IRSTI 31.15.21
Section: Chemistry
Article

Design and industrial verification of the catalytic reforming process

Rizagul Dyussova[1]*, Gaini Seitenova[2], Moldir Borashova[3], Yekaterina Zhakmanova[4], Yakobs Sergeyevs[1]

[1]Toraighyrov University, Pavlodar, Kazakhstan; dyussova_rm@enu.kz; Ya.sergeevs@pnhz.kz
[2]The Association of Producers and Consumers of Petrochemical Products (Petrochemical Association), Astana, Kazakhstan; seitenova_gzh@enu.kz
[3]Atyrau Oil and Gas University, Atyrau, Kazakhstan; borasheva_23@aogu.edu.kz
[4]L.N. Gumilyov Eurasian National University, Astana, Kazakhstan; 980815450705@enu.kz
*Correspondence: dyussova_rm@enu.kz

Abstract: Catalytic reforming with continuous catalyst regeneration (CCR) is one of the key processes in the production of high-octane gasolines. The need to improve its energy and resource efficiency while complying with modern environmental standards remains a relevant and pressing issue. Particularly challenging is the development of accurate mathematical models of this process under industrial operating conditions, considering catalyst degradation, fluctuations in feedstock composition, and significant thermal effects. The purpose of the article is to develop and calibrate a mathematical model of the CCR reforming process using Aspen Hysys, demonstrated through a case study of the Atyrau Refinery. The research methodology includes the collection of operational data (feedstock composition, reactor parameters, catalyst properties), construction of a detailed process flowsheet, thermodynamic modeling, and calculation of material and energy balances. The developed model was calibrated using actual industrial data and tested for reproducibility and predictive accuracy. The results confirm that the proposed model reliably predicts reformate yield and octane number, as well as identifies optimal process parameters under variable production conditions. The article emphasizes the technological advantages of CCR reforming, including high process stability, extended catalyst service life, and improved energy efficiency. The practical significance of the research lies in the possibility of applying the developed model to optimize the operation of existing CCR units and for the training of engineering personnel. The proposed approach can also be adapted for other refineries with similar technological configurations.

Keywords: catalytic reforming, continuous catalyst regeneration, Aspen Hysys, mathematical modeling, process optimization, high-octane gasoline.

Citation: Dyussova, R., Seitenova, G., Borashova, M., Zhakmanova, Ye., Sergeyevs, Ya. (2025). Design and industrial verification of the catalytic reforming process. Bulletin of the L.N. Gumilyov ENU. Chemistry. Geography. Ecology Series, 152(3), 74-89. https://doi.org/10.32523/2616-6771-2025-152-3-74-89

Academic Editor:
E.Ye. Kopishev

Received: 28.08.2025
Revised: 15.09.2025
Accepted: 15.09.2025
Published: 30.09.2025

1. Introduction

The current level of development of world economic systems is accompanied using oil refining and petrochemical products everywhere. The international petroleum products market is among the most investment-intensive sectors of global trade. Over a hundred countries are involved in producing refined petroleum, regardless of whether they possess their own hydrocarbon reserves. In some states, petroleum products are primarily manufactured for export, whereas in Southeast Asia and the Pacific region the focus remains on satisfying domestic demand (Ivanchina et al., 2021; Ivashkina et al., 2023). Given the unique performance characteristics and relatively low cost of petroleum-based products, the oil refining and petrochemical industries are expected to retain their strategic importance for the foreseeable future (Muhammad Nadeem Khalid, 2023). Currently, three oil refineries operate in Kazakhstan (Atyrau, Pavlodar, Shymkent). The total capacity of the three main oil refineries in Kazakhstan for oil refining as of 2024 is 16.7 million tons per year (Annual Report, 2024).

The catalytic reforming process is the basic process to produce high-octane components of motor gasoline and aromatic hydrocarbons for most oil refineries in Kazakhstan. However, modern environmental requirements increasingly limit the content of aromatic hydrocarbons in gasoline and force oil refineries to introduce new processes that provide the necessary octane characteristics. At the same time, it is impossible to completely abandon the production of reformate. At present, this is the cheapest and most traditional way of upgrading the straight-run gasoline fraction of 85–180°C. In addition, for many enterprises, this is the only way to produce hydrogen, which is increasingly required with the constant growth of capacities for hydrodesulfurization of gasoline and diesel fuels (Lopes et al., 2020; Orazbayev et al., 2021).

The method of mathematical modeling is the most cost-effective in terms of economic costs and efficiency. In the work (Ivashkina et al., 2023), engineering models of oil refining are considered as a method for increasing the efficiency of multi-stage gasoline production. The application of engineering mathematical models in oil refining makes it possible to optimize the composition of commercial gasolines by reducing the reliance on costly additives. This is achieved through a more rational use of reformate and catalytic cracking gasoline in fuel blending, which can lower production costs by approximately 0.1–1.0%. With such models, it becomes feasible to predict the composition of gasolines with required properties based on known parameters of the components, including octane number, yield, and the content of aromatics, benzene, olefins, and sulfur. The performance of the final fuel depends not only on the quality of each component, but also on the characteristics of the mixture, which are influenced by hydrocarbon interactions during catalytic processes (reforming, isomerization, catalytic cracking, hydrocracking) as well as during compounding. By accounting for changes in feedstock composition, engineering models enable the calculation of gasoline blends that meet modern environmental requirements while simultaneously lowering production costs through reduced use of expensive streams and minimizing excess margins in key quality indicators such as octane number, sulfur content, and aromatic hydrocarbons.

The study (Ivanchina et al., 2021) presents an approach to optimizing the SRR catalytic reforming process. The approach is based on the use of a mathematical model. The model considers the activity of the catalyst, the instability of its operation, and changes in the hydrocarbon composition of the feedstock. The model allows monitoring the production process and finding the optimal operating mode, which is determined by the conditions of equilibrium of the coke formation reactions and hydrogenation of intermediate pressing products. Using a mathematical model, it is possible to improve the technical indicators of the production process, such as the yield and octane number of the product. In addition, mathematical modeling allows assessing the efficiency of the catalyst and can help decide on replacing it with a new one. According to the research of (Orazbayev et al., 2022), an efficient methodology was proposed for building a system of interconnected process unit models based on diverse sources of data, including fuzzy information. This approach enabled the creation of hybrid models capable of predicting both the yield of catalyzate and its quality parameters. Furthermore, a scheme was developed to integrate the

models of the main units of a catalytic reforming plant into a unified modeling framework. The resulting system provides a comprehensive tool for simulating plant operations, enhancing production efficiency by increasing the output of target products and improving their quality characteristics.

Modern research in the field of catalytic reforming and modeling of oil refining processes demonstrates a steady interest in the development of new catalysts and digital optimization tools. Thus, significant progress has been made in the field of catalyst technologies for producing high-octane gasoline (Gupta & Gupta, 2022; Jarullah et al., 2023; Velázquez et al., 2023; Wei et al., 2008), including approaches to prolonging service life and improving regeneration methods. It was shown in (Boukezoula et al., 2022; Ma et al., 2024; Mokheimer et al., 2024; Pasandide & Rahmani, 2021; Wu et al., 2025; Yang et al., 2022) that the introduction of improved mathematical models and hybrid optimization algorithms can reduce energy costs, reduce coking, and improve the accuracy of forecasting process parameters. At the same time, the direction of integrating machine learning with process modeling is developing (Garma et al., 2024; Moon et al., 2025; Naderi et al., 2025; Samad et al., 2023), which opens new prospects for creating intelligent control and forecasting systems in conditions of uncertainty. These results validate the significance of employing Aspen HYSYS in combination with the adaptation of models to real industrial data, while also underscoring the potential of integrating conventional modeling techniques with advanced digital technologies.

The purpose of this paper is to analyze and critically assess existing mathematical models of the catalytic reforming process with continuous catalyst regeneration, to identify their inherent limitations, and to highlight approaches that improve process efficiency, selectivity, and catalyst performance through advanced simulation and modeling strategies.

2. Materials and methods

The object of the study is the catalytic reforming unit with continuous catalyst regeneration with a benzene extraction unit of Atyrau Oil Refinery LLP (ANPZ). The licensor of the processes and the developer of the basic design package is Axens (France). The working design, supply of equipment and construction of the complex were performed by Sinopec Engineering Co. Ltd (Group). The year of commissioning of the complex is 2014 (Seitenova G.Zh., Dyussova R.M., et al., 2023).

The catalytic reforming unit with continuous catalyst regeneration with a benzene extraction unit consists of the following sections:

- section 100 – catalytic reforming, for obtaining high-octane components of gasoline (or raw materials for the future aromatics complex) and raw materials of section 300;
- section 200 – continuous regeneration of the catalytic reforming catalyst;
- section 300 – extractive distillation of Morphylane, for obtaining a benzene-toluene fraction;
- section 400 – separation (rectification) of the benzene-toluene fraction, obtaining benzene and toluene; - section 500 - auxiliary section (Zainullin et al., 2020).

The feedstock for the catalytic reforming unit consists of a mixture of stabilized heavy naphtha, obtained from the gasoline hydrotreating and fractionation unit, as well as from the naphtha hydrotreating unit. The processing capacity of the catalytic reforming unit (section 100) is 1,000 tons per year, determined by the volume of feedstock available at the plant. The nominal capacity of section 300, dedicated to extractive distillation using the Morphylane process, is 417 tons per year, while section 400, responsible for separating the benzene–toluene fraction to produce commercial benzene, has a capacity of 133 tons per year. The operational flexibility of the complex allows for throughput fluctuations in the range of 50–100%, which defines the selection of process equipment and automated control systems to ensure stable operation within the specified limits. The total number of operating hours amounts to 7,920 annually.

Reforming reactions take place in reactors with a moving catalyst bed, from which the

catalyst is removed for regeneration and returned to the reactors again. The circulation and regeneration of the catalyst is carried out on a continuous basis with fully automated control of all operations. To facilitate chemical reactions that contribute to an increase in octane number, elevated temperatures of approximately 500 °C are required, which necessitates preheating of the feedstock. Moreover, several key reactions are highly endothermic and consume significant amounts of heat. As a result, the catalyst bed is distributed across multiple reactors, with inter-reactor furnaces installed to compensate for heat losses and maintain the required reaction conditions (Orazbayev et al., 2021).

As we know, high efficiency of the reforming process mainly occurs with a combination of high temperature and low operating pressure. These parameters lead to a short operating life of the catalyst in traditional fixed-bed reactors. Therefore, the advantage of this reforming unit compared to traditional units is the continuous regeneration of the catalyst. The main research method is mathematical modeling of the catalytic reforming unit using the Aspen Hysys model developed by Aspen Tech (Rekoske et al., 2017; Sapre & Katzer, 2020; Smith et al., 2022).

3. Results

The catalytic reformer model was created using the Distributed Control System (DCS) diagrams, process and instrumentation diagrams, column and reactor specifications, catalyst loading, laboratory analysis data, hourly average unit data, and daily material balances.

Modeling steps:

1. Data collection
2. Review and analysis of the obtained data:
- Structuring, grouping, and validation;
- Application of standard methodology for concluding;
- It is essential that it is applied by process experts and, with good engineering judgment (a thorough understanding of the process and data quality);
- The accepted conclusions can be revised at;
- Optimizer task (automatic calibration tool);
- Verification of results.
3. Entering reactor data
4. Calibrating the reformer reactor (Calibration Environment)
5. Within the Simulation Environment:
- Building the rest of the scheme;
- Performing simulation runs to assess the reliability of reactor predictions;
- Setting up a Case Study (e.g. to generate linear programming data).

The HYSYS model consists of three sections:

1. Plant data analysis (red rectangle in Figure 1).
2. Linear programming (green rectangle in Figure 1).
3. Reactor, furnaces, fractionation columns and hydrogen recycle loop with blowdown.

Refinery System (RefSYS) reactors are operational models, meaning they are not very sensitive to reactor designs and catalyst compositions. Essentially, the model theory is distorted to match the actual data (Figure 2). This is done in the Calibration Environment and using the measured Net Product (Measurement) as the target.

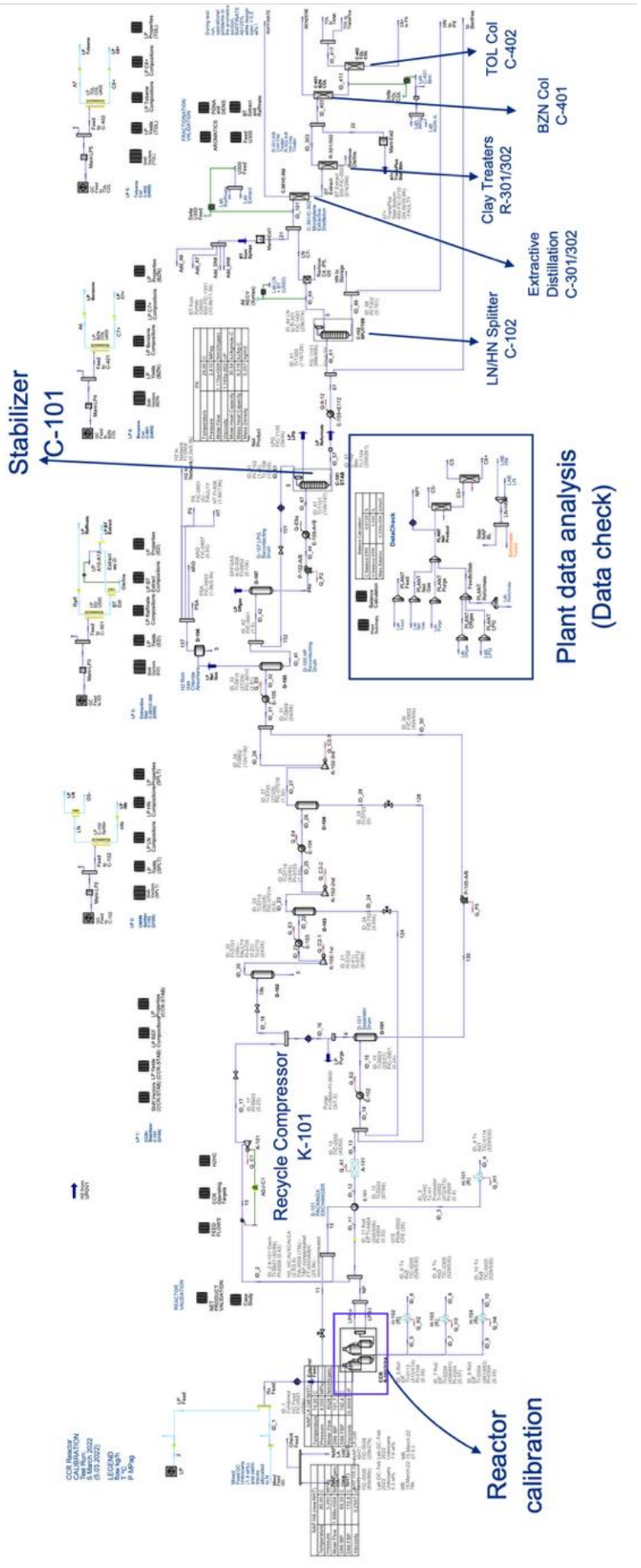
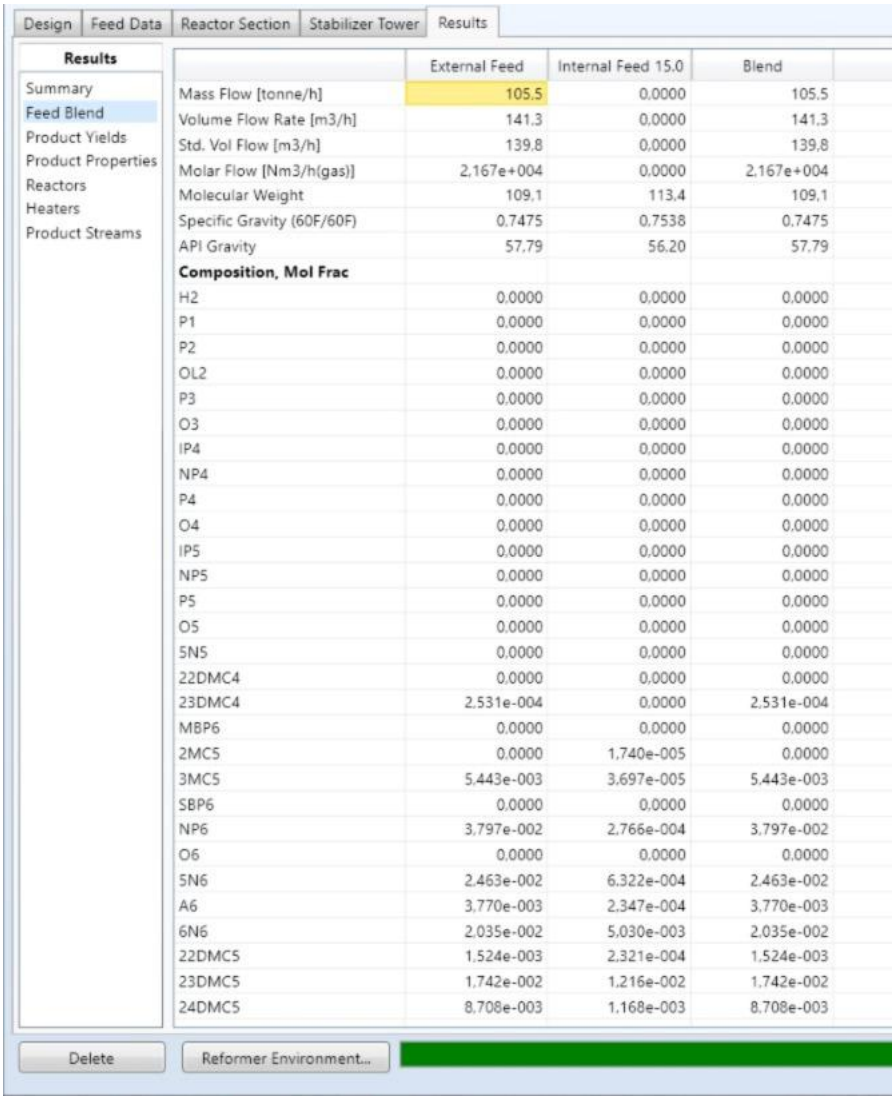


Figure 1. The catalytic reformer process flow diagram



	External Feed	Internal Feed 15.0	Blend
Mass Flow [tonne/h]	105.5	0.0000	105.5
Volume Flow Rate [m3/h]	141.3	0.0000	141.3
Std. Vol Flow [m3/h]	139.8	0.0000	139.8
Molar Flow [Nm3/h(gas)]	2.167e+004	0.0000	2.167e+004
Molecular Weight	109.1	113.4	109.1
Specific Gravity (60F/60F)	0.7475	0.7538	0.7475
API Gravity	57.79	56.20	57.79
Composition, Mol Frac			
H2	0.0000	0.0000	0.0000
P1	0.0000	0.0000	0.0000
P2	0.0000	0.0000	0.0000
OL2	0.0000	0.0000	0.0000
P3	0.0000	0.0000	0.0000
O3	0.0000	0.0000	0.0000
IP4	0.0000	0.0000	0.0000
NP4	0.0000	0.0000	0.0000
P4	0.0000	0.0000	0.0000
O4	0.0000	0.0000	0.0000
IP5	0.0000	0.0000	0.0000
NP5	0.0000	0.0000	0.0000
P5	0.0000	0.0000	0.0000
O5	0.0000	0.0000	0.0000
5N5	0.0000	0.0000	0.0000
22DMC4	0.0000	0.0000	0.0000
23DMC4	2.531e-004	0.0000	2.531e-004
MBP6	0.0000	0.0000	0.0000
2MC5	0.0000	1.740e-005	0.0000
3MC5	5.443e-003	3.697e-005	5.443e-003
SBP6	0.0000	0.0000	0.0000
NP6	3.797e-002	2.766e-004	3.797e-002
O6	0.0000	0.0000	0.0000
5N6	2.463e-002	6.322e-004	2.463e-002
A6	3.770e-003	2.347e-004	3.770e-003
6N6	2.035e-002	5.030e-003	2.035e-002
22DMC5	1.524e-003	2.321e-004	1.524e-003
23DMC5	1.742e-002	1.216e-002	1.742e-002
24DMC5	8.708e-003	1.168e-003	8.708e-003

Figure 2. Dialog box «Measured net product»

The reforming model uses a fixed set of components suitable for the reforming process. This set is based on the standard list of components of the gasoline reformer REFSRK.

Aspen reforming components are grouped based on carbon number (Table 1).

Table 1. Components grouped

№	Components in program	Reforming components
1	MBP	Highly branched iso-paraffins
2	SBP	Single side chain iso-paraffins
3	5N	5-carbon (cyclopentane) naphthenes
4	6N	6-carbon (cyclohexane) naphthenes
5	N	Grouped 5- and 6-carbon naphthenes
6	NP	Normal paraffins
7	P	Grouped iso- and normal paraffins
8	O	Olefins
9	A	Aromatics

Depending on the carbon number, the component will either be a pure component (e.g. nP_4)

or a group of pure components with a similar structure (e.g. MBP7). All A8 isomers are presented as pure components.

Additional pure components for C_6 and C_7 are added so that individual iso-paraffins can be accounted for in the fractionation section that processes the product from the reactor block.

The full list of components processed by the reforming unit is given in Table 2.

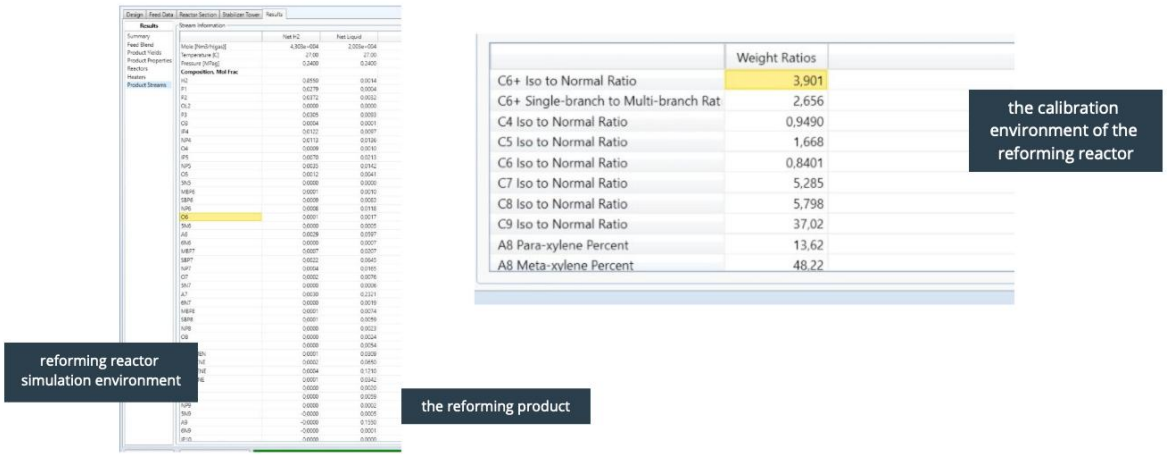


Figure 3. Isomer ratios

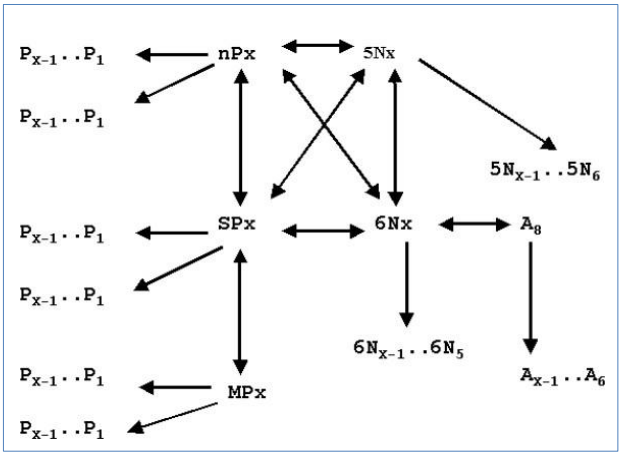


Figure 4. Reforming reaction routes

Table 2. List of components processed by the reforming unit

№	Formula	Hysys Components	№	Formula	Hysys Components
1	H_2	Hydrogen	39	$5N_7$	Branched 7 carbon cyclopentanes
2	P_1	Methane	40	A_7	Toluene
3	P_2	Ethane	41	$6N_7$	Methylcyclohexane
4	OL_2	Ethylene (C_2H_4)	42	MBP_8	Multi-branch 8 carbon paraffins
5	P_3	Propane	43	SBP_8	Single-branch 8 carbon paraffins
6	O_3	Propylene (C_3H_6)	44	O_8	Octenes (C_8H_{16})
7	IP_4	Isobutane	45	NP_8	n-Octane
8	NP_4	n-Butane	46	$5N_8$	Branched 8 carbon cyclopentanes
9	P_4	Total butanes	47	ETHYLBEN	Ethyl-benzene
10	O_4	Butylenes (C_4H_8)	48	O-XYLENE	1,2-dimethylbenzene

11	IP_5	Isopentane	49	M-XYLENE	1,3-dimethylbenzene
12	NP_5	n-Pentane	50	P-XYLENE	1,4-dimethylbenzene
13	P_5	Total pentanes	51	A_8	8 Carbon aromatics
14	O_5	Pentylenes (C_5H_8)	52	$6N_8$	8 Carbon cyclohexanes
15	$5N_5$	Cyclopentane	53	IP_9	9 Carbon isopar affins
16	$22DMC_4$	22-Dimethylbutane	54	NP_9	9 Carbon normal paraffins
17	$23DMC_4$	23-Dimethylbutane	55	$5N_9$	9 Carbon cyclopentanes
18	MBP_6	Multi-branch butanes	56	A_9	9 Carbon aromatics
19	$2MC_5$	2-Methylpentane	57	$6N_9$	9 Carbon cyclohexanes
20	$3MC_5$	3-Methylpentane	58	IP_{10}	10 Carbon isoparaffins
21	SBP_6	Single-branch pentanes	59	NP_{10}	10 Carbon normal paraffins
22	NP_6	n-Hexane	60	$5N_{10}$	10 Carbon cyclopentanes
23	O_6	Hexenes (C_6H_{12})	61	A_{10}	10 Carbon aromatics
24	$5N_6$	Methylcyclopentane	62	$6N_{10}$	10 Carbon cyclohexanes
25	A_6	Benzene	63	IP_{11}	11 Carbon isoparaffins
26	$6N_6$	Cyclohexane	64	NP_{11}	11 Carbon normal paraffins
27	$22DMC_5$	22-Dimethylpentane	65	$5N_{11}$	11 Carbon cyclopentanes
28	$23DMC_5$	23-Dimethylpentane	66	A_{11}	11 Carbon aromatics
29	$24DMC_5$	24-Dimethylpentane	67	$6N_{11}$	11 Carbon cyclohexanes
30	MBP_7	Multi-branch 7 carbon paraffins	68	P_{12}	12 Carbon paraffins
31	$2MC_6$	2-Methylhexane	69	N_{12}	12 Carbon naphthenes
32	$3MC_6$	3-Methylhexane	70	A_{12}	12 Carbon aromatics
33	$3EC_5$	3-Ethylpentane	71	P_{13}	13 Carbon paraffins
34	SBP_7	Single-branch 7 carbon paraffins	72	N_{13}	13 Carbon naphthenes
35	NP_7	n-Heptane	73	A_{13}	13 Carbon aromatics
36	O_7	Heptene (C_7H_{14})	74	P_{14}	14 Carbon paraffins
37	DMCP	Dimethycyclopentane	75	N_{14}	14 Carbon naphthenes
38	ECP	Ethylcyclopentane	76	A_{14}	14 Carbon aromatics

The detailed kinetic scheme includes 50 kinetic groups that are linked by a network of 112 reactions. The reaction routes used for C_6-C_8 are shown in the following diagram. As the carbon number increases above 8, the complexity of the pathways decreases.

Coke formation in a reformer is modeled by reacting paraffins, C_5 cyclic naphthenes, and aromatics in a first-order reaction mechanism. All C_5 cyclic naphthenes have a common activation energy, as do the aromatics and paraffins. The frequency coefficients vary with carbon amount and type.

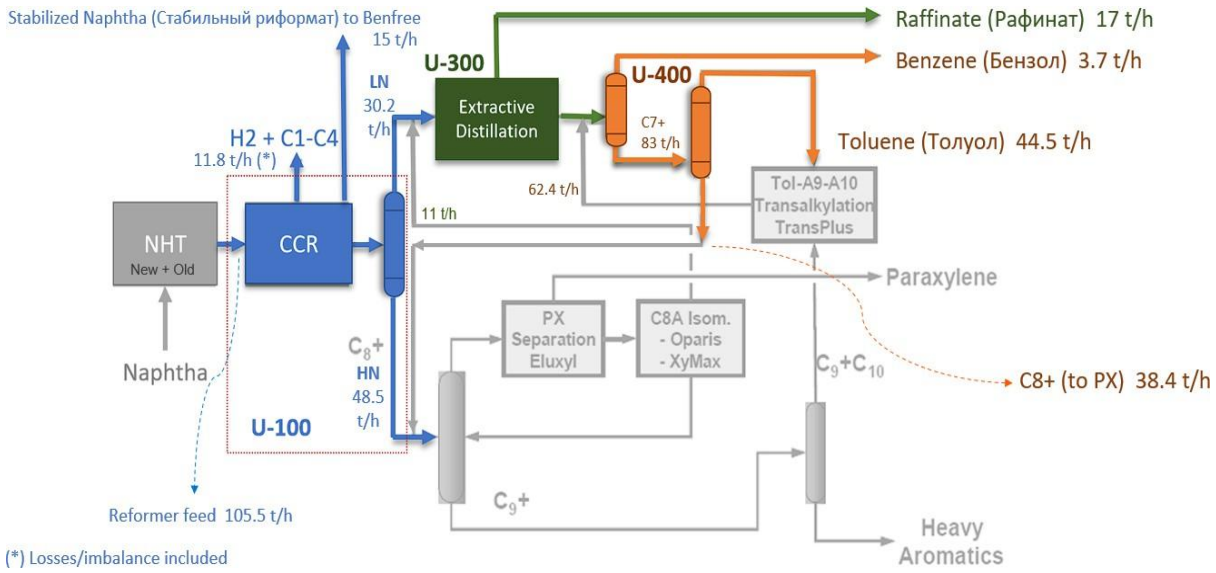


Figure 5. Model boundaries

Figure 5 shows the simulation boundaries of the three units implemented in the HYSYS reforming model: U-100 (blue), U-300 (green) and U-400 (orange). A portion of the stabilized reformate is sent to Benfree (15 t/h), and two external feed streams (62.4 t/h with Trans Plus and 11 t/h with XyMax) contribute to the final products. The reforming unit (U-100) includes the following units:

1. Reactor (R-101/2/3/4)
2. Stabilization (C-101)
3. Reformate separation (C-102)

The purpose of U-100 is to obtain a reformate fraction rich in aromatic compounds with a high octane number, along with high-purity hydrogen, LPG and a light reformate fraction rich in toluene (A_7).

The reformer catalyst regeneration loop (U-200) and the water-chloride balance are not included in the model. The HYSYS reactor model assumes that operators will control the catalyst chlorination according to the catalyst supplier's specifications. The activity of the chlorinated catalyst is determined during calibration based on measured values of light ends, reactor temperature drop, and coke yield. The reformer (U-100) is typically modeled as a single unit in planning models (i.e., as a single lp submodel). An example of a simplified scheme is shown below in figure 6.

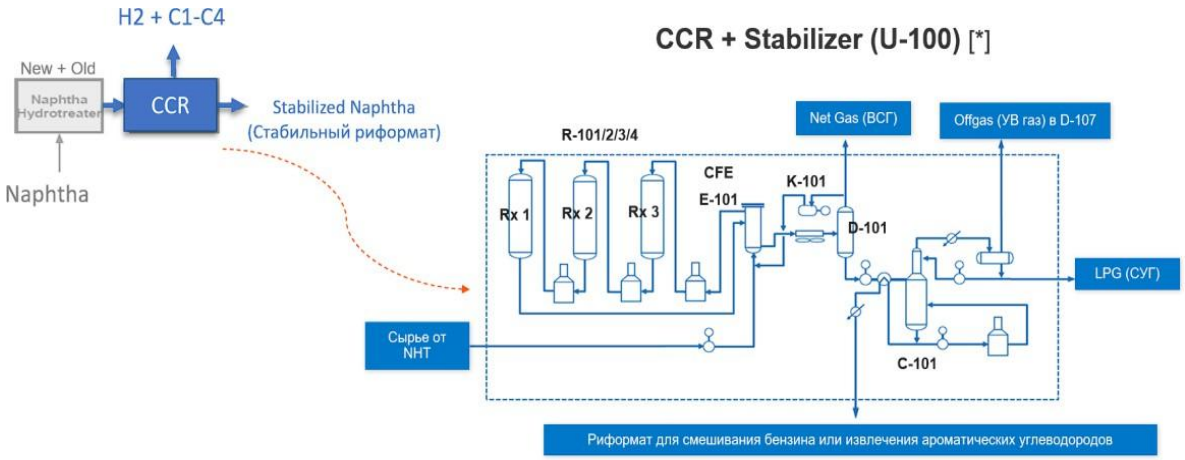


Figure 6. CCR Simplified Schematic

When the reformer operates in gasoline mode, the stabilized reformate from the C-101 stabilizer still is sent to the gasoline blending park or tank. An alternative mode of operation was chosen for calibration of the HYSYS model: the aromatic mode. Light gasoline (LN) from the reformate splitter overhead and BT (benzene-toluene) from the XyMax are processed in the Morphylane section (U-300). This is an extractive distillation, which is modeled by the HYSYS component splitter. The aromatic extract from the extractive distillation section is clay scrubbed in R-301/R-302. Hot clay scrubbing (R-302) converts traces of olefins (and/or diolefins) into higher boiling components via olefin alkylation (Figure 7). Some of the valuable aromatic product produced by catalytic reforming is lost to remove olefinic impurities.

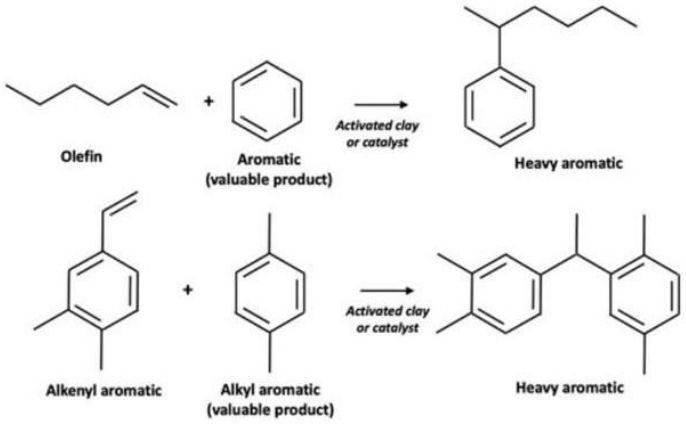


Figure 7. Alkylation of olefins (R-302)

Finally, the processed U-300 extract is combined with A7+ from the TransPlus stabilizer bottoms (U-700), and valuable aromatics are recovered in the benzene and toluene column sections (U-400).

The quality of the CCR reactor feed is determined by a mixture of hydrotreated (HT) streams:

1. Straight-run gasoline.
2. Gasoline from the DT GO unit (Prime D).
3. Cracking gasoline from the FCC unit (Prime G).
4. Coker gasoline (which is processed in the “old” gasoline hydrotreater).
5. Raffinate (which is processed in the “new” gasoline hydrotreater).

The HYSYS standard reformer block was used to model the 4-bed CCR catalytic reformer. This block includes the reactor, product separator and hydrogen recirculation loop integrated with the model block. The feed-to-product heat exchanger (CFE E-101) is modeled internally as a simple heat exchanger with a hot side approach.

The reformer has 2 products: H_2 Product and Net Liquid. These streams are calculated using the internal instantaneous vapor-liquid equilibrium model and considering the pressure and temperature specified for the product separator (Reactor Control parameter in the Reactor Section tab). In the reformer, the H_2 recycle is assumed to come from the top of this separator. The H_2 product is the "net" gas phase produced (i.e. excluding H_2 recycle).

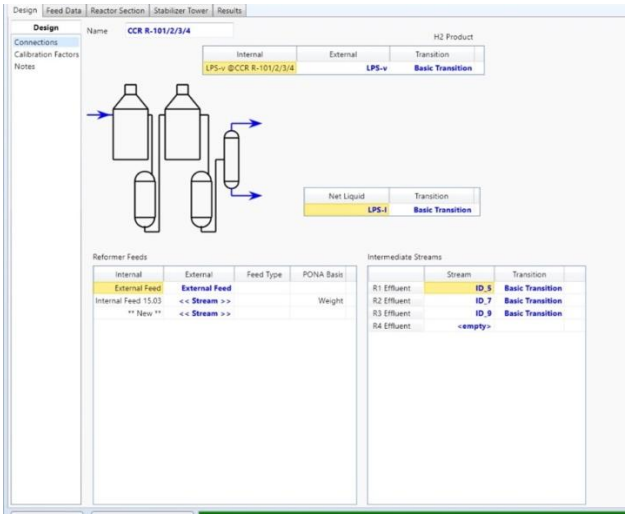


Figure 8. Reforming products

The reactor product gas portion leaving the product separator (D-101) is recycled to the reactor inlet, with the flow rate typically adjusted to obtain the desired H_2HC ratio. This ratio is important for catalyst stability and the effect of removing reaction products and condensables from the catalyst and supplying the catalyst with available hydrogen. Increasing the H2HC ratio will move the naphtha through the reactors at a higher rate and provide greater heat removal for the endothermic heat of reaction.

Key reactor operating parameters can be entered in the CR Operating Targets spreadsheet:

1) Inlet weighted average temperature (ºC).

2) Product separator (D-101) pressure (MPa g) and temperature (ºC).

3) H_2HC (Recycle compressor flow rate (Nm^3/h) can be entered as an alternative).

For the CFE (E-101) and preheater (H-101) simulations, the effluent from reactor №4 was reconstructed by adding 61 kNm^3/h (approximately 18 t/h) to the product H_2 (Figure 8). The H_2HC ratio was determined to be 2.6 mol/mol in the reactor block, resulting in a calculated H_2 recycle purity of 89 mol.% in D-101 once the recycle loop converges. The reformers are continuous catalyst regeneration (CCR) units; Axens process with 4 radial flow reactors. Only catalyst is injected into the reactors; this is used to calculate the weighted average inlet temperature.

The vessel volume is necessary when modeling reactors in a steady state, since it determines the residence time. The effective reactor volume (catalyst volume) is calculated based on the mass of the catalyst and the density of the catalyst particles.

4. Discussion

The results of catalytic reforming modeling showed high accuracy in reproducing material and energy balances, predicting the yield of the reformate and its octane number. This is consistent with studies (Ivanchina et al., 2021; Ivashkina et al., 2023), which demonstrated that engineering models allow for the degradation of the catalyst, fluctuations in the composition of raw materials, and thereby increase the efficiency and cost-effectiveness of production. A comparison with (Orazbayev et al., 2021, 2022) confirms that the integration of industrial statistics with thermodynamic modeling is a universal method for optimizing the operation of CCR installations and can also serve as a tool for training engineering personnel and digitalizing processes at refineries.

However, there are still areas for further work – more detailed modeling of catalyst deactivation and coke formation (Zainullin et al., 2020), as well as the use of hybrid methods combining mechanistic modeling and machine learning. This will expand the applicability of the developed model to various refineries and increase its predictive value in the context of changing raw material composition and stricter requirements for sustainable development.

5. Conclusion

The model developed for the purpose of optimal control of a catalytic reformer is a good calibration of the available data and is therefore adequate for updating the linear programming submodel.

As a rule, when performing new calibrations, it is important to check the hydrogen balance "original" and "corrected" (i.e. after adjusting the material balance). A reasonable range for this is from 98% to 102%. If the material balance is confirmed to be good, but this value is bad, the GC data should be reviewed, the feed and product analyses may be inconsistent. An error does not always mean that the hydrogen yield itself is incorrect.

The default material balance reconciliation performed by the reformer model consists of distributing the material balance error across all products by normalizing their consumption upward or downward by the same factor. This approach is not recommended when the hydrogen or carbon imbalance is high.

The amount of final product obtained has a direct impact on its final quality. Therefore, reconciliation should be performed with reasonable calculation when balance errors are too large.

It is recommended to recalibrate once a year when major changes occur in the plant or when forecasts seem to diverge from actual operation.

The review of existing models for catalytic reforming with continuous catalyst regeneration has demonstrated the growing importance of advanced simulation tools for understanding and optimizing this complex process. While many models effectively describe reaction kinetics and product distribution, challenges remain in the accurate representation of catalyst deactivation, heat integration, and multi-reactor system dynamics. Integrating empirical data, kinetic modeling, and digital tools such as Aspen Plus and machine learning approaches opens new perspectives for improving predictive accuracy and operational efficiency. Future research should focus on refining model parameters through real-time plant data and exploring hybrid modeling techniques that combine mechanistic and data-driven methods.

6. Supplementary Materials: All figures in a high quality version are given here (https://drive.google.com/drive/folders/1ThEVonP1sjC5Z2VuF9csILHiiMU3hHg6)

7. Author Contributions

Research concept, text writing - R.D.; project administration - G.S.; data analysis - M.B.; data collection and processing, illustrations - Y.S.; data collection and processing - Y.Zh.

8. Author Information

Dyussova, Rizagul – postdoctoral fellow, Toraighyrov University, 64, Lomov str., Pavlodar, Kazakhstan, 140000; email: dyussova_rm@enu.kz, https://orcid.org/0000-0003-3083- 5255.

Seitenova, Gaini – Head of the project office, Association of Producers and Consumers of Oil and Gas Chemical Products (Oil and Gas Chemical Association), 8 Kunayev St., Astana, Kazakhstan, 010000; e-mail: seitenova_gzh@enu.kz, https://orcid.org/0000-0001-6202-3951.

Borashova, Moldir – doctoral student, Atyrau Oil and Gas University, 1 Azattyk Avenue, Atyrau, Kazakhstan, 060000; borasheva_23@aogu.edu.kz, https://orcid.org/0009-0009-2842-0078.

Zhakmanova, Yekaterina – doctoral student, L.N. Gumilyov Eurasian National University, Kazhymukan st., 13, Astana, Kazakhstan, 010000; e-mail: 980815450705@enu.kz, https://orcid.org/0000-0003-0545-5912.

Sergeyevs, Yakobs – doctoral student, Toraighyrov University, 64 Lomov str., Pavlodar, Kazakhstan, 140000; email: Ya.sergeevs@pnhz.kz, https://orcid.org/0009-0009-2090-9143.

9. Funding: This research was funded under grant funding for research of young scientists under the project "Zhas Galym" for 2023-2025, implemented by the Science Committee of the Ministry

of Education and Science of the Republic of Kazakhstan, under the program AP19175752 "Scientific and technical support for energy saving and resource efficiency of the technology for the preparation of high-octane gasoline and aromatic hydrocarbons".

10. Acknowledgements: Gratitude for assistance in conducting research to the General Director of the Association of Legal Entities "Association of Producers and Consumers of Petrochemical Products" (Petrochemical Association) Tolkimbaev Gabit Azhdarovich.

11. Conflicts of Interest: No conflict of interest between the authors.

12. References

1. Boukezoula, T.F., Bencheikh, L., Belkhiat, D.E.C. (2022). 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* 135(5), 2323–2340. https://doi.org/10.1007/S11144-022-02257-Z/FIGURES/5
2. Garma, R., Sioud, D., Binous, H., Bellagi, A. (2024). Introduction to the modeling of complex chemical reaction equilibrium using gPROMS® and GAMS®. *Computer Applications in Engineering Education* 32(3), e22714. https://doi.org/10.1002/CAE.22714
3. Gupta, A., Gupta, S.K. (2022). Catalyst regeneration techniques in naphtha reforming: Short review. *Chemical and Process Engineering* 43(2), 101-108. https://doi.org/10.24425/CPE.2022.140813
4. Ivanchina, E., Chernyakova, E., Pchelintseva, I., Poluboyartsev, D. (2021). Mathematical modeling and optimization of semi-regenerative catalytic reforming of naphtha. *Oil and Gas Science and Technology* 76. https://doi.org/10.2516/OGST/2021041
5. Ivashkina, E.N., Koksharov, A.G., Ivanchina, E.D., Chuzlov, V.A., Nazarova, G.Y., Chernyakova, E.S., Dolganov, I.M. (2023). Engineering models of oil refining: increasing the efficiency of multi-stage gasoline production. *Bulletin of the Tomsk Polytechnic University, Geo Assets Engineering* 334(4), 195–208. https://doi.org/10.18799/24131830/2023/4/3793
6. Jarullah, A.T., Ahmed, A.N., Altabbakh, B.A., Ahmed, A.M. (2023). Design of New Composites Nano-Catalysts for Naphtha Reforming Process: Experiments and Process Modeling. *Tikrit Journal of Engineering Sciences* 30(2), 46–59. https://doi.org/10.25130/tjes.30.2.6
7. Lopes, I.S., Figueiredo, M.C., Sá, V. (2020). Criticality Evaluation To Support Maintenance Management of Manufacturing Systems. *International Journal of Industrial Engineering and Management* 11(1), 3–18. https://doi.org/10.24867/IJIEM-2020-1-248
8. Ma, X.C., He, C., Chen, Q.L., Zhang, B.J. (2024). Modeling and optimization for the continuous catalytic reforming process based on the hybrid surrogate optimization model. *Computers & Chemical Engineering* 191, 108841. https://doi.org/10.1016/J.COMPCHEMENG.2024.108841
9. Mokheimer, E.M.A., Shakeel, M.R., Harale, A., Paglieri, S., Mansour, R.Ben. (2024). Fuel reforming processes for hydrogen production. *Fuel* 359, 130427. https://doi.org/10.1016/J.FUEL.2023.130427
10. Moon, J.A., Syauqi, A., Lim, H. (2025). Multi-objective optimization of hydrogen production based on integration of process-based modeling and machine learning. *Chemical Engineering Journal* 520, 166148. https://doi.org/10.1016/J.CEJ.2025.166148
11. Naderi, M., Rashidi, H., Reynolds, A., Doherty, W. (2025). Aspen Plus modelling of the MILENA dual fluidised bed biomass gasifier technology. *International Journal of Thermofluids* 29, 101334. https://doi.org/10.1016/J.IJFT.2025.101334

12. Orazbayev, B., Zhumadillayeva, A., Kodanova, S., Iskakova, S., Orazbayeva, K. (2021). Improving the efficiency of technological units for the production of high-quality motor fuels using fuzzy mathematics methods. *E3S Web of Conferences* 288, 01020. https://doi.org/10.1051/E3SCONF/202128801020
13. Orazbayev, B., Zhumadillayeva, A., Orazbayeva, K., Iskakova, S., Utenova, B., Gazizov, F., Ilyashenko, S., Afanaseva, O. (2022). The System of Models and Optimization of Operating Modes of a Catalytic Reforming Unit Using Initial Fuzzy Information. *Energies* 15(4), 1573. https://doi.org/10.3390/EN15041573
14. Pasandide, P., Rahmani, M. (2021). Simulation and optimization of continuous catalytic reforming: Reducing energy cost and coke formation. *International Journal of Hydrogen Energy* 46(58), 30005–30018. https://doi.org/10.1016/J.IJHYDENE.2021.06.151
15. Rekoske, J.E., Abrevaya, H., Bricker, J.C., Zhu, X., Bricker, M. (2017). Advances in Refining Technologies. *Advances in Refining Catalysis*, 3–58. https://doi.org/10.1201/9781315370125-2/ADVANCES-REFINING-TECHNOLOGIES-JAMES-REKOSKE-HAYIM-ABREVAYA-JEFFERY-BRICKER-XIN-ZHU-MAUREEN-BRICKER
16. Samad, A., Ahmad, I., Kano, M., Caliskan, H. (2023). 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* 177, 1403–1414. https://doi.org/10.1016/J.PSEP.2023.07.046
17. Sapre, A.V., Katzer, J.R. (2020). Some Aspects of Modeling in Petroleum Processing. *Computer-Aided Design of Catalysts*, 553–602. https://doi.org/10.1201/9781003067115-13
18. Smith, J.M., Van Ness, H.C., Abbott, M.M., Swihart, M.T. (2022). *Introduction to chemical engineering thermodynamics*, 762.
19. Velázquez, H.D., Cerón-Camacho, R., Mosqueira-Mondragón, M.L., Hernández-Cortez, J.G., Montoya de la Fuente, J.A., Hernández-Pichardo, M.L., Beltrán-Oviedo, T.A., Martínez-Palou, R. (2023). Recent progress on catalyst technologies for high quality gasoline production. *Catalysis Reviews* 65(4), 1079–1299. https://doi.org/10.1080/01614940.2021.2003084
20. Khalid M.N. (2023). View of Analysis of the world production of petroleum products. https://doi.org/https://doi.org/10.32523/2789-4320-2023-2-108-118
21. Wei, W., Bennett, C.A., Tanaka, R., Hou, G., Klein, M.T. (2008). Detailed kinetic models for catalytic reforming. *Fuel Processing Technology* 89(4), 344–349. https://doi.org/10.1016/J.FUPROC.2007.11.014
22. Wu, J., Chen, G., Chen, A., Gao, Z., Wu, X., Cheng, H., Li, Y., Wang, Y., Qian, Z., Zhang, X., Xu, C., Chen, Z., Zhang, L. (2025). Molecular-Level Modeling of Naphtha Continuous Catalytic Reforming Process. *Chemical Engineering Science* 309, 121430. https://doi.org/10.1016/J.CES.2025.121430
23. Yang, X., Wang, S., He, Y. (2022). Review of catalytic reforming for hydrogen production in a membrane-assisted fluidized bed reactor. *Renewable and Sustainable Energy Reviews* 154, 111832. https://doi.org/10.1016/J.RSER.2021.111832
24. Zainullin, R.Z., Zagoruiko, A.N., Koledina, K.F., Gubaidullin, I.M., Faskhutdinova, R.I. (2020). Multi-Criterion Optimization of a Catalytic Reforming Reactor Unit Using a Genetic Algorithm. *Catalysis in Industry* 12(2), 133–140. https://doi.org/10.1134/S2070050420020129/FIGURES/3
25. Annual report (2024). https://www.kmg.kz/ru/company/
26. Seitenova G.Zh., Dyussova R.M., Burumbayeva G.R. (2023). Mathematical modeling of oil refining processes as a method of resource saving and energy efficiency. *Neft I gaz* 133, 10. https://doi.org/10.37878/2708-0080/2023-1.13

Каталитикалық реформалау процесін жобалау және өнеркәсіптік тексеру

Ризагуль Дюсова, Гайни Сейтенова, Мөлдір Борашова, Екатерина Жакманова, Якобс Сергеевс

Аңдатпа: Катализатордың үздіксіз регенерациясы (CCR) каталитикалық риформингі жоғары октанды бензиндерді өндірудегі негізгі процестердің бірі болып табылады. Қазіргі экологиялық стандарттарды сақтай отырып, оның энергетикалық және ресурстық тиімділігін арттыру қажеттілігі өзекті және шұғыл мәселе болып қала береді. Катализатордың деградациясын, бастапқы шикізат құрамының ауытқуын және маңызды жылу әсерлерін ескере отырып, өндірістік жұмыс жағдайында осы процестің нақты математикалық модельдерін жасау өте қиын міндет болып табылады. Мақаланың мақсаты Атырау мұнай өңдеу зауытының мысалында көрсетілген Aspen hysys көмегімен CCR риформинг процесінің математикалық моделін әзірлеу және калибрлеу болып табылады. Зерттеу әдістемесі пайдалану деректерін жинауды (шикізат құрамы, реактор параметрлері, катализатор қасиеттері), егжей-тегжейлі технологиялық схеманы құруды, термодинамикалық модельдеуді және материалдық және энергетикалық баланстарды есептеуді қамтиды. Әзірленген модель нақты өндірістік деректерді қолдана отырып калибрленді және репродуктивтілік пен болжау дәлдігіне тексерілді. Нәтижелер ұсынылған модель риформингтің шығуын және октан санын сенімді түрде болжайтынын, сондай-ақ әртүрлі өндірістік жағдайларда процестің оңтайлы параметрлерін анықтайтынын растайды. Мақалада CCR риформингінің технологиялық артықшылықтары, соның ішінде процестің жоғары тұрақтылығы, катализатордың ұзақ қызмет ету мерзімі және энергия тиімділігінің жоғарылауы көрсетілген. Зерттеудің практикалық маңыздылығы қолданыстағы CCR қондырғыларының жұмысын оңтайландыру және инженерлік персоналды оқыту үшін әзірленген модельді қолдану мүмкіндігі болып табылады. Ұсынылған тәсілді ұқсас технологиялық конфигурациясы бар басқа мұнай өңдеу зауыттарына да бейімдеуге болады.
Түйін сөздер: каталитикалық реформалау, катализатордың үздіксіз регенерациясы, Aspen HYSYS, математикалық модельдеу, процестерді оңтайландыру, жоғары октанды бензин.

Разработка и промышленная проверка процесса каталитического риформинга

Ризагуль Дюсова, Гайни Сейтенова, Молдир Борашова, Екатерина Жакманова, Якобс Сергеевс

Аннотация: Каталитический риформинг с непрерывной регенерацией катализатора (CCR) является одним из ключевых процессов в производстве высокооктановых бензинов. Необходимость повышения его энергетической и ресурсоэффективности при соблюдении современных экологических стандартов остается актуальной и неотложной проблемой. Особенно сложной задачей является разработка точных математических моделей этого процесса в промышленных условиях эксплуатации, учитывающих деградацию катализатора, колебания состава исходного сырья и значительные тепловые эффекты. Целью статьи является разработка и калибровка математической модели процесса риформинга CCR с использованием Aspen HYSYS, продемонстрированной на примере Атырауского нефтеперерабатывающего завода. Методология исследования включает сбор эксплуатационных данных (состав сырья, параметры реактора, свойства катализатора), построение подробной технологической схемы, термодинамическое моделирование и расчет материального и энергетического балансов. Разработанная модель была откалибрована с

использованием реальных промышленных данных и протестирована на воспроизводимость и точность прогнозирования. Результаты подтверждают, что предложенная модель надежно предсказывает выход риформинга и октановое число, а также определяет оптимальные параметры процесса при различных производственных условиях. В статье подчеркиваются технологические преимущества риформинга CCR, включая высокую стабильность процесса, увеличенный срок службы катализатора и повышенную энергоэффективность. Практическая значимость исследования заключается в возможности применения разработанной модели для оптимизации работы существующих установок CCR и для обучения инженерного персонала. Предложенный подход также может быть адаптирован для других нефтеперерабатывающих заводов с аналогичной технологической конфигурацией.

Ключевые слова: каталитический риформинг, непрерывная регенерация катализатора, Aspen HYSYS, математическое моделирование, оптимизация процесса, высокооктановый бензин.