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Simulation and Feasibility Assessment of Normal Butane Substitution for LPG Feed in the Alkylation Unit

Parisa Jalali Nia[1], Mir Mohammad Khalilipour[2]✉, Farhad Shahraki[3], Mohammad Reza Sardashti Birjandi[4]

[1] Chemical Engineering Department, University of Sistan and Baluchestan, Zahedan, Iran. Email: a.khalilipour@gmail.com
[2] Corresponding Author, Chemical Engineering Department, University of Sistan and Baluchestan, Zahedan, Iran. Email: a.khalilipour@eng.usb.ac.ir
[3] Chemical Engineering Department, University of Sistan and Baluchestan, Zahedan, Iran. Email: f.shahraki@eng.usb.ac.ir
[4] Chemical Engineering Department, University of Sistan and Baluchestan, Zahedan, Iran. Email: m.r_sardashti@eng.usb.ac.ir

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ABSTRACT

The strategic demand for propylene in the market leads to the conventional LPG feedstock is now redirected, with the C_3 fraction sent to the Propylene Recovery Unit (PRU). This operational adjustment left the alkylation unit primarily reliant on C_4 feed, prompting a comprehensive investigation of alternative feed scenarios to optimize product yield and process economics. In this study, steady-state process simulations were performed using Aspen HYSYS to evaluate the feasibility of replacing the LPG feed with surplus normal butane in the unit. Three scenarios were investigated: (*i*) baseline operation with standard LPG feed, (*ii*) replacement of the propane fraction with normal butane, and (*iii*) replacement of the isobutane fraction with normal butane. The simulation results demonstrated that the substitution of normal butane for propane in the LPG feed is technically feasible, achieving a net alkylate yield of 15.48ton/h with product quality comparable to industrial benchmarks. However, replacing isobutane with normal butane resulted in a drastic drop in alkylate production, with net output falling to 4.72ton/h, rendering this scenario economically unviable. Validation against plant process flow diagrams (PFDs) confirmed the simulation's reliability within acceptable error margins. The findings also highlight the importance of effective feedstock management in alkylation units while partial replacement of LPG with normal butane can optimize resource utilization and meet operational demands, the critical role of isobutane in achieving high alkylate yield and purity must be preserved. The study offers practical implications for the strategic adaptation of Iranian refineries facing changing feedstock availability and market priorities.

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1. Introduction

The rapid growth in global gasoline demand, driven primarily by the expansion of the automotive sector, has made gasoline one of the most critical products in modern petroleum refineries. In recent decades, conventional atmospheric and vacuum distillation processes have proven insufficient to meet the increasing consumption levels. Consequently, refineries have increasingly relied on advanced conversion technologies such as catalytic cracking, hydrocracking, and alkylation to transform heavy and light hydrocarbon feedstocks into higher-value gasoline components [1]. Among these processes, alkylation is particularly important due to its ability to produce high octane alkylate, which serves as a premium blending component in environmentally compliant gasoline formulations. In petroleum refining terminology, alkylation refers specifically to the reaction of low molecular weight olefins with isoparaffins, most commonly isobutane, to form higher molecular weight isoalkanes. Although the reaction is essentially the reverse of catalytic cracking, early misconceptions regarding the chemical inertness of paraffins delayed the recognition of alkylation's industrial potential until the mid-1930s [1]. The urgent demand for high octane aviation fuels during World War II significantly accelerated the development and commercialization of alkylation technologies [2]. Although the prominence of alkylation temporarily declined in the postwar period, its importance has increased again in recent decades due to increasingly stringent fuel quality and environmental regulations.

Industrial alkylation reactions typically occur at relatively low temperatures in the presence of strong liquid acid catalysts such as sulfuric acid (H_2SO_4) or hydrofluoric acid (HF) [3]. Early research conducted by UOP demonstrated that under these mild operating conditions, isoalkanes react with olefins to produce highly branched, saturated hydrocarbons with superior octane characteristics. The principal product, known as alkylate (represented by the reaction $C_4H_8 + iC_4H_{10} \rightarrow C_8H_{18}$), consists primarily of branched C_8 isoparaffins such as trimethylpentanes (TMP) and dimethylhexanes (DMH). These compounds typically exhibit research octane numbers (RON) exceeding 95, making alkylate one of the most valuable blending components in gasoline production.

Despite these advantages, the use of liquid acid catalysts introduces significant operational, technological, and environmental challenges. These include severe equipment corrosion, high catalyst consumption, complex handling requirements, and strict safety considerations [3,4]. Comparative studies have shown that catalyst costs per unit of product in alkylation processes—particularly those based on sulfuric acid—are considerably higher than those associated with many other refinery conversion processes [5]. Furthermore, catalyst losses and the need for immediate neutralization of acid residues complicate both process design and operational management. Hydrofluoric acid, in particular, is associated with severe toxicity and handling risks, which has led to increasing scrutiny of its industrial use. The gasoline demand in Iran has increased rapidly since the widespread adoption of automobiles, placing the country among the world's largest gasoline consumers. Despite the operation of nine domestic refineries, national gasoline production often struggles to fully satisfy domestic demand. Moreover, the contribution of alkylation to the overall gasoline pool remains relatively limited, with the majority of production relying on catalytic reforming and hydrocracking units. This situation highlights the need for improved process integration and technological optimization within Iranian refineries [6]. For instance, in the Abadan refinery, excess normal butane is frequently flared, representing a loss of potentially valuable feedstock. At the same time, liquefied petroleum gas (LPG) can be marketed externally, creating a strong economic incentive to optimize internal feedstock utilization and improve refinery process efficiency.

Alkylation units play a critical role in upgrading low-value refinery gases, primarily C_3 and C_4 streams, into high-octane gasoline blending components of premium quality. The process relies on the reaction between light olefins and isobutane, typically in the presence of strong acid catalysts, to produce aromatic-free fuels that comply with modern environmental fuel standards. In an environment characterized by volatile petroleum prices and increasing competition, refineries continuously seek cost-effective feedstocks such as propane and butane to improve operational margins and enhance return on investment [3, 7]. The economic attractiveness of alkylation largely stems from its capability to convert relatively low-value light hydrocarbons into high-value gasoline components, thereby improving refinery profitability and operational flexibility. Liquefied petroleum gas (LPG) has gained considerable attention as an energy carrier due to its relatively low cost and the ease with which it can be stored and transported in the liquid phase [8]. In Iran, however, a persistent surplus of normal butane—often vented or flared—indicates an inefficiency in feedstock utilization that negatively affects both economic performance and environmental sustainability. The effective integration of surplus normal butane into alkylation processes offers a promising opportunity to increase product value, enable profitable LPG marketing, and reduce greenhouse gas emissions associated with routine flaring. While a full discounted cash flow analysis is beyond the scope of this study, the substantial differences in net alkylate production (15.48 vs. 4.72ton/h) provide a clear qualitative basis for assessing operational attractiveness.

Research Necessity. Increasingly stringent environmental regulations and industrial performance requirements regarding gasoline composition—particularly concerning oxygenates, aromatics, sulfur content, and fuel volatility—have driven refineries worldwide toward the production of higher-quality gasoline fuels [9]. In this context, alkylation has emerged as a key process due to its ability to produce high-octane, clean-burning gasoline components. Consequently, optimizing feedstock selection and operating conditions in alkylation units has become essential for maximizing product yield, reducing operational costs, and minimizing environmental impacts, thereby supporting both economic competitiveness and long-term refinery sustainability. The primary objective of this study is to evaluate the technical and economic feasibility of substituting normal butane for LPG as the feedstock in the alkylation unit of the Abadan refinery through detailed process simulation using Aspen HYSYS, supported by validation with available plant data. The novelty of this research lies in its practical and industry-oriented approach to addressing a real operational challenge within the refinery. To the best of the authors' knowledge, a comprehensive assessment of such a feedstock substitution strategy has not previously been conducted for the Abadan refinery. By utilizing surplus normal butane as an alternative feedstock, the proposed approach has the potential to simultaneously improve refinery profitability and reduce environmental impacts associated with hydrocarbon flaring.

The progressive expansion of the petrochemical industry, coupled with increasingly stringent environmental legislation, has compelled refineries to produce high-quality gasoline with improved combustion characteristics. Regulatory frameworks require refined gasoline to contain oxygenates, be free of aromatics and sulfur, and exhibit low volatility [10]. Among the advanced conversion processes, alkylation of isobutane with light olefins—catalyzed by hydrofluoric or sulfuric acids—has emerged as one of the most effective strategies for producing high-octane, clean-burning gasoline components [11]. The growing importance of alkylation in recent years is reflected in extensive research efforts aimed at optimizing process efficiency, product quality, and environmental compatibility [12].

Process optimization in alkylation unit focuses on maximizing both yield and octane value while minimizing energy and raw material consumption. Butane, which is more economically accessible compared to propane, has become an increasingly attractive feedstock. In pursuit of improved operational economics, refineries have gradually integrated additional olefin streams (e.g., propylene and butylene), shifting away from traditional butane-butylene mixed feeds [10]. In the Iranian context, limited utilization of LPG as a petrochemical feedstock is primarily attributed to its relatively high market price compared to natural gas, which enjoys broader availability and economic advantage. Conversely, normal butane can be converted to the highly-valued isobutane through isomerization, providing a rich source of octane [12]. However, the use of LPG as alkylation feedstock can limit the availability of critical intermediates such as butylene, ultimately restricting the achievable octane number in the alkylate product and contributing to a global deficit of high-octane blending components [11]. Typical alkylation units, particularly those integrated with fluid catalytic cracking (FCC) processes, preferentially utilize isobutane and light olefins (C_3 and C_4 fractions) as feed. Where FCC is insufficient, additional butane isomerization capacity is required to supply isobutane for alkylation.

Existing literature covers various facets of alkylation process modeling, catalyst innovation, operational optimization, and environmental impact mitigation. Mehdi Zadeh et al. [13] demonstrated alkylation process optimization using real plant data, applying response surface methodology and predictive process modeling to simulate operational parameters and optimize alkylate yield and quality. Atashani et al. [12] investigated the optimal operational window for alkylation using sulfuric acid catalysts, focusing on minimizing side reactions such as polymerization and maximizing product quality. Their analysis, based on actual data from the Abadan refinery, pinpointed the key variables impacting process outcomes. Sahebdel et al. [14] studied the kinetics of benzene alkylation with light olefins over zeolitic catalysts, highlighting the strong influence of reactant molecular size and catalyst pore structure on reaction rates and deactivation phenomena. Kazemi et al. [15] optimized hydrodealkylation of toluene using Aspen HYSYS, systematically evaluating operational and thermodynamic parameters for improved reactor performance. Ivashkina et al. [16] provided a mathematically rigorous description of isobutane alkylation kinetics using sulfuric acid catalysis, delineating the effect of propylene concentration and acid strength on product octane number. Kolbenikova et al. [10] modeled hydrodynamic mixing in alkylation reactors, presenting novel injector configurations that enhance reactant distribution, reduce catalyst circulation rates, and maintain mixing efficiency.

In the context of process modeling and advanced control strategies for complex chemical systems, recent studies have demonstrated the effectiveness of data-driven and state-space approaches. For instance, Kiani Talaei et al. [17] developed an enhanced soft sensor framework integrating the state-dependent parameter method with a dynamic data reconciliation filter, which successfully mitigated measurement noise and improved estimation accuracy in nonlinear chemical processes. Furthermore, Kharaji et al. [18] introduced a centralized non-minimal state space proportional-integral-plus (NMSS-PIP) control structure for reactive distillation processes, which eliminated oscillatory behavior and achieved superior disturbance rejection compared to conventional PI controllers. These methodologies offer valuable insights for the monitoring and optimization of alkylation units, where precise control and noise reduction are critical for maintaining product quality and operational stability.

While significant advancements have been attained in the refinement and modeling of alkylation processes globally, direct studies investigating the replacement of LPG with surplus normal butane as feedstock in the alkylation unit—particularly in the context of Iranian refinery operations—remain limited. The present study addresses this gap

through a simulation-based assessment of the Abadan refinery's alkylation unit. It aims to validate the technical and economic viability of this feed replacement and its benefits for process efficiency and environmental impact.

2. Process description and simulation methodology

2.1. Overview of Abadan refinery alkylation unit

The alkylation unit at Abadan Refinery is designed to produce high-octane gasoline blending components (alkylate) by reacting isobutane with light olefins (mainly propylene and butylene). In industrial practice, these reactions occur at low temperatures and are catalyzed by concentrated sulfuric acid—contrasting with the non-catalytic, high-temperature conditions of laboratory alkylation reactions. The core alkylation process yields branched alkanes suitable for gasoline blending, with detailed boiling range and octane ratings of MON 87-95 and RON 90-98. The unit configuration and operational strategy minimizes side reactions, such as olefin polymerization, which increase acid consumption and decrease alkylate quality (elevating FBP and lowering anti-knock index).

2.2. Chemical reactions and catalyst management

The idealized alkylation reactions involve propylene, butenes, and pentenes combining with isobutane to produce high-value alkylate molecules. In practice, the reaction network is far more complex, yielding a broad hydrocarbon cut. The catalyst in Abadan's alkylation unit is concentrated sulfuric acid (98.5wt%), which must be continuously regenerated and re-circulated due to unavoidable losses in acid strength caused by side reactions and trace contaminants in feed streams. Alkylation occurs in a biphasic (emulsion) medium with acid as the dominant phase, requiring constant agitation to prevent acid phase separation. Side reactions—particularly polymerization among olefins—result in higher acid consumption and diminished product quality. Steady acid injection and online control are essential for sustainable operation.

2.3. Key operating variables

The quality and yield of alkylate are controlled by several critical process variables:

- **Isobutane concentration:** High isobutane levels suppress undesired polymerization and promote selective alkylation. The feed ratio of isobutane to olefins typically ranges from 7:1 to 10:1, with excess isobutane being recovered and recycled.
- **Olefin space velocity:** Lower space velocities increase the interaction probability between isobutane and olefins, improving product selectivity. Defined as volumetric olefin feed per unit acid inventory (m^3/h).
- **Reaction temperature:** Low temperatures (7-16°C depending on feed) inhibit side reactions. Excessively low temperatures (below 4°C for butylene systems) result in acid carry-over due to poor phase separation.
- **Mixing intensity:** Sufficient agitation ensures intimate contact between reactants, enhancing alkylation yield and reducing mass transfer limitations.
- **Acid strength:** Acid strength should be maintained at 93-96wt% for optimal performance; lower strengths increase polymerization risk and complicate reaction control ("acid runaway").

2.4. Process control

The alkylation unit employs rigorous process control to stabilize operating conditions and ensure product quality. Key control tactics include:

- Maintaining acid strength above 93wt% in the final reactor stage.
- Utilizing refrigeration to cool recycled isobutane and feeds, minimizing water content and acid dilution.
- Ensuring a dominant acid phase in all reactor emulsions (design target: 55vol% acid).
- Maximizing the isobutane-to-olefin ratio and circulation rates for improved selectivity.
- Using caustic washing stages and mesh pads to neutralize acid carryover and prevent downstream fouling.

The reactor system is equipped with process instrumentation, circulation pumps, static mixers, and chillers for robust emulsion management.

2.5. Unit configuration and streams

The alkylation unit consists of five main sections: reactors, washing systems, separation, blow-down, and refrigeration. FCC-derived C_3 and C_4 streams are separately introduced, optimized, and maintained using level controllers and in-line analyzers. Isobutane is pre-cooled and split into parallel flows for injection and thorough mixing; downstream separation towers (RIF, IBF, Propane Depropanizer, n-Butane Debutanizer) accomplish product purification and recycling of key streams.

2.6. Simulation methodology

2.6.1. Simulation objectives

Given surplus normal butane available in Abadan Refinery, this study aims to assess the technical and economic feasibility of substituting LPG with normal butane as feedstock for alkylation. The unit is simulated under two scenarios:

- Base Case: Alkylation unit fed with conventional refinery LPG
- Alternative Case: Alkylation unit fed with normal butane

2.6.2. Simulation platform and thermodynamics

Process flowsheets as can be seen in Fig. 1 were simulated in Aspen HYSYS using the Peng–Robinson equation of state. This model is appropriate due to the hydrocarbon-dominated nature of the feed and modest deviations from ideal liquid-phase behavior. Only the vapor phase shows non-ideality meriting advanced modeling.

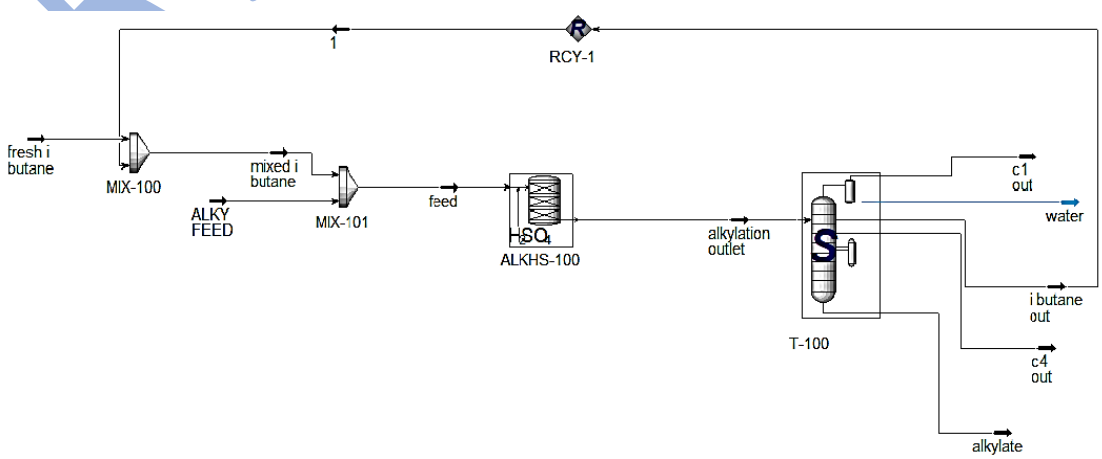

Fig. 1. Aspen-Hysys Process Flow Diagram (PFD) of the alkylation unit using refinery feedstock

2.6.3. Feed compositions

Three principal feed streams were modeled:

- **Pure isobutane:** Total flow rate of 24 ton/h (recycled to reach 103 ton/h after convergence with fresh feed).
- **Butane-butene mix:** Flow rate of 12 ton/h with detailed molar composition (Table 1).
- **LPG:** Flow rate 20-25 ton/h with significant molar fractions of propane (14%), isobutane (20%), and normal butane (66%)—(Table 2)

Feed blends for simulation are termed "alkylation feed".

Table 1. Composition of the butane–butene feed

Components	Mole fraction
Methane	0
Ethane	0
Propane	0.004
i-Butane	0.05393
n-Butane	0.0739
tr2-Butene	0.1266
1-Butene	0.1674
cis2-Butene	0.0836
3M-1-butene	0.0052

Table 2. Composition of the LPG feed

Components	Mole fraction
Methane	0
Ethane	0
Propane	0.1394
i-Butane	0.2023
n-Butane	0.6573
tr2-Butene	0.0002
1-Butene	0.0002
cis2-Butene	0.0001
3M-1-butene	0
22-Mpropane	0.0003
i-Pentane	0.0002

2.6.4. Feed substitution scenarios

To simulate feasibility of normal butane replacement, two main cases were set up:

- **Case 1 (n-butane replaces isobutane):** Feed adjusted to 90% n-butane and 10% i-butane due to simulation constraints.
- **Case 2 (n-butane replaces propane):** Feed compositional changes detailed in Table 3.

Material and energy balances, selectivity, and process controllability were compared for both base and alternative cases. Results are presented in subsequent sections and analyzed for process, economic, and operational impacts.

3. Results and discussion

This section presents and discusses the simulation results of the Abadan Refinery alkylation unit under different feedstock scenarios. The base case utilizes the conventional refinery LPG feed, while two alternative scenarios investigate the substitution of normal butane for (*i*) isobutane and (*ii*) propane. The primary evaluation criteria are alkylate yield, alkylate purity, and overall process feasibility.

Table 3. Composition of the n-butane replacing propane in LPG feed

Components	Mole fraction
Methane	0
Ethane	0
Propane	0
i-Butane	0.2023
n-Butane	0.7967
tr2-Butene	0.0002
1-Butene	0.0002
cis2-Butene	0.0001
3M-1-butene	0
22-Mpropane	0.0003
i-Pentane	0.0002

3.1. Simulation with conventional refinery LPG feed

Simulation of the alkylation unit with the standard refinery LPG feed produced the outlet composition summarized in Table 4. The product stream contains a wide range of hydrocarbons, from unreacted light components to heavier branched paraffins. The alkylate fraction is defined here as the C_6+ hydrocarbons represented by NBP cuts from NBP[88] onward, which are the desired products of the alkylation reaction.

Table 4. Product composition at the alkylation outlet using refinery LPG feed. Alkylate fraction is defined as hydrocarbons with normal boiling point (NBP) cuts corresponding to C_6+ components (NBP ≥ 88°C)

Components	Mole fraction	Components	Mole fraction
NBP: 41°C	0	Propene	0.0394
NBP: 56°C	0	i-Butene	0.0359
NBP :72°C	0	1-Butene	0.0185
NBP :88°C	0.0114	tr2-Butene	0.0257
NBP :104°C	0.053	cis2-Butene	0.0251
NBP :120°C	0.237	1-Pentene	0.00046
NBP :136°C	0.106	2M-1-butene	0.00032
NBP :151°C	0.0001	3M-1-butene	0.00032
NBP :167°C	0.0515	2M-2-butene	0.00032
NBP :183°C	0.00017	tr2-Pentene	0.00046
NBP :199°C	0.0054	cis2-Pentene	0.00046
NBP :215°C	0.00025	i-Butane	0.38698
NBP :231°C	0.00006	n-Butane	0.00127
NBP :247°C	3.9E-8		
NBP :262°C	7.8E-9		

Table 4 indicates that branched C_6+ components constitute 46.5% of the total outlet stream, while a significant portion of isobutane remains unreacted and must be recovered and recycled to the reactor inlet. This behavior is consistent with industrial alkylation practice, where excess isobutane is required to suppress polymerization and enhance selectivity. Components with zero mole fraction in the simulation results (e.g., NBP cuts at 41°C, 56°C, and 72°C) are retained in the table to maintain the complete NBP reporting framework, but they indicate the absence of detectable quantities under the simulated conditions.

Following downstream separation, the refined alkylate composition is reported in Table 5. Light hydrocarbons and unreacted species are effectively removed, resulting in a final alkylate purity of 96.23%. The corresponding alkylate mass flow rate was calculated as 65.72ton/h, while the net alkylate product, accounting for separation losses, reached 63.24ton/h. These results confirm the effectiveness of the separation section in producing a high-purity alkylate stream.

Table 5. Refined alkylate composition and flowrate under LPG feed. Alkylate fraction is defined as hydrocarbons with normal boiling point (NBP) cuts corresponding to C_6^+ components (NBP ≥ 88°C)

Components	Mole fraction
NBP: 88°C	0.0235
NBP: 104°C	0.10967
NBP: 120°C	0.491
NBP: 136°C	0.219
NBP: 151°C	0.0003
NBP: 167°C	0.106
NBP: 183°C	0.0003
NBP: 199°C	0.0113
NBP: 215°C	0.0005
NBP: 231°C	0.0001

3.1.1. Simulation validation

To validate the simulation model, the alkylate purity obtained from the simulation was compared with design data reported in the process flow diagram (PFD). As shown in Table 6, the relative deviation between the simulated alkylate purity (96.23%) and the PFD value (88.95%) is 7.56%. Given the simplifying assumptions of the thermodynamic and kinetic models, this level of deviation is considered acceptable and confirms the reliability of the simulation for comparative feedstock evaluation.

Table 6. Simulation validation

Alkylate percentage in the Simulation	Alkylate percentage in the PFD	Difference (%)
96.23	88.95	7.56

3.2. Simulation: Replacement of isobutane with normal butane

In the first substitution scenario, isobutane in the feed was largely replaced by normal butane (90% n-butane and 10% i-butane). The resulting outlet composition is presented in Table 7. Compared to the base case, the proportion of C_6^+ hydrocarbons decreased sharply to 21%, indicating a severe reduction in alkylation effectiveness. Consequently, the net alkylate production dropped to only 4.72ton/h. This pronounced decline can be attributed to the lower reactivity of normal butane relative to isobutane, which plays a critical role as both a reactant and a diluent in alkylation chemistry. The results clearly demonstrate that substituting isobutane with normal butane leads to unacceptable losses in alkylate yield and quality, rendering this scenario technically and economically infeasible.

Table 7. Product composition with n-butane substitution for isobutane. Alkylate fraction corresponds to the C_6^+ hydrocarbons represented by NBP cuts ≥ 88°C

Components	Mole fraction
NBP: 104°C	0.00727
NBP: 120°C	0.0603
NBP: 136°C	0.142
NBP: 151°C	0.0002
NBP: 167°C	0
NBP: 183°C	0
NBP: 199°C	0
NBP: 215°C	0.0002
NBP: 231°C	0.0002

Note: Mole fractions reported as zero are < 1×10^{-6} in the simulation output.

3.3. Simulation: Replacement of propane with normal butane

In the second scenario, propane in the LPG feed was replaced with normal butane, while maintaining isobutane in the feed. The product composition obtained from this simulation is summarized in Table 8.

Table 8. Product composition with n-butane substitution for propane. Alkylate fraction corresponds to the C_6^+ hydrocarbons represented by NBP cuts ≥ 88°C

Components	Mole fraction
NBP: 104°C	0.007
NBP: 120°C	0.58
NBP: 136°C	0.237
NBP: 151°C	0.0003
NBP: 167°C	0
NBP: 183°C	0
NBP: 199°C	0
NBP: 215°C	0.0003
NBP: 231°C	0.00008

In contrast to the previous scenario, the C_6^+ fraction remained high at 89.27%, and the purified alkylate flow rate reached 15.48 ton/h. The distribution of NBP cuts indicates that the dominant alkylate components were preserved, with no significant deterioration in product quality. These results suggest that propane plays a less critical role in alkylation reactions compared to isobutane. Therefore, its replacement with normal butane does not significantly disrupt reaction pathways or selectivity.

3.4. Comparative Analysis and Discussion

Propane does not participate directly in the alkylation reaction as either an olefin or an isoparaffin; its role in the LPG feed is primarily as an inert diluent. Therefore, replacing propane with normal butane does not remove any reactive species essential to alkylation chemistry. In contrast, isobutane is the sole isoparaffin that reacts with olefins to form highly branched C8 alkylate molecules. Substituting isobutane with normal butane—which cannot undergo hydride transfer or form the necessary tertiary carbocation intermediates—eliminates the primary alkylation reactant, leading to the drastic yield reduction observed. A comparative assessment of the three feed scenarios reveals the following key findings:

- **Base case (Refinery LPG feed):** High alkylate purity and yield, consistent with industrial design data.
- **Isobutane replacement:** Severe reduction in alkylate yield and C_6^+ fraction, confirming the indispensable role of isobutane in alkylation chemistry.
- **Propane replacement:** Acceptable alkylate yield and composition maintained, demonstrating the technical feasibility of this substitution.

Overall, the simulation results confirm that normal butane can feasibly replace propane but not isobutane in the alkylation feed. The validated model provides a reliable basis for refinery decision-making regarding feedstock flexibility and optimization. Summary of Simulation Results under Different Feed Scenarios are depicted in Table 9.

Table 9. Summary of simulation results under different feed scenarios

Scenario	Feed composition	C_6^+ fraction in product (%)	Final alkylate purity (%)	Net alkylate flowrate (ton/h)	Relative difference vs. PFD (%)	Technical / Operational feasibility
Base case – Refinery LPG feed	Conventional LPG (per refinery specification)	46.5	96.23	63.24	7.56	✓ Feasible – baseline operation
Scenario 1: *Replacement of i-C_4 with n-C_4*	90% n-butane + 10% i-butane	21.0	—	4.72	—	✕ Not feasible – major alkylate loss
Scenario 2: *Replacement of propane with n-C_4*	LPG with propane fully substituted by n-butane	89.27	—	15.48	—	✓ Feasible – acceptable yield and purity

* Alkylate fraction is defined as hydrocarbons with NBP ≥ 88 °C (corresponding to C_6^+ cuts). Flowrates represent net alkylate production after product separation. Relative difference refers to deviation between simulated and design (PFD) alkylate purities.

4. Conclusion

In the Abadan refinery, the LPG stream from the FCC unit is first treated for H_2S and mercaptan removal in the amine and Sulfrex units. The treated stream is then routed to the fractionation tower, where C_3 and C_4 fractions are separated. According to the original design, the C_3 stream was intended as feedstock for the C_3 section of the alkylation unit, while the C_4 stream supplied the C_4 section. As a result, the C_3 section of the alkylation unit has remained inactive since the plant's commissioning. The simulation results obtained in this study indicate that the C_3 section of the alkylation unit can potentially operate using the C_4 feed, thereby providing greater operational flexibility in refinery production planning. Such a configuration would enable the refinery to continue prioritizing propylene recovery while maintaining the option to utilize the C_3 section for gasoline production when required by domestic fuel demand.

It is important to note that the simulation scenarios assume the C_3 section of the alkylation unit, originally designed for propane/propylene feed but currently inactive, is made available for processing the modified C_4-rich feed. This reactivation is technically straightforward, as the equipment remains in place and only feed routing would need adjustment. The main objective of this research was to evaluate the feasibility of replacing LPG with normal butane as the feedstock for the alkylation unit. Process simulation results demonstrate that replacing propane with normal butane in the LPG feed is technically feasible. Under this scenario, the net alkylate production reached approximately 15.48 ton/h, while the resulting product composition remained within acceptable industrial quality standards. This indicates that normal butane can be effectively integrated into the alkylation process as a partial substitute for propane without significantly compromising product quality or process performance. In contrast, the replacement of isobutane with normal butane resulted in a substantial decline in alkylate production, reducing the net yield to approximately 4.72ton/h. Such a reduction is incompatible with the operational and economic objectives of the alkylation unit. Since the primary function of the alkylation process is to maximize both the yield and quality of high-octane alkylate, this substitution strategy is considered neither technically feasible nor operationally justified, as the severe yield reduction would undermine the unit's primary objective.

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