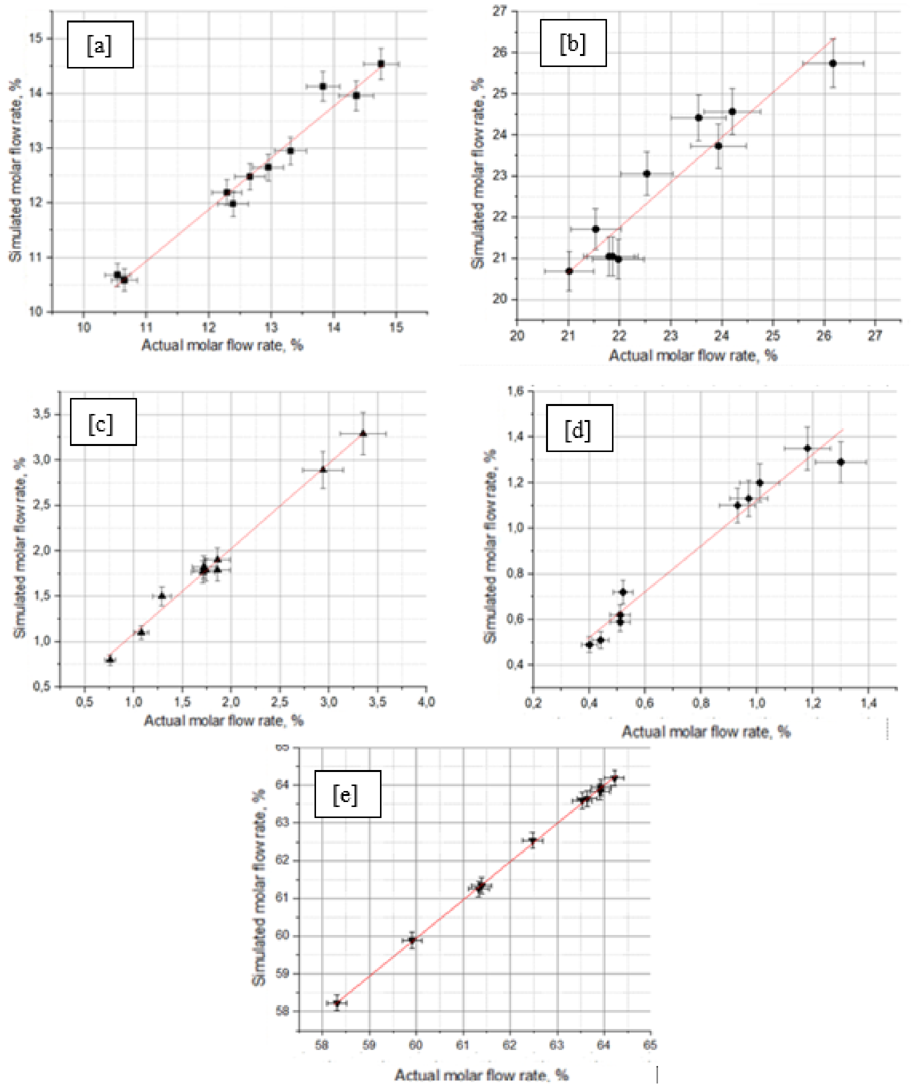

Figure 4.
Comparison between calculated and experimental values of catalytic reforming parameters.
[a] n-paraffins, [b] i-paraffins, [c] five-membered naphthenes, [d] six-membered naphthenes, [e] aromatics.

Figure 4 shows a comparison of experimental data and predicted reforming molar composition for several selected hydrocarbon types. The calculated values agree well with the experimental information, with a deviation of less than 3%. In particular, the composition of aromatic hydrocarbons coincides with the experimental data, with a maximum deviation of less than 1%.

The 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 their use for modeling 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 significantly more experimental data. However, as shown in Figure 4, the results demonstrate that the developed kinetic model is sufficiently detailed to consider the kinetic parameters independent of the feedstock composition.

4. Discussion

Table 1 shows the composition of the feedstock, demonstrating that n-paraffins, iso-paraffins, naphthenes, and aromatics play distinct roles in the reforming process. Feedstocks with high n-paraffin and naphthene content are particularly advantageous for producing high-octane products due to their efficient conversion to aromatic hydrocarbons. However, monitoring the process to prevent coke formation is critical to maintaining efficiency.

Figure 4 illustrates the validation of the developed model by comparing experimental data with predicted reforming parameters. The results show that the predicted parameters closely align with the experimental data, with deviations consistently under 3%. The exceptionally high agreement for aromatic hydrocarbons (deviation below 1%) underscores the model's reliability and accuracy. This alignment demonstrates the model's robustness, especially given its ability to generalize kinetic parameters across different feedstock compositions.

Figure 4 further highlights that, despite the complexity of reforming kinetics, the developed model achieves an effective balance between simplicity and detail. By incorporating sufficient detail into the kinetic parameters, the model remains applicable across diverse feed conditions without requiring excessive experimental data. The predictions for n-paraffins, iso-paraffins, naphthenes, and aromatics, as shown in Figure 4, align well with experimental results, reflecting the model's reliability.

Overall, the results highlight the practicality and adaptability of the developed model in improving catalytic reforming outcomes. The capability to predict and optimize process performance across varying conditions ensures its utility in enhancing high-octane fuel production while maintaining cost and operational efficiency.

5. Conclusion

- A kinetic model for the catalytic reforming process was developed based on data from a commercial fixed-bed catalyst plant. The parameters of this model were determined by minimizing the discrepancies between the calculated values of the model and real data.
- Using this model, the influence of feedstock compositions on the quality of the catalytic reforming product - reformate - has been investigated, and predictive calculations using the model have been performed, considering catalyst deactivation. It is demonstrated that the mathematical model allows us to consider the influence of feedstock on the yield and quality of reformate and also corresponds to the catalyst used.
- The kinetic model proposed in this work combines the simplicity of generalized approaches with the capabilities of more complex models, as it can accurately predict the reformate composition and considers key process variables affecting the behavior of the reacting system. Validation and use of the model are carried out using real data from both laboratory isothermal experiments and commercial plants.
- The software product developed based on the presented mathematical model showed a high degree of adequacy: the overall error was less than 3%, and the error of the main reforming target product—aromatic compounds—was less than 1%. This indicates a high level of detail and accuracy of the presented model.

Symbols

Symbol	**Definition**
α	Degree of change in the number of moles of hydrocarbons.
N_v	HBG circulation rate
v_b	Hydrogen-containing gas (HCG) flow rate.
V_L	volumetric feed rate of liquid raw material
C_p	Heat capacity of the reaction mixture
E_a	Activation energy
R	Universal gas constant
c_i	Molar concentration ofi -th component in the reaction mixture
r_v	Rate of change in the number of moles of hydrocarbons
v_L	Raw material consumption
Ea_i	is activation energy,
k_i	The reaction rate constant,
N	naphthenes
P	Paraffins
$P(j)$	The absolute partial pressure of component j
P_k	Catalyst bulk density
R	The universal gas constant
$r(i)$	The rate of reaction
r_v	Rate of change in the number of moles of hydrocarbons
s	The number of carbon atoms
W_i	The resulting rate of change of the concentration of the i-th component
Y_i	Mole fraction of the i-th component in a hydrocarbon mixture
ΔG_j	Changing of the gibbs free energy forj -th reaction
Δt	Time interval between experimental points in the coke combustion experiments (s)
ξ	Dimensionless catalyst bed height.
τ	Contact time
A	Aromatics
P	Total pressure
R	Catalyst bed radius
T	Temperature

i	The number of reactions; s is the number of carbon atoms.
q	The reaction heat effect.
t	Time

References

[1] Y. M. Zhorov, Y. N. Kartashev, G. Panchenkov, and G. Tatarintseva, "Mathematical model of platforming under stationary conditions with allowance for isomerization reactions," *Chemistry and Technology of Fuels and Oils,* vol. 16, no. 7, pp. 429-432, 1980. https://doi.org/10.1007/BF00726749

[2] J. Henningsen and M. Bundgaar, "Catalytic reforming," *British Chemical Engineering,* vol. 15, no. 11, pp. 1433-1438, 1970.

[3] M. P. Ramage, K. R. Graziani, and F. Krambeck, "6 Development of mobil's kinetic reforming model," *Chemical Engineering Science,* vol. 35, no. 1-2, pp. 41-48, 1980. https://doi.org/10.1016/0009-2509(80)80068-6

[4] M. P. Ramage, K. R. Graziani, P. H. Schipper, F. J. Krambeck, and B. C. Choi, "KINPTR (Mobil's kinetic reforming model): a review of Mobil's industrial process modeling philosophy," *Advances in Chemical Engineering,* vol. 13, pp. 193-266, 1987. https://doi.org/10.1016/S0065-2377(08)60018-6

[5] D. Bommannan, R. Srivastava, and D. Saraf, "Modelling of catalytic naphtha reformers," *The Canadian Journal of Chemical Engineering,* vol. 67, no. 3, pp. 405-411, 1989. https://doi.org/10.1002/cjce.5450670309

[6] M. A. Rodríguez and J. Ancheyta, "Detailed description of kinetic and reactor modeling for naphtha catalytic reforming," *Fuel,* vol. 90, no. 12, pp. 3492-3508, 2011. https://doi.org/10.1016/j.fuel.2011.05.022

[7] M. Z. Stijepovic, A. Vojvodic-Ostojic, I. Milenkovic, and P. Linke, "Development of a kinetic model for catalytic reforming of naphtha and parameter estimation using industrial plant data," *Energy & Fuels,* vol. 23, no. 2, pp. 979-983, 2009. https://doi.org/10.1021/ef800771x

[8] W. Wei, C. A. Bennett, R. Tanaka, G. Hou, and M. T. Klein, "Detailed kinetic models for catalytic reforming," *Fuel Processing Technology,* vol. 89, no. 4, pp. 344-349, 2008. https://doi.org/10.1016/j.fuproc.2007.11.014

[9] W. Wei, C. A. Bennett, R. Tanaka, G. Hou, M. T. Klein Jr, and M. T. Klein, "Computer aided kinetic modeling with KMT and KME," *Fuel Processing Technology,* vol. 89, no. 4, pp. 350-363, 2008. https://doi.org/10.1016/j.fuproc.2007.11.015

[10] R. Sotelo-Boyás and G. F. Froment, "Fundamental kinetic modeling of catalytic reforming," *Industrial & Engineering Chemistry Research,* vol. 48, no. 3, pp. 1107-1119, 2009. https://doi.org/10.1021/ie800607e

[11] H. D. Velázquez *et al.*, "Recent progress on catalyst technologies for high quality gasoline production," *Catalysis Reviews,* vol. 65, no. 4, pp. 1079-1299, 2023. https://doi.org/10.1080/01614940.2021.2003084

[12] A. V. Sapre and J. R. Katzer, *Some aspects of modeling in petroleum processing," in Computer-Aided Design of Catalysts*. United States: CRC Press, 2020, pp. 553–602.

[13] D. Uner, *Advances in refining catalysis*. New York Routledge, 2017.

[14] H. Arani, M. Shirvani, K. Safdarian, and E. Dorostkar, "Lumping procedure for a kinetic model of catalytic naphtha reforming," *Brazilian Journal of Chemical Engineering,* vol. 26, pp. 723-732, 2009. https://doi.org/10.1590/S0104-66322009000400011

[15] M. Wei, M. Yang, F. Qian, W. Du, W. He, and W. Zhong, "Dynamic modeling and economic model predictive control with production mode switching for an industrial catalytic naphtha reforming process," *Industrial & Engineering Chemistry Research,* vol. 56, no. 31, pp. 8961-8971, 2017. https://doi.org/10.1021/acs.iecr.7b02610

[16] E. M. A. Mokheimer, M. R. Shakeel, A. Harale, S. Paglieri, and R. B. Mansour, "Fuel Reforming Processes for Hydrogen Production," *Fuel,* vol. 359, p. 130427, 2024. https://doi.org/10.1016/j.fuel.2023.130427

[17] I. Elizalde and J. Ancheyta, "Dynamic modeling and simulation of a naphtha catalytic reforming reactor," *Applied Mathematical Modelling,* vol. 39, no. 2, pp. 764-775, 2015. https://doi.org/10.1016/j.apm.2014.07.013

[18] A. T. Jarullah, A. N. Ahmed, B. A. Ahmed, and A. M. Ahmed, "Design of new composites nano-catalysts for naphtha reforming process: Experiments and process modeling," *Tikrit Journal of Engineering Sciences,* vol. 30, no. 2, pp. 46-59, 2023. https://doi.org/10.25130/tjes.30.2.6

[19] H. G. Krane, A. Groh, B. L. Schulman, and J. H. Sinfelt, "4. Reactions in catalytic reforming of naphthas," Retrieved: https://api.semanticscholar.org/CorpusID:93026176. [Accessed 1959.

[20] T. Boukezoula, L. Bencheikh, and D. Belkhiat, "A heterogeneous mathematical model for a spherical fixed bed axial flow reactor applied to a naphtha reforming process: Enhancing performance challenge using a non-uniform catalyst distribution in the pellet," *Reaction Kinetics, Mechanisms and Catalysis,* vol. 135, no. 5, pp. 2323-2340, 2022. https://doi.org/10.1007/s11144-022-02257-z

[21] O. D. Sparkman, Z. E. Penton, and F. G. Kitson, "Gas chromatography and Mass spectrometry: A practical guide," *Gas Chromatography and Mass Spectrometry: A Practical Guide,* pp. 1–611, 2011. https://doi.org/10.1016/C2009-0-17039-3

[22] R. Sundari and P. D. Vaidya, "Reaction kinetics of glycerol steam reforming using a Ru/Al2O3 catalyst," *Energy & Fuels,* vol. 26, no. 7, pp. 4195-4204, 2012. https://doi.org/10.1021/ef300658n

[23] A. Russel, S. Gupta, and G. Deo, "The rate determining steps and rate equation for the oxidative dry reforming of methane over supported Ni catalyst," *Journal of Environmental Chemical Engineering,* vol. 11, no. 5, p. 110479, 2023. https://doi.org/10.1016/j.jece.2023.110479

[24] Z. Chen, Y. Wang, Y. Li, J. Wu, and L. Zhang, "Explicit molecule-based reaction network simplification: Theory and application on catalytic reforming," *Chemical Engineering Science,* vol. 277, p. 118833, 2023. https://doi.org/10.1016/J.CES.2023.118833

[25] P. Pasandide and M. Rahmani, "Simulation and optimization of continuous catalytic reforming: Reducing energy cost and coke formation," *International Journal of Hydrogen Energy,* vol. 46, no. 58, pp. 30005-30018, 2021. https://doi.org/10.1016/j.ijhydene.2021.06.151

[26] X. Yang, S. Wang, and Y. He, "Review of catalytic reforming for hydrogen production in a membrane-assisted fluidized bed reactor," *Renewable and Sustainable Energy Reviews,* vol. 154, p. 111832, 2022. https://doi.org/10.1016/j.rser.2021.111832

[27] A. Samad, I. Ahmad, M. Kano, and H. Caliskan, "Prediction and optimization of exergetic efficiency of reactive units of a petroleum refinery under uncertainty through artificial neural network-based surrogate modeling," *Process Safety and Environmental Protection,* vol. 177, pp. 1403-1414, 2023. https://doi.org/10.1016/J.PSEP.2023.07.046

[28] X. C. Ma, Q. Zhang, C. He, Q. L. Chen, and B. J. Zhang, "Computer-aided naphtha liquid–liquid extraction: Molecular reconstruction, sustainable solvent design and multiscale process optimization," *Fuel*, vol. 334, p. 126651, 2023. https://doi.org/10.1016/J.FUEL.2022.126651

[29] D. Iranshahi, M. Karimi, S. Amiri, M. Jafari, R. Rafiei, and M. R. Rahimpour, "Modeling of naphtha reforming unit applying detailed description of kinetic in continuous catalytic regeneration process," *Chemical Engineering Research and Design*, vol. 92, no. 9, pp. 1704-1727, 2014. https://doi.org/10.1016/j.cherd.2013.12.012

[30] M. R. Rahimpour, M. Jafari, and D. Iranshahi, "Progress in catalytic naphtha reforming process: A review," *Applied Energy*, vol. 109, pp. 79-93, 2013. https://doi.org/10.1016/J.APENERGY.2013.03.080

[31] A. Gupta and S. Gupta, "Catalyst regeneration techniques in naphtha reforming: Short review," *Chemical and Process Engineering*, vol. 43, no. 2, pp. 101-108, 2022. https://doi.org/10.24425/cpe.2022.140813