JOURNAL OF MULTIDISCIPLINARY SCIENCES AND INNOVATIONS
VOLUME 5, ISSUE 02
MOPNTHLY JOURNALS
ISSN NUMBER: 2751-4390
IMPACT FACTOR: 9,08

ENHANCING THE EFFICIENCY OF AROMATIC HYDROCARBON SEPARATION PROCESSES THROUGH MODELING SOFTWARE

Gaybullaev Saidjon Abdusalimovich
Asia International University

Annotation

Ways to enhance the efficiency of benzene recovery processes from aromatic-rich distillate fractions via selective solvent extraction have been analyzed using process modeling software. The study examines the feasibility of ensuring continuous production of products that meet regulatory quality standards while utilizing existing technological equipment, as well as the potential for expanding the product slate of the unit. Furthermore, reconstruction and modernization recommendations aimed at improving both qualitative and quantitative process performance indicators have been developed to ensure optimal process operation.

Keywords

Benzene separation, reformate stabilization, aromatic hydrocarbon separation, precise rectification, optimal temperature, process modeling software.

INTRODUCTION

The rapid increase in the number of motor vehicles has led to a significant rise in toxic emissions released into the environment, resulting in substantially stricter regulations on exhaust emissions and more stringent quality requirements for motor fuels.

Modern automotive and aviation gasolines represent complex mixtures of base components – such as straight-run gasoline, cracking products, catalytic reforming products, and polymer gasoline–along with iso-paraffins and various additives. Their highly diverse chemical composition exerts a decisive influence on the anti-knock (detonation) characteristics of the fuel.

The gasoline fraction primarily consists of three main groups of hydrocarbons: alkanes, cycloalkanes, and aromatic hydrocarbons of the benzene series. Major global automotive and engine manufacturers in the United States, Western Europe, and Japan adhere to international fuel quality specifications aligned with the European environmental program, which limits the aromatic hydrocarbon content in gasoline - particularly benzene - to no more than 1 wt.% (European standard EN 228).

The object of the present study is an extraction unit designed for the separation of lower aromatic hydrocarbons from base gasoline components. Aromatic hydrocarbons are obtained by selective solvent extraction of various stabilized distillates rich in arenes, followed by separation into individual components [1].

At the same time, the rapid development of the petrochemical and gas chemical industries has led to a sharp increase in the demand for aromatic hydrocarbons, especially benzene. Benzene is widely used as a primary feedstock in the production of polymers, synthetic fibers, dyes, pharmaceuticals, and high-octane fuel components. Therefore, the development of efficient and economically viable industrial methods for benzene separation remains a pressing scientific and technological challenge.

LITERATURE REVIEW AND METHODOLOGY

Enhancement of aromatic hydrocarbon recovery efficiency is achieved through the optimization of catalytic reforming processes using advanced catalysts that ensure high yields and selectivity, the application of improved separation techniques such as selective extraction and solvent treatment, and the implementation of integrated purification technologies aimed at producing high-purity products required for the petrochemical industry. Within these technological schemes, impurity removal—particularly sulfur compounds—and deep distillation processes play a decisive role.

Analysis of operational data from industrial units has demonstrated that the stability of the individual aromatic hydrocarbon separation block (benzene and toluene) is periodically disrupted due to various process disturbances, resulting in the production of off-specification materials. Specifically, instances were recorded in which the toluene content in benzene exceeded 0.11 wt.%, while the benzene content in toluene surpassed 0.10 wt.%.

Moreover, cases were observed where the product quality failed to fully comply with regulatory and technical documentation requirements. Although the necessary quality margin for stabilized reformate was ensured in the stabilization column, the separation efficiency with respect to the overhead product remained unsatisfactory: the content of C_6 and heavier hydrocarbons reached 20 wt.% compared to the specified regulatory limit of 5 wt.%.

Accordingly, the primary objective of this study was defined as the development and implementation of a set of measures aimed at optimizing the operating parameters of the extraction unit for the separation of aromatic hydrocarbons from arene-rich distillates, thereby ensuring rational utilization of resources. In addition, the study seeks to maintain product quality within regulatory specifications in the secondary distillation block, including under conditions of increased feedstock throughput.

The study thoroughly investigated the sequential separation processes in the extraction unit for narrow-cut stabilized reformate, including stabilization of the reforming catalyst, selective extraction of the stabilized reformate, and secondary distillation of the extract to obtain individual aromatic hydrocarbons. In research conducted by A.T. Jalilov, K.M. Akhmerov, A. Ikromov, S.E. Nurmonov, L.R. Jo‘rayeva, and O.Sh. Qodirov, the optimization problem was addressed using a decomposition approach, taking into account the complexity of the technological system. In this method, each individual process block was solved separately, and the results were subsequently coordinated considering their interdependencies. According to the authors, the extremely large scale of optimization tasks in petroleum refining makes the practical application of integral computational methods excessively labor-intensive.

In industrial practice, the improvement of aromatic hydrocarbon recovery efficiency from various distillates is carried out along the following main directions:

In industrial practice, improving the efficiency of aromatic hydrocarbon recovery from various distillates is carried out along the following principal directions:

Catalytic Reforming

- *Advanced catalysts:* Utilization of highly active and selective catalysts capable of increasing the yield of aromatic hydrocarbons—benzene, toluene, and xylenes—from reformate.
- *Optimization of operating conditions:* Selection of optimal temperature, pressure, and feed rate parameters to maximize aromatic formation.

Extraction and Separation

- *Selective extraction:* Application of selective solvents to separate aromatic hydrocarbons from non-aromatic components.
- *Integrated purification:* Removal of sulfur-containing compounds from extracts followed by deep fractionation.

Process Technology Improvement

- *Automation and control:* Real-time monitoring and control to maintain optimal operating parameters.
- *Process integration:* Integration of reforming, extraction, and purification stages into a unified and efficient technological complex.

Significance of This Approach:

Increasing the Yield of High-Purity Aromatic Hydrocarbons: Benzene, toluene, and xylenes serve as essential feedstocks for the production of plastics, synthetic fibers, solvents, and other petrochemical products.

Reducing Production Costs: Increased process efficiency and higher yields contribute to lowering manufacturing expenses.

Improving Product Quality: Ensures the production of aromatic hydrocarbons with high purity levels, which are essential for subsequent synthesis stages.

The significance of these approaches lies in increasing the yield of high-purity aromatic hydrocarbons. Benzene, toluene, and xylenes serve as essential feedstocks for the production of plastics, synthetic fibers, solvents, and other petrochemical products. Furthermore, improved process efficiency and higher yields contribute to reduced production costs and ensure the production of aromatics with purity levels suitable for subsequent synthesis stages.

RESULTS

The results of model calculations indicate that:

- increasing the reflux rate of the stabilization column from the specified 6–7 m^3/h to 10–12 m^3/h allows the content of heavy components in the light fraction to be reduced to the regulatory limit of 5% by mass;
- the initial boiling point of the raffinate remains within the permissible range;
- it is possible to switch to a single-column scheme for fractionation while maintaining compliance with quality regulations.

Based on feedstock composition data, mathematical models of the relevant technological units were developed using the HYSYS® process simulation software package [2]. The adequacy of the models was verified by comparing simulated results with actual operational data, with relative errors not exceeding 3% [3].

The first stage of optimization is the stabilization block, designed to separate C_1–C_5 hydrocarbons from the reforming product. The principal technological scheme of this block is shown in Figure 1.

The target fraction of this block is the stabilized reformate, which is directed to the extraction unit for aromatic hydrocarbon recovery. In addition, light stabilized fractions and hydrocarbon gases are produced as by-products.

Under current production conditions, cases have been observed in which the product quality does not fully meet the requirements of regulatory and technical documentation.

Maintaining a reflux rate of 6–7 m^3/h provides the necessary quality reserve for a stable catalyst. However, the precision of separating the light fraction at the top of the stabilization column remains very limited. Consequently, the proportion of C_6 and heavier hydrocarbons frequently exceeds 20% by mass. Furthermore, regulatory limits dictate that losses of benzene with the light fraction represent a significant share of the annual yield, making these parameters particularly important in evaluating process performance.

If the process scheme is modified to use a single column, the load on the reboiler at the bottom of the column increases. At the same time, the rise in reflux rate leads to changes in the vapor–liquid traffic within the stabilization column. The permissible values of vapor–liquid loads were verified following the methodology outlined in [4], and it was established that, at the required reflux rate, there is sufficient margin to ensure stable operation of the column's downcomer.

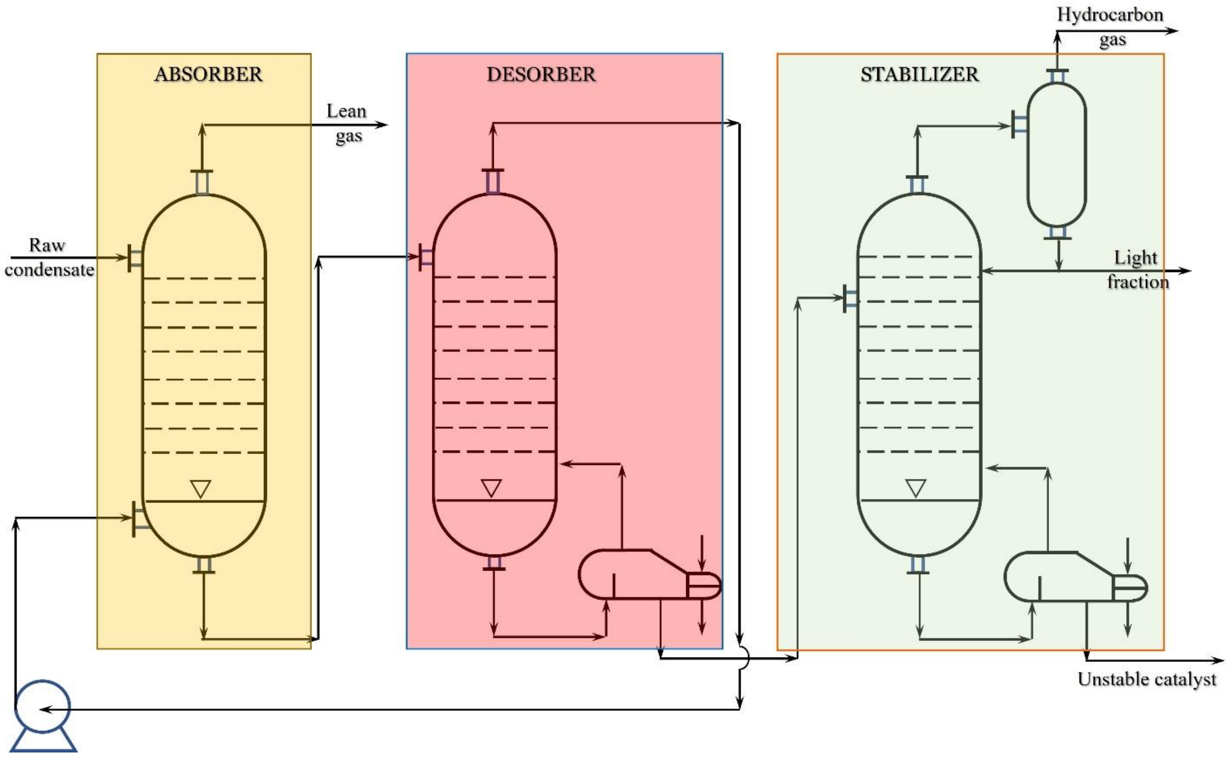

Figure 1. Technological Scheme of the Catalyst Stabilization Block

Furthermore, the feasibility of transitioning from the outdated three-column separation scheme to a single-column process, which demands lower operational variability, was evaluated. Considering the increased load on the stabilizer when the two columns intended for pre-separation of gases are removed, it was confirmed that the reboiler at the bottom of the column can deliver the necessary heat duty to maintain proper operation.

The calculation results were confirmed during active experimental trials in the current production process. According to the conducted tests, transitioning to a single-column stabilization scheme was shown to allow compliance with the regulatory and technical requirements for product quality (Figure 2).

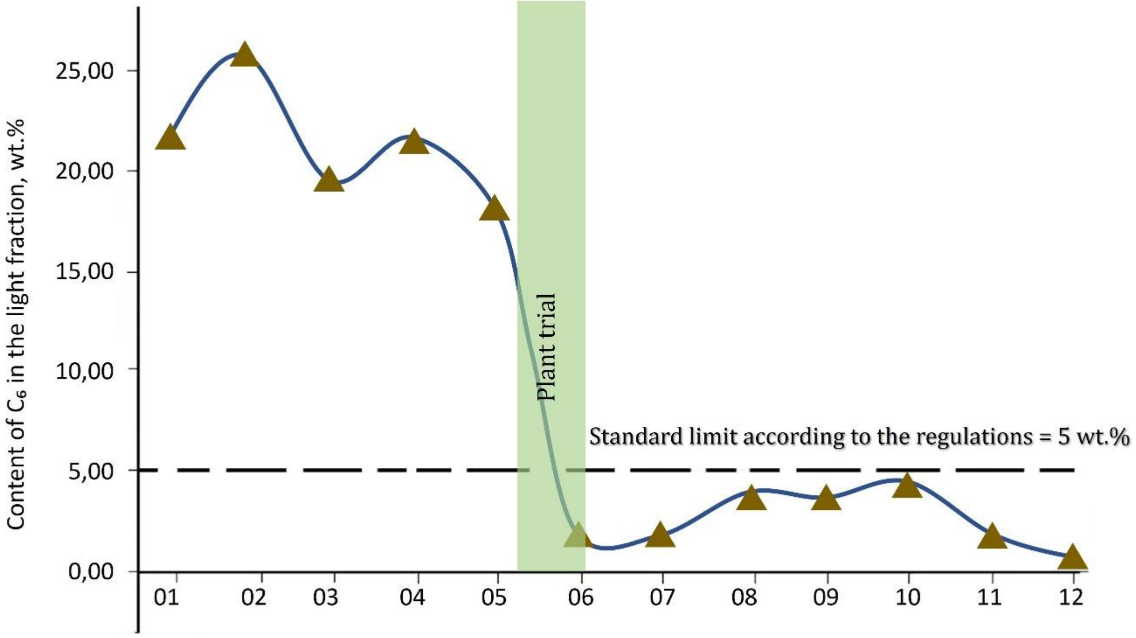

Figure 2. Changes in the quality of the light fraction from the stabilizer as a result of adjustments to the technological regime.

At present, work is underway to substantiate these proposals. Particular attention is being given to converting the unit to a single-column operational mode during the reconstruction process, while adjusting the technological regime in accordance with the recommended parameters. This, in turn, enables the content of C_6 and heavier hydrocarbons in the reflux to be reduced to less than 1% by mass, significantly minimizing losses of the target products.

The next identified issue is related to the periodic deterioration in the quality of commercial benzene and toluene, which are separated in the secondary drive unit using precise rectification methods, as illustrated in Figure 3.

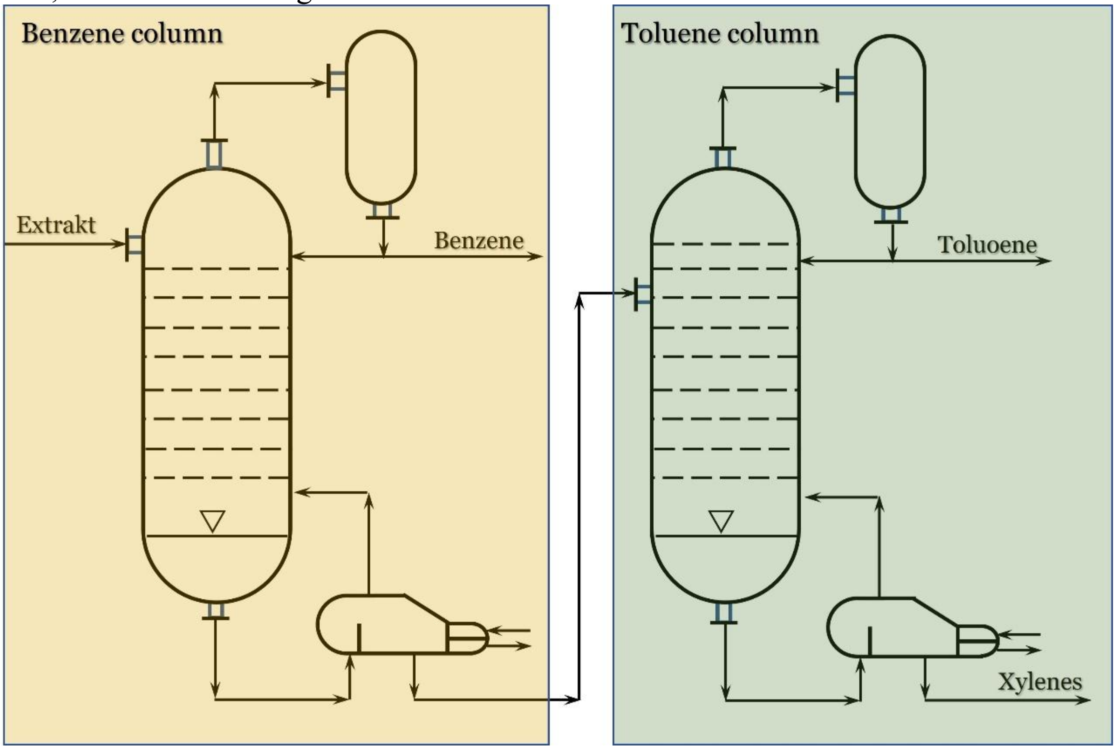

Figure 3. Principal technological scheme of the secondary drive unit.

During the operation with feedstocks of varying composition, monitoring of process parameters and product stream quality identified the bottleneck in the secondary separation system-the benzene separation column.

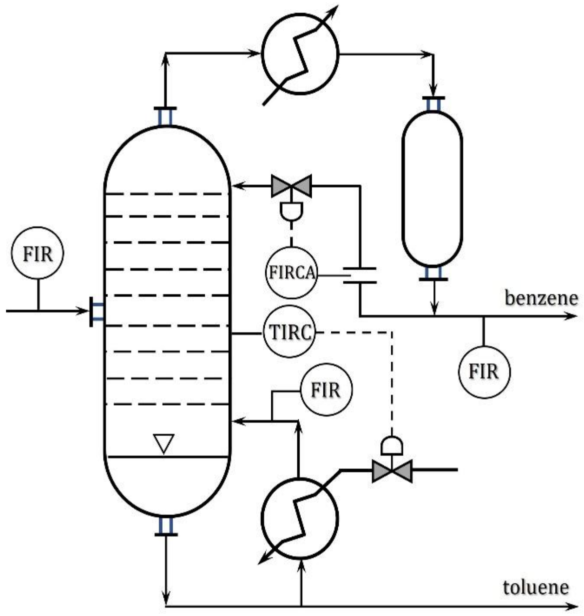

Figure 4. Control system of the benzene separation column.

Factors affecting product quality were determined and classified into two groups:

- **Controllable parameters**: heat carrier flow to the column bottom, reflux rate, and temperature;
- **Feedstock characteristics**: feed flow rate and benzene-to-toluene ratio.

The control scheme for the column apparatus is shown in Figure 4.

Analysis of the rectification process revealed the main cause of reduced separation efficiency in the column: when the benzene content in the feed increases, the unit experiences excessive vapor loading (Figure 5).

A list of factors affecting the final product quality was compiled, and the benzene flow in the feed was identified as the most influential factor on the separation performance. Based on this indicator, and taking into account the variability of the sharp reflux temperature in the stream, the optimal reflux rate was determined using the relationship $F_{refl.}=f(F_{C_6H_6})$.

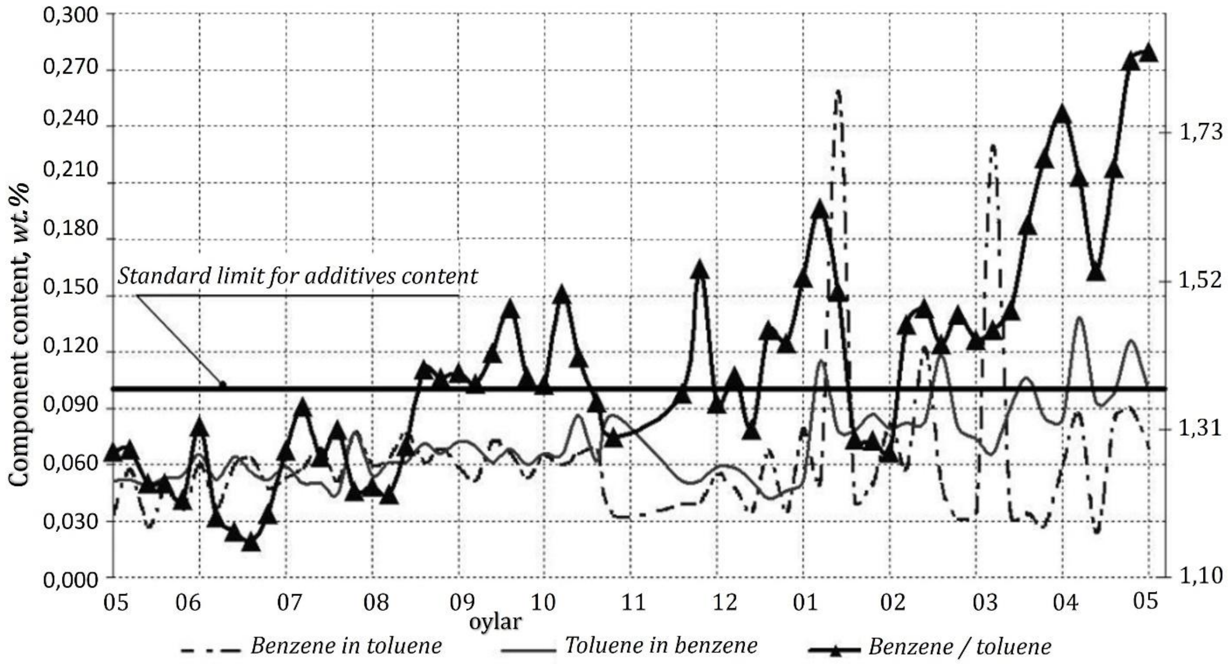

Figure 5. Variation in product quality during unit operation.

According to calculations based on this formula, the highest vapor load occurs on the second tray from the top, as determined from the heat balance condition [5]. Specifically, maintaining the vapor load on the second tray at the stable (nominal) operating level ensures reliable column performance. This is because, for each specific feed composition, the optimal reflux rate is calculated and set accordingly.

Where:

$F_{C_6H_6}$ – benzene flow rate, t/h;

$F_{bug'_2}$ – vapor flow rate on the second tray, determined based on model calculations, t/h;

$$\Delta T = T_2 - T_{refluyks} \approx 86 - T_{refluyks}, \quad ^\circ C$$

Where, T_2 denotes the temperature corresponding to the liquid–vapor phase transition of the component mixture on the second tray at the given pressure. In the nominal (base) operating mode, ($T_2 \approx 86\ ^\circ C$).

$\tilde{C}_{er}$ – average isobaric heat capacity, J/(kg·°C).

λ – thermal conductivity coefficient, W/(m·°C).

The reduction of the distillate stream temperature prior to its entry into the reflux drum is ensured by the operation of an air-cooling unit. During the summer season, under conditions of elevated ambient air temperatures, certain operational difficulties arise due to fluctuations in the temperature of the reflux irrigation stream, which affect phase equilibrium in the upper section of the apparatus. The value of this parameter is taken into account in relation (1) as a correction coefficient.

The vapor flow rate and the temperature at the upper tray were set at the levels recorded under steady-state operating conditions, at which the quality of the product streams complied with regulatory specifications with a significant margin. This operating mode was adopted as the base case.

A hypothesis was proposed that maintaining a constant vapor load is one of the necessary conditions for meeting impurity concentration constraints in the product streams under conditions of varying feedstock parameters.

Thus, in accordance with relation (1), the constancy of the vapor load can be ensured by adjusting the reflux flow rate in response to changes in ambient conditions and feedstock characteristics.

As the second control parameter for the benzene separation column, the flow rate of the hot stream supplied to the bottom tray of the column was selected. This parameter enables modification of the temperature profile of the column apparatus.

As a result of processing the experimental data, a relationship (2) was obtained that allows determination of the optimal temperature value at the 22nd control tray as a function of the load and feedstock quality, taking into account pressure corrections for the existing ranges of parameter variations.

$$T^2_{maqb} = 105{,}33 + 0{,}47 \cdot (Z - 17) - 1{,}55 \cdot (B - 10)$$

Where, Z denotes the total load, t/h, and B denotes the benzene load, t/h.

After the possibility of improving the quality of the product streams had been confirmed by calculations, the proposed approach was tested at an operating industrial facility. The experiment aimed at implementing the proposed control scheme was conducted over a period of 10 days. During this time, the composition of the feedstock varied over a wide range; specifically, the benzene-to-toluene ratio fluctuated between 1.0 and 1.6.

Throughout the experiment, in accordance with the calculation results, it became possible to reduce the toluene content in the commercial benzene product from approximately 0.06 wt.% to 0.03 wt.%. These values meet the requirements for a high-quality product grade, namely **“highly**

purified benzene." At the same time, the quality of the toluene product remained within the limits specified by the operating regulations (Fig. 6).

When setting the temperature value at the control tray, it is necessary to correct the calculated value in accordance with the pressure prevailing in the system, which is explained by the linear relationship between these parameters (3):

where **ΔP** is the difference between the actual pressure in the column and the base pressure value.

After completion of the experiment, recommendations were developed to adjust the operating mode of the process unit. The temperature profile along the entire column was reduced by 4–7 °C; in particular, the temperature at the 22nd control tray is currently maintained within the range of 104–109 °C (prior to the experiment, this value was 108–114 °C). At the same time, a high level of product quality is preserved, with a stable average toluene content in benzene of less than 0.03 wt.%.

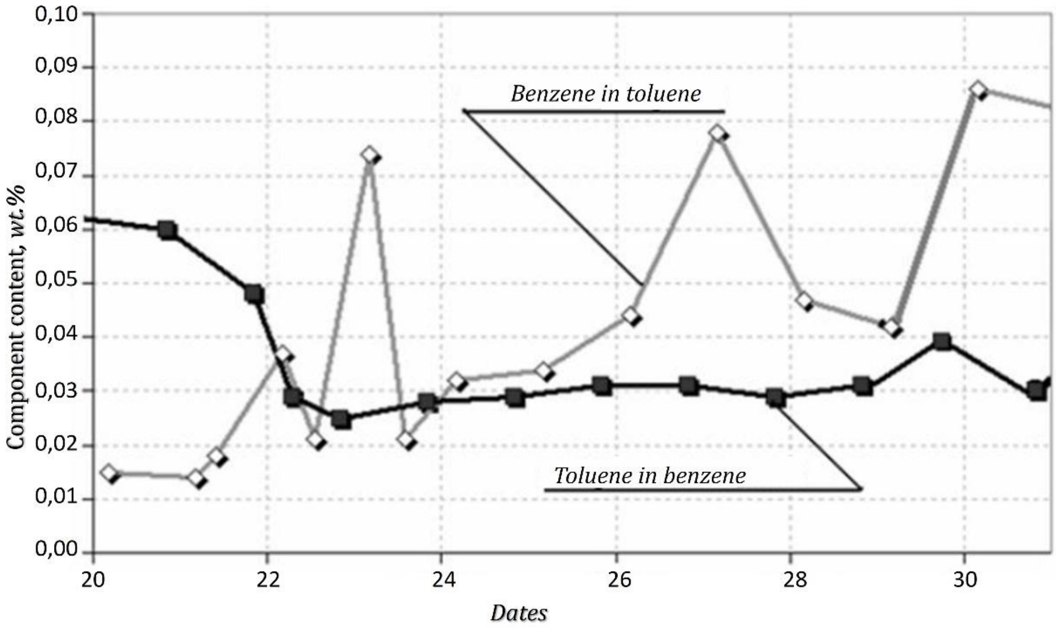

Figure 6. Variability of product quality during the experimental campaign

Conclusions and Recommendations

After completion of the experiment and during the transition to the new control system settings, minor operational disturbances may occur solely due to potential malfunctions of auxiliary equipment.

The obtained results demonstrate that the recommended column operating settings ensure the guaranteed production of products meeting standard quality requirements and enable the manufacture of high-quality products, namely benzene of the *"highly purified"* grade.

Since the unit blocks operate under strict interconnections, it is possible to accurately predict the parameters of technological streams based on the operating conditions of the upstream processing stages. This makes it feasible to timely adjust control commands supplied to regulators in accordance with changes arising at earlier stages, thereby ensuring uninterrupted production of products of the required quality.

Thus, the objective of maintaining quantitatively specified product quality and producing premium-grade benzene has been successfully achieved.

In addition, the study considered the possibility of increasing unit throughput while simultaneously improving the quality of individual product streams. By adjusting operating conditions in the stabilization block, it was possible to reduce losses of marketable products and enhance the quality of by-products, as well as to facilitate the operation of adjacent process units. As a result of stabilizing the operation of the benzene separation column and increasing separation efficiency, the production rate of commercial benzene was increased by 10%.

At the final stage of the study, further analysis of the extraction block operation is being conducted in order to identify opportunities for improving the efficiency of aromatic component recovery.

References:

1. Yulduz Malikjon Qizi Murodova, & Saidjon Abdusalimovich G'Aybullayev (2022). BENZOLNING NEFTKIMYOVIY SINTEZDA QO'LLANILISHI. Scientific progress, 3 (1), 79-86.
2. Urunov N. S. et al. PIROKONDENSAT TARKIBINING KIMYOVIY TAHLILI //Science and Education. – 2021. – T. 2. – №. 3. – C. 32-40.
3. Sadriddinovch S. M. et al. INFLUENCE OF THE QUANTITY OF BENZENE ON THE PERFORMANCE CHARACTERISTICS OF GASOLINE //Euro-Asia Conferences. – 2021. – T. 4. – №. 1. – C. 188-192.
4. Гайбуллаев С. А., Турсунов Б. Ж. Пироконденсат-важнейшее сырье химического синтеза //Universum: технические науки. – 2020. – №. 6-2 (75). – С. 84-86.
5. Абдулазизов С. С. Ў., Шарипов М. С., Ғайбуллаев С. А. МОЙ ФРАКЦИЯЛАРИНИНГ КИМЁВИЙ ТАРКИБИ ВА РЕОЛОГИК ХОССАЛАРИ //Science and Education. – 2021. – Т. 2. – №. 3.
6. Zaripov, M. X. O. G. L., & G'Aybullayev, S. A. (2021). PIROLIZ KINETIKASINING MATEMATIK MODELI. Academic research in educational sciences, 2(9), 619-625.
7. Jumaev, A. V. O. G. L., & G'Aybullayev S. A. (2021). Adsorbentlarning turlari va tasnifi. Science and Education, 2 (9), 145-154.
8. Raupov, B. K. O. G. L., Mavlonov, B. A., & G'Aybullayev S. A. (2021). Bitumlarning ekspluatatsion xossalari va ularni yaxshilash. Science and Education, 2 (9), 170-179.
9. Mizrobjon Xalim O'G'Li Zaripov, & Saidjon Abdusalimovich G'Aybullayev (2021). UGLEVODORODLARNING TERMIK PIROLIZI MAHSULOTLARI HOSIL BO'LISHIGA REAKSIYA SHAROITINING TA'SIRI. Academic research in educational sciences, 2 (11), 723-731.
10. Nodir Sirojiddinovich Hasanov, & Saidjon Abdusalimovich G'Aybullayev (2022). Neft mahsulotlarini gidrotozalashning nazariy asoslari. Science and Education, 3 (1), 229-237.
11. Nodir Sirojiddinovich Hasanov, & Saidjon Abdusalimovich G'Aybullayev (2022). Neft mahsulotlari tarkibidagi oltingugurtli birikmalar va ularning xossalari. Science and Education, 3 (1), 137-146.