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

Study of the effectiveness of the deisohexanizer and its impact on the isomerate quality of the Algiers refinery

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Résumé* —Ce document porte sur l'optimisation des performances du désisohexaniseur (DIH) de l'unité d'isomérisation de la raffinerie d'Alger. La modélisation et l'analyse des performances de l'unité ont été réalisées à l'aide du logiciel de simulation Hysys. Dans un premier temps, une simulation sans désisohexaniseur a permis d'établir une base de référence. L'étude se poursuit par une seconde simulation intégrant le désisohexaniseur. Cette étape permettra de mesurer l'impact de son intégration sur l'efficacité globale du système. Des ajustements ont été apportés aux paramètres de fonctionnement du désisohexaniseur afin d'améliorer la séparation des composés et d'optimiser les cycles de recyclage. Un rapport final présente plusieurs points d'optimisation et des recommandations formulées à l'intention de Sonatrach.

Mots-clés : Performances du désisohexaniseur, unité d'isomérisation, modélisation et performances.

***Abstract* — This document focuses on optimizing the performance of the deisohexanizer (DIH)** in th**e isomerization unit of the Algiers refinery. Using the Hysys simulation software, modeling and performance analysis of the unit were conducted. Initially, a simulation without the deisohexanizer was carried out to establish a baseline for performance. The study will continue with a second simulation, where the deisohexanizer was integrated. This part will allow measuring the impact of its inclusion on the overall system efficiency. Adjustments were made to the operating parameters of the deisohexanizer, aimed at improving the separation of compounds and optimizing recycling cycles. A final report presents several optimal points and recommendations that we proposed to Sonatrach**

Keywords — **Performance of the deisohexanizer , isomerization unit , modeling and performance .**

I. INTRODUCTION

Crude oil is a mixture of different hydrocarbon products, usable in various branches of industry and combustion engines.
Oil refining is a key industrial process that aims to satisfy economic demands and positively influence the daily lives of individuals within their societies, by providing energy products essential to the propulsion of our modern world.
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, naphtha, kerosene, diesel

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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. This process is generally accompanied by a decrease in the octane rating.

So the current problem for refineries is to produce gasoline with a high octane rating and an adequate REID Vapor Pressure (TVR) containing fewer aromatic compounds.

One possible solution is to recover the naphtha and treat it by two separate processes, namely isomerization and catalytic reforming.

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

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

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 [1] .

The efficiency of heat exchange equipment in industry is an important factor that directly influences the performance of industrial installations. In most refining or petrochemical units, the supply of thermal energy required by the process is made through various equipment, including electric superheaters in which the energy produced by the 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 encounter various technical problems, as equipment failure or the failure of one of its components leads to a plant shutdown, and the consequences of such a shutdown or reduced efficiency have a significant impact on production.

In our study, particular attention was paid to the simulation of the isomerization unit and to studying the influence of the deisohexanizer column on the quality of isomerate recovered from this unit.

II. Description of the Isomerization Unit

In order to carry out the isomerization process, the Algiers refinery has put in place a whole installation of necessary equipment.

flow diagram (PFD) is a detailed illustration of the necessary equipment and instrumentation used in the process.

It is an essential tool for engineers and operators to understand and optimize process parameters , such as temperature, pressure, and flow rates, to ensure the quality and yield of the desired product. [4]

The sections of the isomerization unit:

The isomerization unit consists of the following sections:

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

A. 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).

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- This mixture is transferred by the isomerization charging pumps to the series dryers via a downward flow to remove moisture, thus protecting the isomerization catalyst from damage caused by water, which is harmful to the catalyst.

B. 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.

C. 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 $kg/cm^2.g$.

III. SIMULATION AND OPTIMIZATION OF RESULTS

A. *Problematic*

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

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

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

The problem encountered by the Algiers refinery is that the current yield of the isomerization unit is not optimal; this is due to poor separation within the deisohexanizer.

This work, carried out using the Aspen HYSYS V14 simulator, aims to demonstrate the paramount importance of the Deisohexanizer in this unit, as well as to determine the optimal operating conditions leading to a better isomerate yield at the outlet of this unit.

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 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, with a density of 72 m^2/h.

B. *Simulation of the isomerization unit without a deisohexanizer*

B.1 Simulation of the reaction section:

a. Simulation of the first reactor:

Table 1
Sizing of the first reactor

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

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

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Composition	Entrance to the first reactor	First Reactor Exit
H2	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	

The first reactor is used to carry out the hydrogenation of benzene 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 the conversion of linear hydrocarbons into branched isomers is verified by calculating the octane number, which is 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 leads to a total conversion of benzene to cyclohexane.
The conversion of benzene to cyclohexane can be verified as follows:

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

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 represents the results of the partial isomerization, by determining the octane number of the effluent from the first reactor.

Table 3
Octane rating results from the first reactor simulation

	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

The increase in octane rating in the first isomerization reactor indicates an improvement in the quality of the fuel produced. The four naphthenes present in the isomerization feedstock are cyclopentane (CP), methyl cyclopentane (MCP), cyclohexane (CH), and methylcyclohexane. These compounds undergo secondary

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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%)

b. Simulation of the second reactor:
The second reactor in the unit's reaction section is used to complete the isomerization not achieved by the first reactor, while simultaneously increasing the octane number of the resulting products. To verify the efficiency of the hydrocarbon conversion, we consider the octane number as an indicator. The results are presented in Table 4 below.

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

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

An increase in octane rating is observed, indicating improved fuel quality in terms of knock resistance and engine performance. This suggests that the second isomerization reactor has been adjusted to further increase the conversion of linear alkanes to high-octane cyclic isomers.
In the second reactor, we note that the majority of the input and output fractions remained quite similar, which explains why most of the isomerization takes place in the first reactor.
The increase in octane number in the second isomerization reactor indicates a successful molecular transformation of linear components into high-octane cyclic isomers, leading to improved 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, thus contributing to an increase in the measured octane rating.

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C. Variation of TVR and RON as a function of temperature

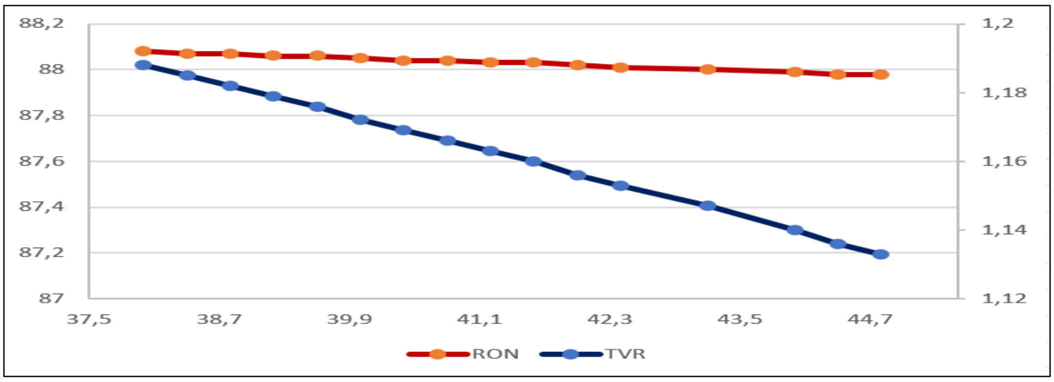

Fig. 2 *Variation of TVR and RON as a function of temperature*

This graph shows that increasing the temperature of the tank (510-D-006) leads to a considerable decrease in TVR from 1.188 to 1.13. This is explained by the effect of heating the tank, which helps to remove the light fractions.

Simultaneously, a slight decrease in the octane rating is also observed, dropping from 88 to 87.2. To optimize stabilizer performance, it is important to find a temperature that balances the TVR reduction with maintaining the octane rating. Specifically, when the TVR reaches 1.13 and the RON is 88.7, the optimal temperature is 44.8.

IV. CONCLUSIONS

The objective of our final year project was to study the isomerization unit, more specifically the impact of the deisohexanizer on this unit. Indeed, we performed a simulation for this study, optimizing the operating parameter values that were not consistent with the design data.

Using the ASPEN HYSYS V14 software, we were able to compare the results in the design case and in the real case, which allowed us to determine the optimal points of each parameter by varying the data while respecting a margin of precise values for the different installations.

For the Deisohexanizer section we optimized the Temperature as well as the reflux rate after calculating it.

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 percentage of benzene at the outlet of the first reactor must meet current requirements, with an permissible benzene level in the isomerate of 2%.
- The increase in octane number in the first reactor indicates an improvement in the quality of the isomerate produced. Naphthenes present in the isomerization feed underwent hydrogenation reactions to form paraffins, which in turn were transformed into isomers.
- 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 demonstrates a successful molecular transformation of the linear components into high-octane cyclic isomers, thus 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 in order to regulate the Reid vapor pressure (TVR) 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

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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 provided by HYSYS, plotting curves with Excel software to better understand the behavior of the TVR and RON values and 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.

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