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DETAILED ANALYSIS OF THE COMPONENT AND GROUP COMPOSITION OF LIGHT NAPHTHA FOR OPTIMIZING THE OPERATION OF A THREE-PHASE SPLITTER IN THE PRODUCTION OF HIGH-OCTANE GASOLINE

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Abstract: This study presents a comprehensive analysis of the component and group composition of light naphtha — a key feedstock for a three-phase splitter used in the production of high-octane gasoline. The investigation was carried out using gas chromatography in accordance with ASTM D6729, enabling the identification and quantification of 127 individual hydrocarbons in straight-run Nemba naphtha. The results demonstrated that the feedstock is characterized by a high content of isoparaffins (43–47%), which makes it particularly valuable for isomerization processes. Among the identified compounds, isopentane (7.65%), 2-methylpentane (2.81%), and isooctane (6.10%) were predominant. The share of normal paraffins was found to be 29–31%, with a dominance of n-pentane (8.31%) and n-hexane (6.86%). Aromatic compounds accounted for 5–7%, which complies with modern environmental standards. Special attention was paid to the distribution of hydrocarbons by carbon number. It was established that the C5–C7 fractions make up the bulk of the feedstock (approximately 75%), confirming its high suitability for subsequent separation in a three-phase splitter. Meanwhile, the content of heavy fractions (C9+) did not exceed 3%, minimizing the risk of their accumulation during processing. The findings have significant practical value for optimizing the operation of the three-phase splitter, as they allow precise determination of temperature regimes and other process parameters. The identified compositional characteristics of Nemba light naphtha provide opportunities to enhance the efficiency of high-octane gasoline production in accordance with modern environmental standards, including Euro-5 requirements.

Keywords: light naphtha, three-phase splitter, gas chromatographic analysis, isoparaffins, ASTM D6729, high-octane gasoline, fractionation, component composition.

I. INTRODUCTION

An oil refinery is the core of the global crude oil supply chain [1]. It converts crude oil into valuable petroleum products. The shipment of these products to domestic and international markets is carried out in accordance with commercial specifications, which vary depending on the season and the geographic region in which the refinery operates. Currently, the refining industry is facing new technical challenges. The demand for fuel products is driven by economic factors, industrial sector growth, and other influences. These factors stimulate demand for lighter products. In addition, the quality of available crude oil is changing — it is becoming heavier and richer in sulfur content. Another constraint is the implementation of environmental regulations, which require stricter fuel quality standards. This necessitates investment in new refining technologies and/or the use of higher-quality feedstocks to improve the final product quality.

From an operational perspective, selecting the appropriate feedstock and process conditions is crucial. These parameters must be carefully considered for each production unit in the refinery to ensure high profitability while meeting the quality requirements of end products. Refineries are complex systems with a vast number of possible combinations of flows, blend compositions, products, and scenarios involving the sale or purchase of energy resources. This complexity makes decision-making extremely challenging [2–8], especially in the presence of uncertainties in feedstock specifications, product demand, and economic parameters [9]. Plant-wide optimization is a key prerequisite for making strategic decisions to overcome these challenges, achieve high operational efficiency, and maintain competitiveness in the market [10; 11]. Such optimization enables the determination of the optimal feedstock blend and facilitates effective blending of gasoline and distillates [12]. Furthermore, it helps minimize fuel overproduction and excessive quality margins, while ensuring efficient energy consumption management [13].

Light naphtha (C5–C12 fraction) is a valuable feedstock for producing high-octane gasoline components. Its composition directly affects the efficiency of the three-phase splitter — a unit that separates naphtha into narrow fractions for subsequent isomerization and reforming. This study provides a comprehensive analysis of the feedstock with the identification of components that influence key technological parameters of the process.

II. METHODS AND MATERIALS

A. Feedstock Characterization

The object of the study was light naphtha of the Nemba grade, obtained by atmospheric distillation of crude oil at an industrial unit. The main characteristics of the feedstock are as follows:

- Boiling range: 35–180°C
- Density at 20°C: 0.678 g/cm³
- Sulfur content: <0.01 wt.%
- Reid vapor pressure: 82 kPa

Samples were collected in accordance with GOST 2517-2012 ("Petroleum and petroleum products. Sampling methods") using hermetically sealed stainless-steel samplers.

B. Equipment and Reagents

The following equipment was used for analysis:

1. **Gas Chromatograph: Agilent 7890B with mass spectrometric detector Agilent 5977A**
    - Capillary column: PAC (Petrocol^{TM} DH 50.2)
    - Length: 50 m
    - Internal diameter: 0.2 mm
    - Film thickness: 0.5 μm
    - Temperature program:
    - Initial temperature: 35°C (held for 5 min)
    - Ramp: 3°C/min up to 300°C
    - Final hold: 20 min
2. **Auxiliary equipment:**
    - Hamilton microsyringes (1 μL volume) for sample injection
    - Gerstel MPS sample preparation system
    - Standard hydrocarbon mixtures from Restek for calibration

C. Analytical Procedure

The study was conducted in accordance with ASTM D6729 ("Detailed Hydrocarbon Analysis by Gas Chromatography") with the following modifications:

Sample preparation:

- Degassing at 0°C for 15 minutes
- Filtration through a 0.45 μm membrane

Chromatography:

- Injection volume: 0.2 μL (split ratio 1:50)
- Injector temperature: 250°C
- Carrier gas (helium) flow rate: 1.2 mL/min

Component identification:

- Comparison of retention times with reference standards
- Use of NIST 2020 mass spectral library
- Calculation of linear Kovats indices

Quantitative analysis:

- Internal standard method (n-decane)
- Response factor correction for each hydrocarbon class

D. Data Processing

Statistical processing was performed using:

- Agilent MassHunter (chromatographic data)
- Petrosoft DHA (group composition analysis)
- OriginPro 2022 (graph plotting)

Method precision:

- For components >0.1%: ±2% relative
- For components <0.1%: ±5% relative

E. Quality Control

To ensure reproducibility:

- Daily calibration using Restek DHA Calibration Mix
- Blank run after every 5 samples
- Participation in interlaboratory comparisons (ASTM D02.H0 program)

This methodology ensures selective identification of 127 individual hydrocarbons with a detection limit of 0.01 wt.%, which is critical for optimizing the operation of the three-phase splitter.

III. RESULTS AND DISCUSSION

A. Component Composition of Light Naphtha

Gas chromatographic analysis revealed a complex hydrocarbon composition in the studied light naphtha of Nemba grade. A total of 127 individual compounds were identified, belonging to the following classes:

1. **Isoparaffins (43–47 wt.%):**
   - Major components: isopentane (7.65±0.15%), 2-methylpentane (2.81±0.06%), isooctane (6.10±0.12%)
   - Particular attention is drawn to the high concentration of 2,2,4-trimethylpentane (isooctane), the reference compound used for octane number determination.
2. **n-Paraffins (29–31 wt.%):**
   - Major components: n-pentane (8.31±0.17%), n-hexane (6.86±0.14%), n-heptane (5.27±0.11%)
   - Linear alkanes in this fraction are of particular interest as feedstock for isomerization processes.
3. **Naphthenes (18.1±0.4 wt.%):**
   - Dominant compounds: methylcyclohexane (2.21±0.05%), cyclohexane (3.20±0.07%)
   - Naphthenes contribute to enhanced thermal stability of fuels.
4. **Aromatic hydrocarbons (6.3±0.2 wt.%):**
   - Main constituents: benzene (1.87±0.05%), toluene (0.20±0.01%), xylenes (2.89±0.08%)
   - Benzene content is within Euro-5 regulatory limits (<1 vol.%).

B. Carbon Number Distribution

The distribution of hydrocarbons by carbon number showed the following:

- C5–C6 fraction: 75.2±1.5 wt.% — optimal feedstock for isomerization
- C7–C8 fraction: 22.1±0.9 wt.% — promising for catalytic reforming
- C9+ fraction: 2.7±0.3 wt.% — undesirable heavy components

C. Key Technological Parameters

Based on the obtained data, the following technological conclusions can be drawn:

1. The C5–C6 fraction, which constitutes approximately 75% of the feedstock, is the most valuable for isomerization processes. Its high isoparaffin content (up to 47%) allows forecasting:
   - Isomerate yield with an octane number of 88–92 (RON)
   - Reduction in process energy consumption by 15–20%
2. The C7–C8 fraction (22%) is suitable for reforming, as it contains:
   - 12.8 wt.% of isoalkanes
   - 6.3 wt.% of aromatic hydrocarbons
   - 3.1 wt.% of naphthenes
3. The heavy fraction (C9+) accounts for less than 3%, which:
   - Minimizes the risk of coke formation
   - Allows reduction of the bottom column temperature by 15–20°C

IV. CONCLUSIONS

The qualitative composition of the studied naphtha demonstrates optimal characteristics for processing in a three-phase splitter. The high content of isoparaffins (43–47 wt.%) is of particular value, making this feedstock especially promising for the production of high-octane gasoline. Moreover, the low concentrations of aromatic hydrocarbons (5–7 wt.%) and olefins (<2.2 wt.%) fully comply with the stringent requirements of modern environmental standards. The analysis of the technological advantages of the feedstock revealed a favorable distribution of hydrocarbons by carbon number, with a clear predominance of C5–C6 fractions accounting for 75 wt.% of the product. This distribution makes the naphtha an ideal feedstock for isomerization processes. Special attention should be given to the minimal content of heavy C9+ fractions (<3 wt.%), which significantly reduces the risk of coke formation and simplifies the fractionation process. Additionally, the notable concentration of isooctane (6.10 wt.%) highlights the high potential of the feedstock for producing premium-grade fuels. Based on the conducted research, specific recommendations were developed for optimizing the operation of the three-phase splitter. To achieve maximum yield

of target fractions, the following optimal process parameters are proposed: top column temperature of 65–70°C and bottom column temperature of 175–180°C, with pressures maintained at 2.1–2.5 bar at the top and 3.5–3.8 bar at the bottom of the unit. Particular emphasis is placed on the proposed fractionation scheme involving separate recovery of C5–C6 fractions (for isomerization) and C7–C8 fractions (for catalytic reforming). The practical application of the obtained results offers significant prospects for the refining industry. Implementation of the proposed solutions will allow for a 15–20% increase in the yield of high-octane components, while ensuring full compliance of the products with Euro-5 standards. The findings provide a scientific basis for the modernization of existing process schemes, which is especially relevant in the context of tightening environmental regulations and increasing demand for high-quality motor fuels.

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