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Impact Analysis of Deisohexanizer Fractionation On Isomerate Research Octane Number At The Algiers Refinery

Etude d'éfficacité du Déisohexaniseur et son impact sur la qualité d'isomérat de la raffinerie d'Alger

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ABSTRACT. This study investigates the optimization of the light naphta isomerization process at the Algiers Refinery, with a focus on the operational efficiency of the Deisohexanizer (DIH) column. Isomerization is a critical refinery process that upgrades low-octane linear alkanes into high-octane branched isomers, thereby enhancing the Research Octane Number (RON) of the gasoline pool.
The research methodology employed Aspen HYSYS software to conduct rigorous steady state modeling and performance analysis of the unit. To quantify the added value of the fractionation section, a baseline simulation was first established for a once-through configuration that excluded the DIH. Subsequently, a comprehensive simulation integrated the Deisohexanizer into the process flow to evaluate its impact on the global system efficiency and product quality.
The study focused on the sensitivity analysis of key operating parameters, including reflux ratios, feed tray locations, and reboiler duties. These adjustments aimed to maximize the separation of low-octane normal hexane (nC6) from high-octane dimethylbutanes, thereby optimizing recycling cycles and minimizing energy consumption. The final results identify several optimal operating points and provide a set of technical recommendations proposed to Sonatrach. These suggestions aim to enhance the RON of the final isomerate while maintaining cost-effective energy profiles within the Algiers refinery's current infrastructure.
RÉSUMÉ. Cette étude porte sur l'optimisation du procédé d'isomérisation du naphta léger à la raffinerie d'Alger, et plus particulièrement sur l'efficacité opérationnelle de la colonne de désisohexanisation (DIH). L'isomérisation est un procédé de raffinage essentiel qui transforme les alcanes linéaires à faible indice d'octane en isomères ramifiés à indice d'octane élevé, améliorant ainsi l'indice d'octane recherche (RON) de l'essence.
La méthodologie de recherche a utilisé le logiciel Aspen HYSYS pour réaliser une modélisation rigoureuse en régime permanent et une analyse des performances de l'unité. Afin de quantifier la valeur ajoutée de la section de fractionnement, une simulation de référence a d'abord été établie pour une configuration à passage unique excluant la colonne DIH. Par la suite, une simulation complète a intégré la colonne de désisohexanisation au flux de procédé afin d'évaluer son impact sur l'efficacité globale du système et la qualité du produit.
L'étude s'est concentrée sur l'analyse de sensibilité des principaux paramètres de fonctionnement, notamment les taux de reflux, l'emplacement des plateaux d'alimentation et les puissances du rebouilleur. Ces ajustements visaient à optimiser la séparation de l'hexane normal (nC6) à faible indice d'octane et des diméthylbutanes à indice d'octane élevé, optimisant ainsi les cycles de recyclage et minimisant la consommation d'énergie. Les résultats finaux ont permis d'identifier plusieurs points de fonctionnement optimaux et de formuler des recommandations techniques à l'intention de Sonatrach. Ces suggestions ont pour objectif d'améliorer l'indice d'octane de l'isomérat final tout en maintenant des profils énergétiques compétitifs au sein de l'infrastructure actuelle de la raffinerie d'Alger.
KEYWORDS. Performance of Deisohexaniezr, Isomerization unit, Octane Number, modelling, Algiers Refinery.
MOTS-CLÉS. Performance du désisohexaniseur, unité d’isomérisation, modélisation, indice d’octane, raffinerie d’Alger.

1. Introduction

Crude oil is a mixture of various hydrocarbon components, used in various industries and in combustion engines [1].

Oil refining is a key industrial process that aims to meet economic demands and improve the daily lives of individuals in their societies by providing energy products essential to the functioning of our modern world [2, 3, 4].

This process is a crucial step in converting crude oil into a range of refined products suited to various applications. This transformation involves separating the crude into different fractions called petroleum cuts. These cuts, from lightest to heaviest, are: liquefied petroleum gases (LPG), gasoline, light naphta, kerosene, diesel fuel, and residue. Each is intended for specific uses and requires different processing to meet varying requirements.

Fuels used in automotive engines are generally characterized by their octane rating and Reid vapor pressure. New environmental regulations require fuel reformulation to reduce emissions of volatile compounds and limit the presence of aromatic compounds. A decrease in the octane rating generally accompanies this process.

In recent years, petroleum refining has been characterized by the introduction of new techniques, all aimed at meeting the ever-increasing demands for the quality of refined products. Among these demands, the one that dominates this evolution is the need to produce high-performance gasoline, particularly with increasingly higher-octane ratings, with the lowest possible sensitivity.

So, the current problem for refineries is to produce gasoline with a high-octane rating and an adequate Reid Vapor Pressure (RVP), while containing fewer aromatic compounds.

One possible solution is to recover the naphtha and treat it with two separate processes: isomerization and catalytic reforming.

Faced with this trend, paraffin isomerization constitutes an alternative to the total elimination of lead, as well as to limitations on aromatic hydrocarbons, olefins, benzene and sulfur; it is a complementary process to catalytic reforming.

As part of the gradual adaptation of gasoline specifications to global standards, SONATRACH has made an isomerization unit available as part of the refinery rehabilitation, thereby increasing the octane rating of light gasoline.

The utility of isomerization in refining lies in its ability to raise gasoline octane levels by converting straight-chain paraffins into branched forms. This chemical shift not only improves fuel performance but also reduces emissions. [5]

The isomerization of linear-chain paraffins is an important reaction in petroleum-derived chemistry. This process involves the transformation, with minimal cracking, of low-octane linear paraffins into their branched counterparts or into higher-octane isomers.

To enhance octane numbers through molecular rearrangement, catalytic reforming and isomerization remain the primary industrial [6, 7]. While reforming also serves to crack larger hydrocarbons into high-value molecules [8], it faces limitations when handling naphta rich in normal paraffins. Furthermore, the resulting reformate often exceeds legal benzene limits. In contrast, isomerization offers a more refined and cost-effective alternative for octane boosting. The quality of the isomerate is governed by temperature, naphthene content, and Liquid Hourly Velocity (LHSV); higher temperatures accelerate the reaction rate, excessive naphthene levels increase hydrogen demand for ring opening, and overly low LHSV can lead to channeling [9]. Many studies have been done to improve the performance of the isomerization process [10, 11]. Recent research, such as the

comprehensive review by Naqvi et al. [12], continues to optimize this process. Notably, Nikitav Checantsev and Gyngazova [13] developed a mathematical model for light naphta units that accurately predicts isomerate composition across various feedstocks, allowing for better process optimization and efficiency comparisons in schemes involving n-pentane recycling.

Hamadi and Kadhim introduced a material balance and kinetic model for Penex isomerization. Within this framework, material balance calculations were performed to predict kinetic parameters, including the rate constants for n-paraffin-to-olefin (K1) and olefin-to-i-paraffin (K2) conversions, as well as the corresponding activation energies. Their study showed that increasing temperature results in an increase in K_1 and a decrease in K_2 [14]. The optimization of process variables was introduced by Shahata et al. In 2018, researchers optimized the factors that determine the octane numbers of isomerization products (feed composition, temperature, H2/feed ratio, and LHSV) using response surface methodology (RSM) [15].

Zaidoon et al. in 2020 developed a detailed kinetic model using a genetic algorithm to simulate light naphtha isomerization over various Pt/zeolite catalysts. The model, covering 207 reactions for 52 components, showed high accuracy with very low mean absolute errors across six different temperatures [16]

The efficiency of heat-exchange equipment in industry is an important factor directly influencing the performance of industrial installations. In most refining or petrochemical units, the thermal energy required by the process is supplied through various equipment, including electric superheaters, in which energy generated by electrical resistances is transmitted directly to the fluid to be heated [2], [3].

Heat exchange equipment plays a crucial role in petrochemical plants. Operating this equipment can involve various technical problems, such as equipment failure or component failure, which can lead to a plant shutdown. Such a shutdown or reduced efficiency has a significant impact on production.

In our study, particular attention was paid to simulating the isomerization unit and examining the influence of the Deisohexanizer column on the quality of the isomerate recovered from it.

2. Methodology

The Algiers refinery has implemented various chemical processes to improve the quality of gasoline for automotive use, while complying with engine standards and environmental regulations.

To optimize one of the components of this mixture, light naphtha, the refinery has opted for isomerization. This process converts low-octane paraffins into high-octane iso-paraffins. This operation is carried out in catalytic bed reactors operating under specific parameters.

At the outlet of these reactors, a stabilizer separates the unwanted light elements from the desired product, and another separation column, called Deisohexanizer, separates the reacted compounds from the unreacted ones, affecting the quality of the isomerate.

The problem at the Algiers refinery is that the current yield of the isomerization unit is suboptimal, leading to poor separation in the Deisohexanizer.

This work, carried out using the Aspen HYSYS V14 simulator, aims to demonstrate the paramount importance of the Deisohexanizer in this unit and to determine the optimal operating conditions to maximize isomerate yield at the unit's output.

The method used in this work can be summarized in the following steps:

1- Simulation of the isomerization unit without Deisohexanizer;
2- Simulation of the reaction section;
3- Simulation of the first reactor;

4- Simulation of the second reactor;
5- Stabilizer simulation;
6- The optimization of the stabilizer operating parameter;

2.1. *Process description*

To carry out the isomerization process, the Algiers refinery has put in place an entire installation of the necessary equipment.

2.1.1. *The sections of the isomerization unit*

The isomerization unit consists of the following sections:

- dryers and hydrogen dryers;
- Isomerization reactors;
- Stabilizer;
- Deisohexanizer.

2.1.2. *Charge dryers and hydrogen dryers*

- The treated light naphtha from the hydrotreating unit (unit 500) is combined with the recycling product from the Deisohexanizer in the feed tank (510-D-001).
- This mixture is transferred by the isomerization charging pumps (510-P-001-A/B) to the series dryers (510-D-002-A/B) via a downward flow to remove moisture, thus protecting the isomerization catalyst from damage caused by water, which is harmful to the catalyst.

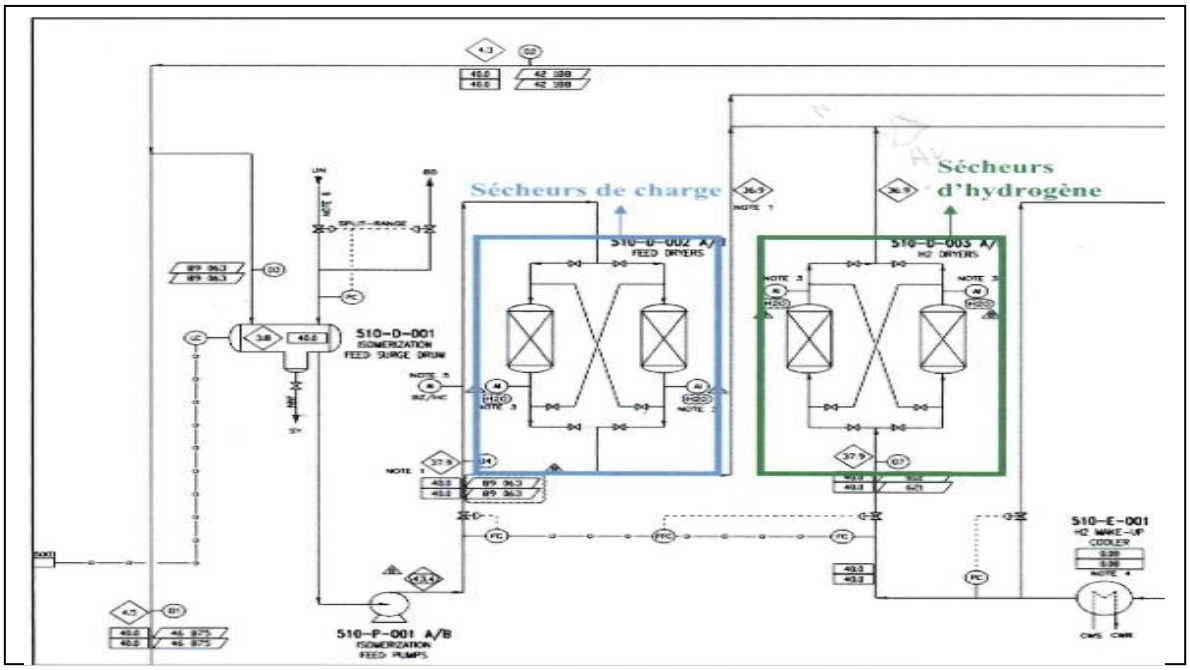

Figure 1. *Dryer section of the isomerization unit*

2.1.3. *Reaction Circuit*

- The process begins by preheating the hydrotreated feed combined with make-up hydrogen from the dryer section in two exchangers.
- Subsequently, the charge intended for the reactor is brought to the required operating temperature, between approximately 112 and 132 °C, by means of medium intermediate pressure (IMP) steam.

- A chlorinating compound is continuously injected into the isomerization reactor feed to maintain the necessary chloride level on the isomerization catalyst, thus compensating for chloride losses in the effluent.
- The treated stream is then routed to the first isomerization reactor (510-R-001), where benzene hydrogenation and isomerization take place.

2.1.4. *Stabilization Circuit*

The effluent from the isomerization reactors feeds the Stabilizer column. The stabilizer's purpose is to remove HCl. The column head pressure is maintained at approximately 18 kg/ cm^2.g·

The initial product is partially condensed in the air condenser (510-EA-001) and cooler (510-E-007) at 40 °C, then collected in the reflux flask (510-D-006). The vapor phase is directed to the scrubber, and the liquid phase is returned to the stabilizer by the reflux pumps (510-P-002A/B).
The stabilizer is heated by intermediate high-pressure (IHP) steam generated by the steam generator

3. Simulation and optimization of results

The HYSYS software allows the simulation of industrial processes in the gas, refining and petrochemical industries in stationary and dynamic modes.

- The user must specify the constituents of the gas, liquid, or mixture.
- He chose a thermodynamic model.
- It must also specify the parameters necessary for calculating each unit operation.
- HYSYS solves the process flow diagram and can also size some equipment.

There are many equations of state to model the behavior of real gases, and Peng Robinson's is particularly useful for predicting the behavior of gases and liquids under high-temperature and high-pressure conditions, such as those found in petrochemical processes, natural gas reservoirs, and other industrial applications.

The isomerization unit is fed with light hydrotreated naphtha from the hydrotreating unit (unit500).

The quantity of crude oil from Sidi Rezin processed in the isomerization unit is designated for a loading rate of 375,000 tonnes/year at a density of 72 m^2/h.

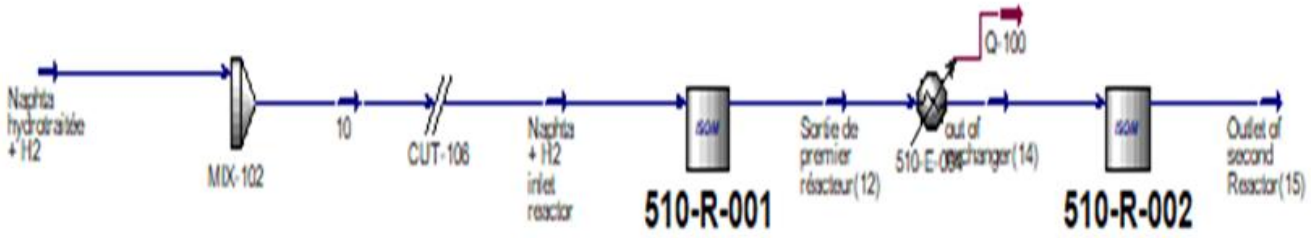

Figure 2. *The simulated reaction section diagram*

3.1. *Simulation of the isomerization unit without a Deisohexanizer*

3.1.1. *Simulation of the reaction section*

3.1.1.1. Simulation of the first reactor

	Values
Reactor diameter (m)	1.8
Reactor length (m)	22.1
Catalyst density (kg/m³)	710
Porosity	0.19

Table 1. *Sizing of the first reactor*

Composition	Entrance to the first reactor	First Reactor Exit
H_2	0.1246	0.0786
P1	0.0024	0.0026
P2	0.0020	0.0022
P3	0.0011	0.0017
iP4	0.0008	0.0048
nP4	0.0064	0.0038
iP5	0.0659	0.1526
nP5	0.1334	0.0579
22DIMETHYLBUTANE	0.0241	0.1512
23DIMETHYLBUTANE	0.0452	0.0465
2-METHYLPENTANE	0.1819	
3-METHYLPENTANE	0.1212	0.1100
nP6	0.1517	0.0636
M cyclopentane 5N6	0.0678	0.0675
BENZENE	0.0163	0.0000
Cyclohexane 6N6	0.0434	0.0657
N heptane nP7	0.0064	0.0065
M cyclohexane 6N7	0.0039	0.0045
TOLUENE	0.0001	
Total (kmol/h)	1242.21	
Total (kg/h)	89,675	

Table 2. *Composition at the inlet and outlet of the first reactor*

We notice the predominant presence of the C5 and C6 components in the load from the first reactor.

The first reactor is used to carry out benzene hydrogenation and most of the isomerization.

In this section, the hydrogenation of benzene is verified by determining the initial mole fraction at the inlet and outlet of the first reactor. Conversely, the efficiency of converting linear hydrocarbons into branched isomers is assessed by calculating the octane number, a key indicator of the conversion.

In the first reactor, benzene and hydrogen react to form cyclohexane according to this reaction:

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

The results of the calculation of the fraction of benzene converted into cyclohexane are given in Table 2. These results indicate that the simulation results in a complete conversion of benzene to cyclohexane.

The conversion of benzene to cyclohexane can be verified as follows:

$$Conversion\ (\%) = [(x_0 - x)/x_0]*100 \quad [1]$$

x: mole fraction of the constituent

x_0 initial mole fraction of the constituent

VOC (%) = [0.0163-0) / 0.0163] *100 = 100%

This means that the reaction has achieved its main objective of transforming benzene into desired products; complete conversion may be important to ensure the quality of the final products.

Table 3 presents the results of the partial isomerization, determined by measuring the octane number of the effluent from the first reactor.

	Reactor inlet R-001		Reactor R-001 Exit	
	HYSYS	Design	HYSYS	Design
MY	64,596	64,596	75.51	74.75
RON	70	70	79.49	78.27

Table 3. *Octane rating results from the first reactor simulation*

The increase in octane rating in the first isomerization reactor indicates improved fuel quality. The four naphthenes present in the isomerization feedstock are cyclopentane (CP), methyl cyclopentane (MCP), cyclohexane (CH), and methylcyclohexane. These compounds undergo secondary reactions, breaking down and hydrogenating to form paraffins (ring opening). These paraffins then undergo molecular rearrangements that lead to the formation of isomers with different chemical structures, as shown in Table 2.

Thus, the increase in NO is due to the compounds shown in orange in Table 2

- i-Pentane, which increases up to 0.1526 (mol%)
- 2,2-Mbutane, which also increases up to 0.1512 (mol%)

3.1.1.2 Simulation of the second reactor

The second reactor in the unit's reaction section completes the isomerization not achieved by the first reactor and simultaneously increases the octane number of the resulting products. To assess the efficiency of hydrocarbon conversion, we use the octane number as an indicator. The results are presented in Table 4 below.

	R-002 reactor inlet	R-002 Reactor Exit
	Simulation	Simulation
MY	75.51	76.41
RON	79.49	80.34

Table 4. *Octane rating at the inlet and outlet of the second reactor*

An increase in octane rating is observed, indicating improved fuel quality with respect to knock resistance and engine performance. This suggests that the second isomerization reactor has been adjusted to increase further the conversion of linear alkanes to high-octane cyclic isomers.

In the second reactor, we note that the input and output fractions remain quite similar, which explains why most of the isomerization occurs in the first reactor. The increase in octane number in the second isomerization reactor indicates successful molecular transformation of linear components into high-octane cyclic isomers, thereby improving fuel quality.

The compounds responsible for this increase are: **2,2-dimethylbutane** and **I-Pentane.**

These cyclic molecules have more compact structures and increased knock resistance, which improves the overall octane rating of the final product. Isomerization of nC5 and nC6 therefore yields hydrocarbons with improved combustion quality and optimized engine performance, thereby increasing the measured octane rating.

	Design case simulation	
Composition	Input R-002	Outlet R-002
Hydrogen	0.0786	0.0783
Methane	0.0026	0.0026
Ethane	0.0022	0.0022
Propane	0.0017	0.0018
I-Butane	0.0048	0.0052
N-Butane	0.0038	0.0036
I-Pentane	0.1526	0.1527
N-Pentane	0.0579	0.0527
2,2-mbutane	0.1512	0.1694
2,3-mbutane	0.0465	0.0469
2-mpentane	0.1803	0.1752
3-mpentane	0.1100	0.1038
N-Hexane	0.0636	0.0563
M cyclopentane	0.0675	0.0597
Benzène	0.0000	0.0000
Cyclohexane	0.0657	0.0734
N-Heptane	0.0065	0.0064
M-cyclohexane	0.0045	0.0046

Table 5. *Molar fraction at the inlet and outlet of reactor r-002*

According to the simulation results, the octane rating reached 88, confirming the need for this column.

3.2. *Stabilizer Simulation*

The stabilizer in the isomerization unit (Fig 3) is an essential part of the hydrocarbon isomerization process. Its main role is to separate the lighter compounds (heads) from the heavier compounds (bottoms) produced during the isomerization operation. This separation allows adjustment of the Reid vapor pressure (RVP).

The stabilizer simulation was performed following the steps described below:

- Define the separator;
- Configure the separator parameters;
- Configure the feed and outlet flows;
- Enter the column dimensions;
- Run the simulation.

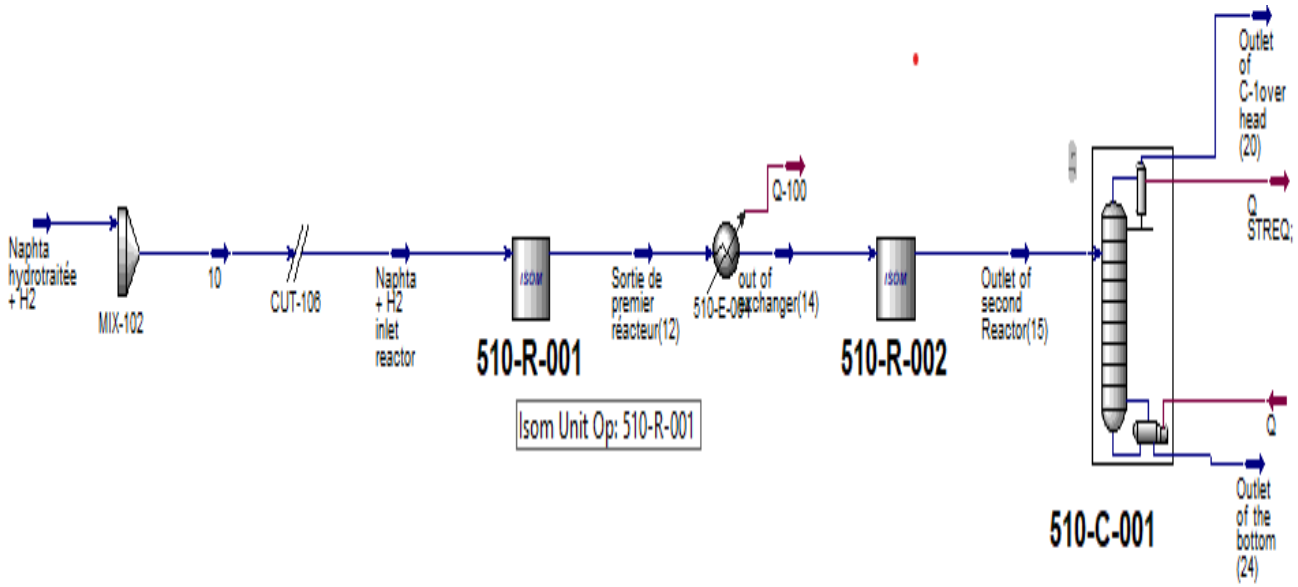

Figure 3. *Stabilizer simulation*

Composition	Input C-001	Bottom C-001
Hydrogen	0.0783	0.0000
Methane	0.0026	0.0000
Ethane	0.0022	0.0000
Propane	0.0018	0.0000
I-Butane	0.0052	0.0001
N-Butane	0.0036	0.0003
I-Pentane	0.1527	0.0000
N-Pentane	0.0527	0.0581
2,2-mbutane	0.1694	0.1886
2,3-mbutane	0.0469	0.0522
2-mpentane	0.1752	0.1952
3-mpentane	0.1038	0.1157
N-Hexane	0.0636	0.0627
M cyclopentane	0.0597	0.0665

Benzene	0.0000	0.0001
Cyclohexane	0.0734	0.0817
N-Heptane	0.0064	0.0072
M-cyclohexane	0.0046	0.0051

Table 6. *Stabilizer inlet and stabilizer outlet composition*

Table 6 shows that the column has removed all light components to regulate the Reid vapor pressure (RVP).

We can say that the increase in RVP is due to the presence of light components. Its regulation determines the quality of the isomerate.

To verify the stabilizer's effectiveness, we use RVP as an indicator. The results are given in Table 7
TVR is measured at a condenser head temperature of 37.8 °C.

RVP Imput C-001	*RVP Bottom C-001*
5.168 Kg/cm^2	0.6593 Kg/cm^2

Table 7. *Reid vapor pressure at the inlet and outlet of the stabilizer*

At the outlet of this circuit, the presence of paraffinic compounds is observed in significant fractions. This is explained by an incomplete isomerization reaction in the reactors, as shown in Table 8

	Reaction circuit input	**Output reaction circuit**
2-mpentane	0.1819	0.1752
N-hexane	0.1500	0.0563
3-mpentane	0.1212	0.1038

Table 8. *Molar composition of partially reacted compounds*

The isomerate obtained is therefore a mixture of high-octane iso paraffins and low-octane n-paraffins.

	Hysys
RON	78,95
MON	77,66

Table 9. *Isomerate octane number obtained from the bottom of the*

The octane values obtained do not sufficiently meet the standards for use. The proposed solution consists of separating unprocessed n-paraffins from the mixture by installing an atmospheric distillation column, called DIH, designed to separate the isomerate fractions based on their boiling points.

The chromatography of this column (Fig 4) shows that the parafinic compounds: 2-methylpentane, 3-methylpentane, and n-hexane, are in the middle of the column. It is then considered to draw a line in the middle of the column to recycle these components for a new reaction.

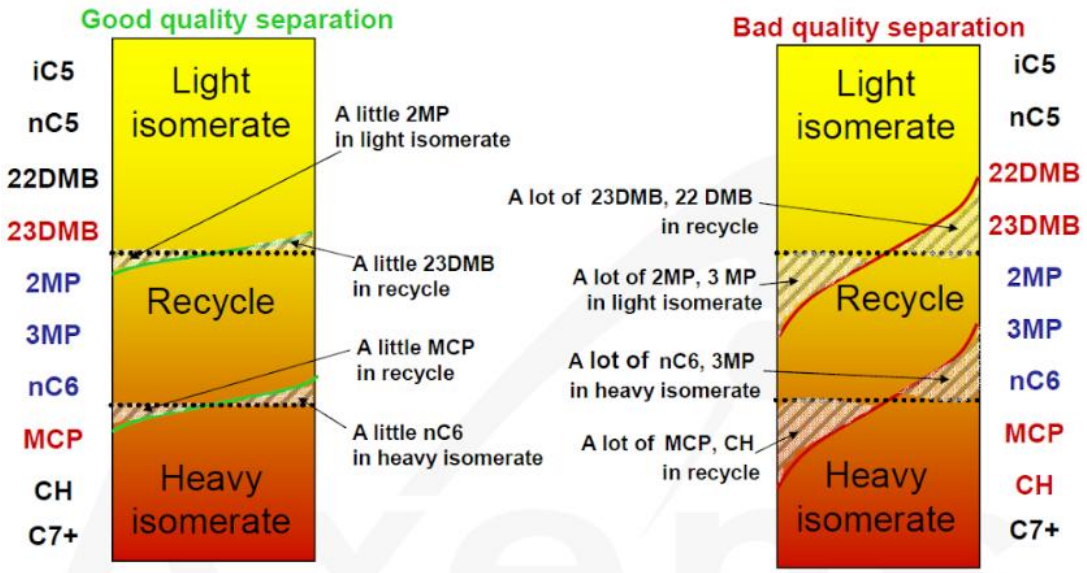

Figure 4. *Separation of the isomerate in the Deisohexanizer column*

The isomerate product is a mixture of the Deisohexanizer distillate and the Deisohexanizer bottoms stream. This is the primary product of the isomerization unit, which will subsequently be sent to the gasoline mixture.

3.4. *Simulation of the isomerization unit with a Deisohexanizer*

The circuit simulation will be carried out as before, with the addition of a distillation column, called a Deisohexanizer, in both the design (Fig 5) and real cases (Fig 6).

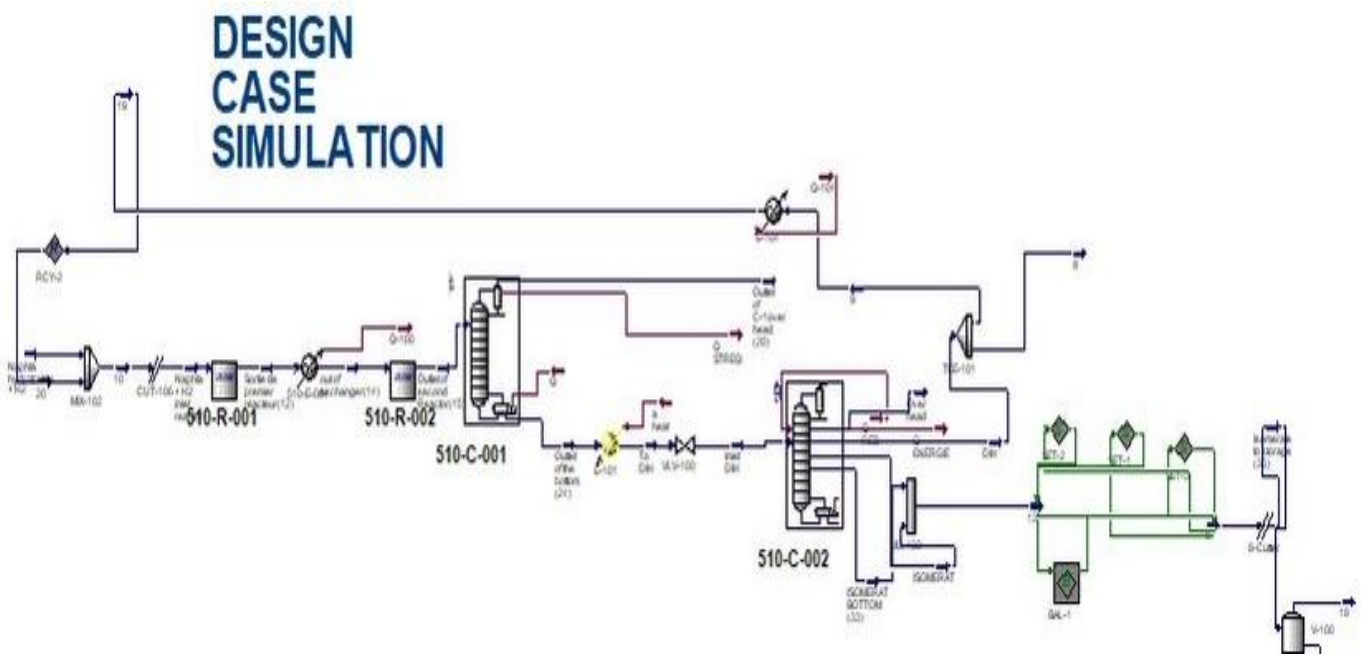

Figure 5. *Simulation of the Deisohexanizer in the design case*

Composition	Product of isomerate after recycling
Hydrogen	0.0000
Methane	0.0000
Ethane	0.0000
Propane	0.0000
I-Butane	0.0001
N-Butane	0.0007
I-Pentane	0.3706
N-Pentane	0.1293
2,2-mbutane	0.3853
2,3-mbutane	0.0334
2-mpentane	0.0437
3-mpentane	0.0019
N-Hexane	0.0000
M cyclopentane	0.0001
Benzene	0.0000
Cyclohexane	0.0182
N-Heptane	0.0096
M-cyclohexane	0.0070

Table 10. *Composition of the isomerate after recycling*

	Entry DIH	Isomerat finale
	Simulation	**Simulation**
MON	77.66	88
RON	78.95	89.5

Table 11. *Isomerate octane number obtained with deisohexanizer*

According to the results of this simulation (Tables 10 and 11), the isomerate product after recycling contains more iso-paraffins, such as I-pentane and 2,2-dimethylbutane, and a small fraction of paraffins. We also see that the octane rating has reached 88.

These results confirm the need for this column.

3.5. *Real case*

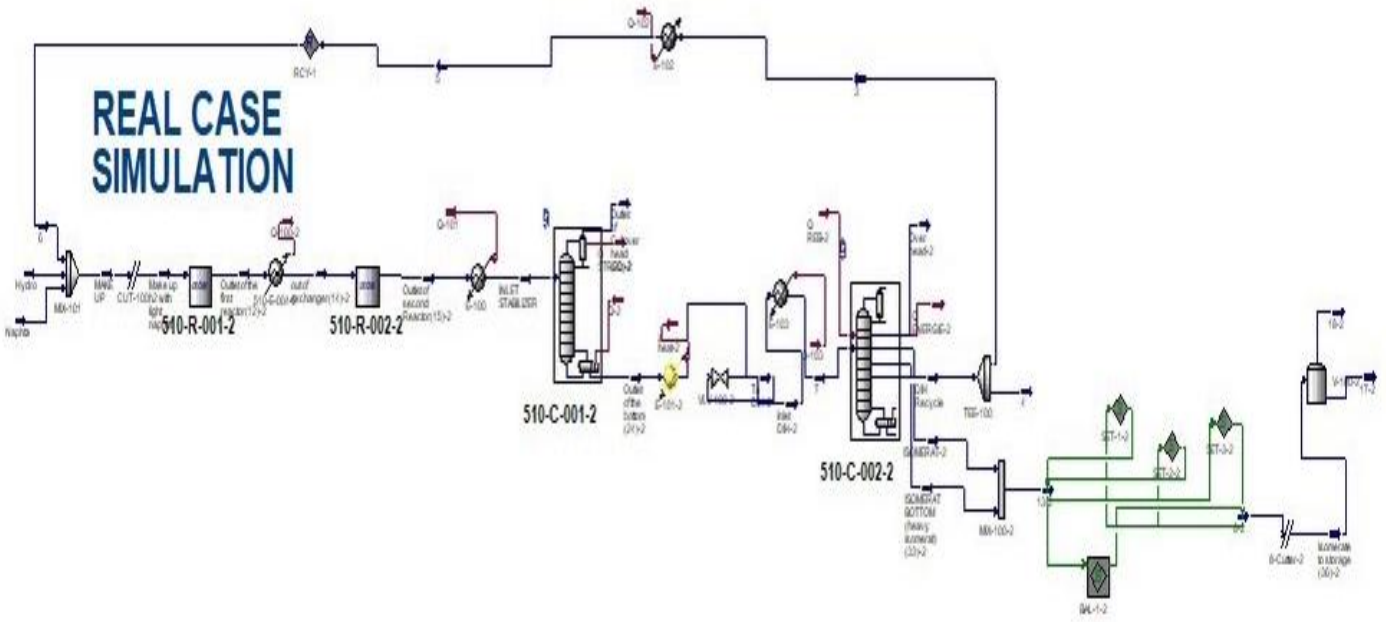

Figure 6. *Simulation of the Deisohexanizer in the real case*

3.6. *The optimization of stabilizer operating parameters*

The parameters that influence the stabilizer's operation are listed in the table below. This table compares the initial design case, the refinery's current situation, and the simulation results.

Some parameters, such as the temperature at the stabilizer inlet (Table 12), have not changed and are identical across the design case, the current case, and the simulation results. Therefore, no optimal points are proposed for these parameters. However, other parameters, such as the reflux flow rate and the balloon temperature, have changed. Thus, a study of the variation in the RVC and the octane number (RON) as functions of these parameters will be carried out to optimize the results.

Parameter	Design	Current	Simulation of a real case	First optimal point
Stabilizer inlet temperature 510-C-001 (°C)	Between (125.2-143.7)	127.1	127.1	127.1
Stabilizer inlet pressure 510-C-001 (Kg/cm^2)	19	18	18	18
Inlet flow rate (m^3/h)	138	111	111	111
Column pressure 510-C-001 (kg/cm^2)	18.9	18.97	18.97	18
Bottoms temperature (°C)	Between (184.8-184.4)	176	176	176
Reflux drum temperature 510-D-006 (°C)	40	43.26	43.26	44.8
Reflux drum pressure 510-D-006 (Kg/cm^2)	18.4	18.97	18.97	18
Reflux flow rate (m^3/h)	46.43	14.88	14.88	39.67
RTV of isomerate (Kg/cm^2)	1.00	1.23	1.214	1.13
octane number	88	88	88.20	88.7

Table 12. *The results of stabilizer operating parameters*

There is a slight decrease in the octane number, from 88 to 87.2.

To optimize the stabilizer's performance, it is important to find a temperature that balances reducing the RVC with maintaining the octane rating. Indeed, when the RVC reaches 1.13 and the RON is 88.7, the temperature is optimal at 44.8.

Conclusions

The objective of our final-year project was to study the isomerization unit, specifically the impact of the Deisohexanizer on it. Indeed, we conducted a simulation for this study, optimizing the operating parameters that were inconsistent with the design data.

Using the ASPEN HYSYS V14 software, we compared the results for the design case and the real case, which allowed us to determine the optimal points for each parameter by varying the data while maintaining a margin of precision for the different installations.

For the Deisohexanizer section, we optimized the temperature and reflux rate after calculating them.

The results of our study led to the following conclusions:

- The simulation of the first reactor shows a complete conversion of benzene to cyclohexane. However, in the current case, the benzene percentage at the outlet of the first reactor must meet current requirements, with a permissible benzene level of 2% in the isomerate.
- The increase in octane number in the first reactor indicates an improvement in the quality of the isomerate produced. Naphthenes in the isomerization feed underwent hydrogenation to form paraffins, which were then isomerized.
- In the second reactor, the input and output fractions remained largely similar, which is explained by the fact that most of the isomerization occurs in the first reactor. The increase in octane number in the second reactor indicates a successful molecular transformation of linear components into high-octane cyclic isomers, thereby improving the quality of the isomerate. The compounds responsible for this increase are **2,2 -dimethylbutane and I-Pentane.**
- A significant fraction of the light compounds at the outlet of the second reactor will be removed using the stabilizer to regulate the Reid vapor pressure (RVP) of the isomerate.
- The values of the temperature and the head reflux flow rate of the stabilizer were optimized using the simulation results of the HYSYS software, after a study of the graphs made on Excel, where the values of the TVR and the RON were discussed.
- The optimal value for temperature is 44.8°C, and that for reflux flow rate is 39.67.
- Simulating the isomerization unit without the Deisohexanizer yielded fraction values at the stabilizer's bottom outlet that were deemed inadequate for automotive engine operating standards. This demonstrated the necessity of integrating the Deisohexanizer into the isomerization unit and its impact on isomerate quality.
- After simulating the unit with the Deisohexanizer column, we observed that certain operating parameter values, such as the temperature and the column head reflux ratio, differed from the design values. These values were then analyzed using data from HYSYS, plotting curves in Excel to better understand the behavior of the RVP and RON values and to determine the optimal points.
- The optimal temperature value is 40.46°C, and the optimal reflux ratio is 6.8.

These were chosen primarily to improve the octane rating.

Bibliographie

[YUS.24] Yusura. Z. A., Abdullayeva. S. A, Gasimova. R. I, Aliyeva. N. F.. "The research of crude oil and investigation of efficient ways of its refinery". PPOR, Vol. 25, No. 3, 2024, pp. 776-785

[TRE. 15] Treese. S.A., Pujadó. P.R., Jones. D.S. J. "Handbook of Petroleum Processing". Second edition. Springer International Publishing Switzerland 2015.

[DS. 15] Jones. D. S. J. "Introduction to Crude Oil and Petroleum Processing". (eds) Handbook of Petroleum Processing. Springer, Cham. 7_24, 2015.

[MUR. 20] Murty. K. G. " Models for Optimum Decision Making; Crude Oil Production and Refining". Springer edition 2020.

[WAL. 23] Walaa.S.O, Fadel.E.A, Shazly.M.S. " Optimum Design of Naphta Recycle Isomerisation Unit with Modification by Adding De-Isopentanizer". Journal Processes , 11(12), 3406. 2023

[OYE. 19] Oyekan.S . "Catalytic Naphtha Reforming Process". Taylor & Francis Group, LLC: Boca Raton, FL, USA, 2019.

[VAL. 13] Valavarasu.G, Sairam.B. "Light Naphtha Isomerization Process: A Review". Pet. Sci. Technol. 31, 580–595, 2013.

[PET. 21] I. Petrov, D. Stratiev, I. Shishkova, D. Yordanov. "A hybrid reformer performance analysis reveals the reason for reformate octane deterioration". Oil Gas Eur. Mag, 47, 14–20, 2021.

[TAM.19] Tamizhdurai. P, Ramesh. A, Krishnan. P, Narayanan. S. "Effect of acidity and porosity changes of dealuminated mordenite on n-pentane, n-hexane and light naphtha isomerization". Microporous Mesoporous Mater, 287, 192–202, 2019.

[SHA.22] Shakor. Z. M., Ramos.M. J., AbdulRazak.A. A. "A detailed reaction kinetic model of light naphtha isomerization on Pt/zeolite catalyst". J. King Saud Univ.-Eng. Sci, 34, 303–308, 2022.

[HAM.23] Hamied.R. S, Z. Shakor. M., Sadeiq. A. H. "Khadim, A.T. Kinetic Modeling of Light Naphtha Hydroisomerization in an Industrial Universal Oil Products Penex Unit". Energy Eng. 120, 1371–1386, 2023.

[NAQ.18] Naqvi S. R., Bibi.A., Nizami. A. S. "New trends in improving gasoline quality and octane through naphtha isomerization: A short review". Appl. Petrochem. Res. 8, 131–139, 2018.

[CHE.24] Chekantsev. N. V, Gyngazova. M. S. "Mathematical modeling of light naphtha (C5, C6) isomerization process". J. Chem. Eng. 238, 120–128, 2024.

[HAM.17] Hamadi.A. S., Kadhim. A. S. "Material Balance and Reaction Kinetics Modeling for Penex Isomerization Process in Daura Refinery". MATEC Web Conf., 111, 02012, 2017.

[SHA.18] Shahata W. M., Mohamed. M.F., Gad. F.K. "Monitoring and modelling of variables affecting isomerate octane number produced from an industrial isomerization process". J. Pet. 27, 945–953, 2018.

[ZAI.20] Zaidoon M. S., Ramos M. J, Adnan. A. A. "A Detailed Reaction Kinetic Model of Light Naphtha Isomerization on Pt/zeolite Catalyst". Journal of King Saud University-Engineering Sciences. 2020

