A THESIS SUBMITTED TO
THE GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES
OF ÇANKIRI KARATEKİN UNIVERSITY

DETERMINATION OF OPTIMUM OPERATING PARAMETERS OF A NAPHTHA REFORMING PROCESS

IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR
THE DEGREE OF MASTER OF SCIENCE
IN
CHEMICAL ENGINEERING

BY

ALI SALIM JUMAAH JUMAAH

ÇANKIRI

2023

DETERMINATION OF OPTIMUM OPERATING PARAMETERS OF A NAPHTHA REFORMING PROCESS

By Ali Salim Jumaah JUMAAH

August 2023

We certify that we have read this thesis and that it is fully adequate, in scope and quality, as a thesis for the degree of Master of Science.

Advisor **:** Asst. Prof. Dr. Haluk KORUCU
Co-Advisor : Assoc. Prof. Dr. Ömer Faruk DİLMAÇ

Examining Committee Members:

Chairman **:** Prof. Dr. Ahmet YARTAŞI
Chemical Engineering
Çankırı Karatekin University

Member **:** Asst. Prof. Dr. Haluk KORUCU
Chemical Engineering
Çankırı Karatekin University

Member **:** Asst. Prof. Dr. Havva MUMCU ŞİMŞEK
Garden Vocational School
Osmaniye Korkut Ata University

Approved for the Graduate School of Natural and Applied Sciences

Prof. Dr. Hamit ALYAR
Director of Graduate School

I hereby declare that all information in this document has been obtained and presented in accordance with academic rules and ethical conduct. I also declare that, as required by these rules and conduct, I have fully cited and referenced all material and results that are not original to this work.

Ali Salim Jumaah JUMAAH

ABSTRACT

DETERMINATION OF OPTIMUM OPERATING PARAMETERS OF A NAPHTHA REFORMING PROCESS

Ali Salim Jumaah JUMAAH

Master of Science in Chemical Engineering

Advisor: Asst. Prof. Dr. Haluk KORUCU

Co-Advisor: Assoc. Prof. Dr. Ömer FARUK DİLMAÇ

August 2023

The process of reforming naphtha is considered one of the important processes in the oil industry. In this process, the molecular structure of hydrocarbon compounds with a low octane number is converted into hydrocarbon compounds with a high-octane number using the catalyst, platinum metal support on alumina. This work focuses on simulating the process of reforming naphtha to increase the octane number and studying the effect of operating conditions on the quantities of products. The study aims to optimize the conditions of the naphtha reforming process and operating conditions inside the reactors to obtain a high-octane number. These conditions are the temperature of the feedstock entering the reactors (RiT), the amount of hydrogen-rich return gas (RG) injected with the naphtha, temperatures of separation vessels (HPS and LPS), and pressure of the stabilizing tower. The optimization process was restricted by determining the minimum amount of reformate (C^{5+}) at least 80% wt.%. In this work, a simulation of the naphtha reforming process was done in the Salah Al-Din/2 refinery in Iraq using the AVEVA PRO/II simulation program and matching the results obtained from the simulation with the real results taken from the factory. The results were getting aromatic content, octane number and hydrocarbon concentrations close to each other. The optimization was carried out using the same program to obtain an increase in octane number, where certain ranges were entered for the operational conditions that directly affect the specifications of the final product, as follows; RiT = (460-500 ºC), LPS Temp = (35-40 ºC), HPS Temp=(35-45 ºC), Tower Pressure=(15-20 barg), RG= (60-120 ton/hr), Feed Quantity= (66-110 m^3/hr). The optimization result was that reducing the amount of RG to 60 tons raises the octane number from (90.5 to 93.7) value with a slight change to other operating conditions.

Among the benefits of the optimization process, an 18,467% improvement was achieved in the heat exchanger and the total amount of energy consumed in the process. In addition, a 22.838% improvement in energy efficiency in compressors and pumps was achieved. These results have shown that the implementation of simulation and optimization can be applied and adapted in the process, which reduces costs in terms of the process and has a positive effect on process efficiency. For this reason, the simulation and optimization work has achieved its goal.

2023, 91 pages

Keywords: Naphtha reforming, Heavy naphtha, Optimization, PRO/II simulation.

ÖZET

BIR NAFTA REFORMİNG PROSESİNİN OPTİMUM İŞLETİM PARAMETRELERİNİN BELİRLENMESİ

Ali Salim Jumaah JUMAAH
Kimya Mühendisliği, Yüksek Lisans
Tez Danişmani: Dr. Öğr. Üyesi Haluk KORUCU
Eş Danişman: Doç. Dr. Ömer Faruk DİLMAÇ
Ağustos 2023

Nafta reform süreci, petrol endüstrisindeki önemli süreçlerden biri olarak kabul edilir. Bu işlemde, düşük oktanlı hidrokarbon bileşiklerinin moleküler yapısı, alümina üzerindeki katalizör platin metal desteği kullanılarak yüksek oktanlı hidrokarbon bileşiklerine dönüştürülür. Bu çalışma, oktan sayısını artırmak için nafta reform sürecini simüle etmeye ve çalışma koşullarının ürünlerin miktarları üzerindeki etkisini incelemeye odaklanmaktadır. Çalışma, yüksek oktanlı bir değer elde etmek için nafta reform sürecinin koşullarını ve reaktörlerin içindeki çalışma koşullarını optimize etmeyi amaçlamaktadır. Bu koşullar, reaktörlere giren hammaddenin sıcaklığı (RıT), nafta ile elde edilen hidrojen açısından zengin geri dönüş gazı (RG) miktarı, ayırma proseslerinin sıcaklıkları (HPS ve LPS) ve dengeleyici kulenin basıncıdır. Optimizasyon süreci, ağırlıkça % 80'den az olmayan minimum reformat miktarı (C^{5+}) belirlenerek sınırlandırılmıştır. Bu çalışmada Irak'taki Salah Al-Din/2 rafinerisinde AVEVA PRO/II simülasyon programı kullanılarak ve simülasyondan elde edilen sonuçların fabrikadan alınan gerçek sonuçlarla eşleştirilerek nafta reform sürecinin simülasyonu yapılmıştır. Sonuçlar; aromatik içerik, oktan sayısı ve hidrokarbon konsantrasyonları birbirine yakın elde edildi. Optimizasyon, nihai ürünün özelliklerini doğrudan etkileyen çalışma koşulları için aşağıdaki gibi belirli aralıkların girildiği oktan sayısında bir artış elde etmek için aynı program kullanılarak; RıT = (460-500 ºC), LPS Sıcaklığı = (35-40 ºC), HPS Sıcaklığı = (35-45 ºC), Kule Basıncı = (15-20 barg), RG = (60-120 ton/saat) ve Besleme Miktarı = (66-110 m^3/saat) olarak gerçekleştirildi. Optimizasyon sonucu, RG miktarının 60 tona düşürülmesinin, diğer çalışma koşullarında hafif bir değişiklikle oktan sayısını (90,5'ten 93,7'ye) yükseltmesiydi. Optimizasyon işleminin faydaları arasında ısı eşanjöründe ve işlemde tüketilen toplam

enerji miktarında%18.467'lik bir iyileşme sağlandı. Ayrıca kompresör ve pompalarda enerji verimliliği açısından %22.838'lik bir iyileşme sağlanmıştır. Bu sonuçlar, simülasyon ve optimizasyonun uygulanmasının süreç içinde uygulanabileceğini ve uyarlanabileceğini, bu da süreç açısından maliyetleri düşürdüğünü ve süreç verimliliği üzerinde olumlu bir etkiye sahip olduğunu göstermiştir. Bu nedenle simülasyon ve optimizasyon çalışmaları amacına ulaşmıştır.

2023, 91 Sayfa

Anahtar Kelimeler: Nafta reformu, Ağır nafta, Optimizasyon, PRO/II simülasyonu.

PREFACE AND ACKNOWLEDGEMENTS

After a year of arduous work, I am finally happy to have ended this thesis. It was an amazing experience, and I will remember it for a long time.

I would like to thank my advisor Asst Prof. Dr. Haluk KORUCU, and my co-advisor Assoc. Prof. Dr. Ömer Faruk DİLMAÇ for their patience, guidance, and understanding.
Finally, I would like to express my endless thanks to my family, who always stood by me and encouraged me throughout my life, especially my parents, for whom I am grateful for their support, motivation, and encouragement to reach my goals and achievements.

Alı Salim Jumaah JUMAAH
Çankırı-2023

CONTENTS

LIST OF SYMBOLS

Ea	Activation energy
Ar	Aromatic
BTX	Benzene, toluene, and xylene
°C	Celsius degree
R	Gas constant
iP	Iso-paraffins
nP	Normal paraffin
N	Naphthenes
O	Olefin
A	Pre-exponential factor
Rx	Reactor

LIST OF ABBREVIATIONS

barg	Bar gauge
CF	Combined feed
CS	Combined stream
EBP	End boiling point.
GC	Gas chromatography
HC	Hydrocarbon
HN	Heavy naphtha
H_2	Hydrogen
H_2/HC	Hydrogen/hydrocarbon mole ratio
HPS	High-pressure separation section
IBP	Initial boiling point
LHSV	Liquid hour space velocity
LPS	Low-pressure separation section
MON	Motor octane number
Mwt.	Molecular weight
Off Gas	Hydrocarbon gases out from stabilizer tower or vessels
PIONA	Paraffin, iso-paraffins, olefin, naphthene, and aromatic
RiT	Reactors inlet temperature
RON	Research octane number
HG	Recycle gas
WHSV	Weight hour space velocity

LIST OF FIGURES

LIST OF TABLES

1. INTRODUCTION

Hydrocarbon compounds are the main components of crude oil and its product; heavy naphtha is the first crude oil out from the top of the distillation tower and has high volatility because initial boiling point it low and it represents between 15 – 30 wt. % of crude oil with a distillation range of (85-180 ^{o}C) by using ASTM D86 method; all these characteristics depend on the specifications and quality of crude oil (Chernyakova *et al.* 2015). Heavy Naphtha it is complex mixture because it consists of groups of different hydrocarbon compounds, which are paraffins, naphthene, olefin, and aromatics), and the numbers of these compounds are in the hundreds (Antos and Aitani 2004).

1.1 Naphtha Catalytic Reforming History

Initially, thermal cracking processes were used, but 1940, catalytic processes were introduced, which had better productivity and higher octane. However, they used molybdenum oxide as a catalyst after that. As a result of continuous development and studies in that period of the last century, platinum metal was used as a catalyst, which proved highly efficient in naphtha reformation processes (Jones and Pujadó 2006).

In 1949, the UOP Company established the first platform for the naphtha reforming process using a monometallic catalyst, which is platinum. Since that time, it has become a standard feature for refineries. After that, it worked to improve the process in two directions: the first was to improve the catalyst, as it was developed and became bimetallic, and the second: was to develop a technology called SR. The company introduced a new CCR technology, which differs from the first in design, operational conditions, and product specifications (Meyers 2016).

1.2 Naphtha Catalytic Reforming Process

Naphtha catalytic reforming is considered one of the most important in oil refineries and petrochemical industries. It works to improve the specifications of gasoline by enhancing the octane number of Heavy Naphtha from a low ^{oc}tane number in the range 30-60 value to high octane number of gasoline normally 100 value, this doing by increasing aromatics and iso-paraffins content which it has a high octane number (Fahim *et al.* 2009).

The product of process known as reformate consists of the hydrocarbon atom starting with (C^{5+} It means the sum of the concentrations of all hydrocarbon compounds that contain five or more carbon atoms), So the fraction of aromatic hydrocarbons ranges between 40-70 wt. %, another product from naphtha reforming like gaseous contains hydrogen 60-90 mol %. Some of the gaseous are recycled again and remain sent to hydrotreating processes, so it is considered a desired product, whereas the liquefied petroleum gas LPG (C^{4+3}) is considered a by-product due to undesired reactions because it decreases the yield of the naphtha reforming product (reformate) (Anabtawi *et al.* 1991). Therefore, gasoline should have the following properties:

- High octane numbers lead to a higher compression ratio, which increases engine efficiency.

- Low vapor pressure must be minimally compatible with room temperature because it leads to losses in vapor.

- Minimum-producing smoke and smog may occur due to forming gums by polymerization of olefins reactions, and this causes damage to the motor. (Antos *et al.* 1995).

The naphtha reforming process consists of many different equipment, such as reactors, which are considered the most important because they have the catalyst, compressors, pumps, separating vessels, and stabilizing tower.

1.3 Naphtha Catalytic Reforming Technology

The process consists of three or four adiabatic reactors. For this reason, it is considered the main section in the naphtha catalytic reforming process, in series with intermediate preheaters (furnaces); these furnaces exist because most of the main reactions that take place inside the reactors are endothermic, except hydrocracking reactions, which it exothermic Therefore, the compounds and reactants leaving the reactors will have a lower temperature than the required temperature when they enter the next reactor (Antos and Aitani 2004).

Therefore, the furnaces will work to raise the temperature of the feedstock inside. The reactor. These reactors are different in volume, contain the catalyst, and operate at temperatures range between 450-520 °C, pressures between 3-35 barg with molar ratios (H_2/HC = 3-8) depending on the design of the process (Shakor *et al.* 2020). Due to the differences in design and operation conditions, the naphtha catalytic reforming process is classified into these types depending on the catalyst regeneration process (Babaqi *et al.* 2016). These types are shown below.

- Semi-Regenerative process, reactor design type (fixed bed catalyst).
- Continuous Catalyst Regeneration process, reactor design type (moving bed catalyst).
- Cyclic Regeneration process, reactor design type (fixed bed catalyst).

1.3.1 Semi-regenerative process (SR)

A semi-regenerative catalytic reforming process usually has three reactors in series with a fixed bed catalyst system and operates continuously, this cycle of operation may be continued for six months to two years times more and this depending on the severity of operation conditions (high temperature, low feed quantity (LHSV) and Heavy Naphtha

quality) these conditions lead to deactivation catalyst which leads to a decrease in the (RON, yield of reformate and decrease in hydrogen yield) (Gary *et al.* 2007). Due to the deposition of coke or sulfur on the surface of the catalyst, so catalyst regeneration process must be done to restore the activity; research octane numbers in this process between 85-100 value (Rahimpour *et al.* 2013).

In Figure 1.1, notice the feed line (heavy naphtha) entering the process. Then, recycled gas rich with hydrogen injected with it, this mixture enters the reactors system, which contains three furnaces and three reactors linked in series, after that, by cooling, it enters a separating container. The gases come out from the top of the container and are separated into two lines (Ancheyta 2011).

The first is recycled gas, and the second is produced gas. As for the liquids, they go to the stabilization tower to stabilize the vapour pressure of the material in the reformate line by removing the light gases that come out from the top of the tower (LPG, Off Gas).

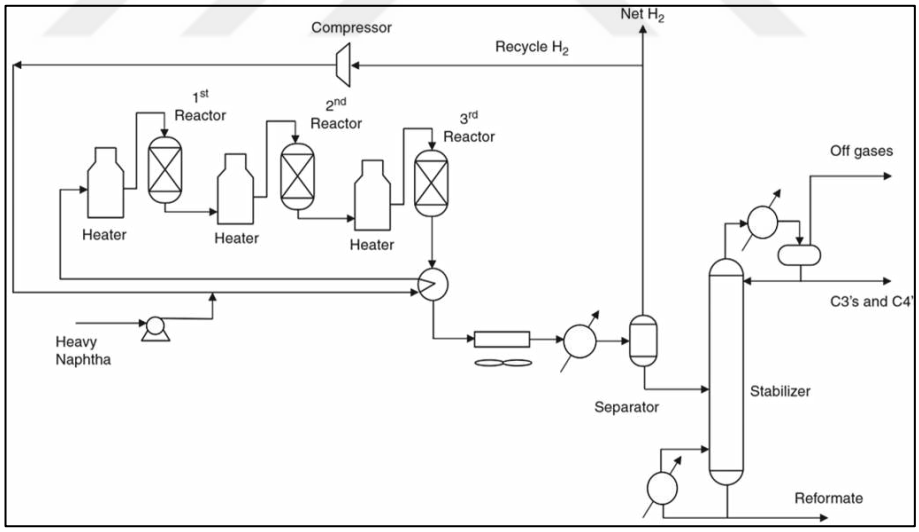

Figure 1.1 Semi-regenerative (SR) catalytic process (Fahim *et al.* 2009)

1.3.2 Continuous catalyst regeneration process (CCR)

CCR units differ from SR units in terms of reactor design, catalyst type, and operating conditions, in addition to the presence of a special tower used to regenerate catalyst continuously and research octane number (RON) in this process type higher than (SR) process range between 95-108 value (Rahimpour *et al.* 2013).

As a result of the continuous catalyst regeneration, the catalyst's activity and selectivity are high, giving acceptable results and high yield. In addition, the low pressure inside the reactors reduces carbon formation on the catalyst's surface, which is considered one of the advantages of the process compared to the high capital costs and low operating costs because of low pressure and hydrogen cycling, which keeps the deposited coke at acceptable limits (Ancheyta 2011, Gary *et al.* 2007). The CCR process consists of three reactors installed, one above the other. The catalyst is in a reactor type of moving bed, so the catalyst bed moves by gravity flow from the first reactor at the top and enters the second reactor to the third reactor after effluent from the bottom third reactor after that (Oyekan 2018).

CCR units are the same as SR units in terms of operating principal feed, which is Heavy Naphtha injected with recycled gas containing hydrogen with purity (80-90% mol), and the combined stream enters the heat exchangers to preheat then to furnaces to increase mixture stream temperature to 500-520 ^{o}C before entering to reactors. After the material out from the reactor section must be cooled, it then enters the separator vessel for separating gas and liquid, Gases are recycled again, and the product hydrogen is sent to other units. Liquid down from the bottom of the vessel goes to the stabilization tower to separate (LPG, Off-Gas) to maintain (RVP) at a constant value of the final product (Reformat), CCR process is shown in Figure 1.2 (Ancheyta 2011).

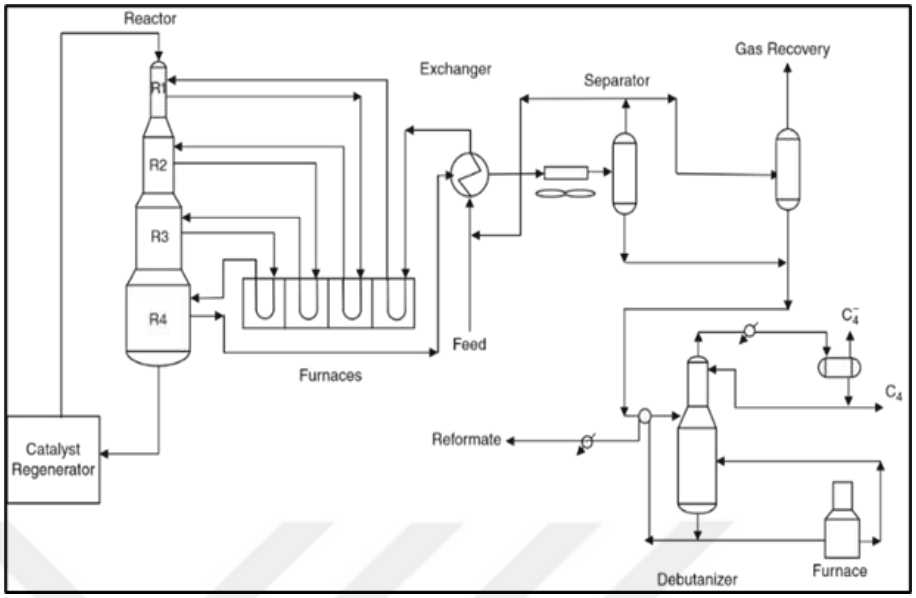

Figure 1.2 Continuous catalyst regeneration (CCR) process (Fahim *et al.* 2009)

1.3.3 Cyclic regeneration process

The cyclic regeneration process has an additional swing reactor, which is used when one of the reactors needs to regenerate, so it must be isolated and enter the swing reactor in work to end the regeneration process. In this process, all reactors are equal in size and characterized by the fact that the octane number and reformate yield, in addition to the produced hydrogen, are higher than the previous two types. Normally, research octane number (RON) in this process has a range of 100-104 value (Ancheyta 2011, Rahimpour *et al.* 2013). The process cyclic regenerative is shown in Figure 1.3 below.

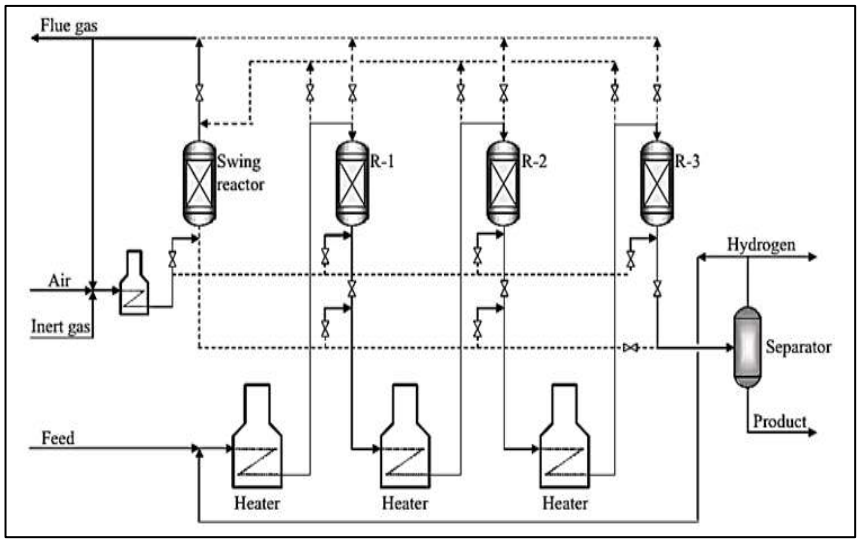

Figure 1.3 Cyclic regenerative process scheme (Ancheyta 2011)

1.3.4 Different between technologies

The catalytic naphtha reforming process combines technology of catalysts, equipment design, and the nature of the operational process to produce a reformate with a high-octane number used as fuel and in petrochemical industrial processes. In addition, it is a source of hydrogen that is used in hydrotreating processes. Are UOP and Axens Companies dominant naphtha catalytic reformers, especially cyclic regenerative (CR), which has about 12% of naphtha catalytic units worldwide (Antos and Aitani 2004).

Table 1.1 show the different between main processes semi-regenerative (SR) and continuous catalytic regenerative (CCR) in licensing the installation and operation, semi-regenerative (SR) has 60%, continuous catalytic regenerative (CCR) has 28% and below will show differences between SR and CCR process.

Table 1.1 Operation condition, product yield for SR and CCR (Antos and Aitani 2004)

PARAMETER	SR UNIT	CCR UNIT
P (barg)	12 – 25	3 – 10
Temperature in (°C)	450– 525	470 – 530
LHSV (h^{-1})	1 – 2	4 – 8
H_2/HC Ratio	4 – 8	2 – 3
Recycle gas: H_2 (vol. %)	70 - 85	85 +
RON	95-100	95-108
C^{5+} yield ((wt. %))	80- 85	90 – 92
H_2 yield ((wt. %))	1,8 – 2,5	3,5 +

1.4 Naphtha Catalytic Reforming Feed

The feedstock enters the catalytic reforming process. Heavy Naphtha is a complex liquid consisting of (paraffin, naphthene, and aromatic) produced by a distillation unit, and it must be treated with hydrogen to reduce contaminant compounds like (sulfur, nitrogen, and oxygen) to lower levels because it deactivates the catalyst efficiency after a short time (Behin and Kavianpour 2009).

Heavy Naphtha has a boiling range between (80-185 ºC), and from this conclude that it is necessary to eliminate the light cut, i.e., the boiling point is between (30-90 ºC) because it will produce light compounds (C_1-C_4), in addition to that, the heavy cut, which Its high boiling point must also be eliminated due to the difficulty of converting it into desirable compounds and the possibility of high cracking reactions, which leads to carbon cocking deposited on the catalyst surface and this leads to reduces it is activity (Antos and Aitani 2004, Antos *et al.* 1995).

1.4.1 Heavy naphtha sources

Heavy Naphtha has many sources, such as (atmospheric distillation units, hydrocracking units, and thermal cracking units) Because of the multiplicity and various sources of Heavy Naphtha, it will vary in physical and chemical properties. Atmospheric distillation units are considered the main source for naphtha catalytic reforming; they are called straight-run of Naphtha and contain 30–70 wt.% paraffin. %, naphthene 15– 45 wt.%, aromatics 5–20 wt.%, and only olefins 0–2 wt.%. These percentages depend on the type of crude oil properties (Yusuf *et al.* 2019).

The hydrocracking and thermal cracking units produce heavy Naphtha with olefin compounds in a high range of 30-50 wt.%, which is undesired feed since it leads to the formation of gums due to polymerization and oxidation reactions. The gum in naphtha leads to hydrogen consumption due to hydrogenation reactions, coking deposition on the catalyst's surface, smoke, smog, and engine damage. Vis-breaker Naphtha is usually limited to small percentages of the feed reformer because it needs severe hydrotreating to prepare a proper reformer feedstock; on the other side, hydrocracking of heavier petroleum fractions rich in naphthene that it is suitable as feed to produce aromatics with high octane (Antos *et al.* 1995).

1.4.2 Heavy naphtha composition

Heavy Naphtha consists of four main hydrocarbon groups that are different in boiling point temperature, density, molecular shape, molecular weight, and concentration due to this, and these differences are different in physical and chemical properties depending on the crude oil source (Fahim *et al.* 2009).

Crude oil produced from oil wells differs in terms of the molecular number of hydrocarbon compounds and their proportions, and for this reason, crude oil may contain proportions of high molecular weight paraffin compounds or so-called polymers, and this gives a high degree of waxy products, motor oils and kerosene, and this type is called oil

paraffin. But if the crude oil contains high percentages of naphthenic compounds or asphalt, then this type of crude oil contains high percentages of light oil products such as heavy and light naphtha, and thus produces high amounts of gasoline and is called naphthenic oil. This type does not contain paraffinic compounds, and it is not good for the manufacture of motor oils (Antos *et al.* 1995).

Paraffins: Formula ($\mathbf{C_nH_{2n+2}}$) saturated hydrocarbons, single bond. There are two types: n-paraffin and iso-paraffins, boiling point of an n-paraffin is always higher than that of the iso-paraffins with the same carbon atom number. It has the same molecular weight but different structure and physical and chemical properties (Antos and Aitani 2004). Some hypothetical shapes of continuous and branched chain paraffin hydrocarbons are shown in Figure 1.4.

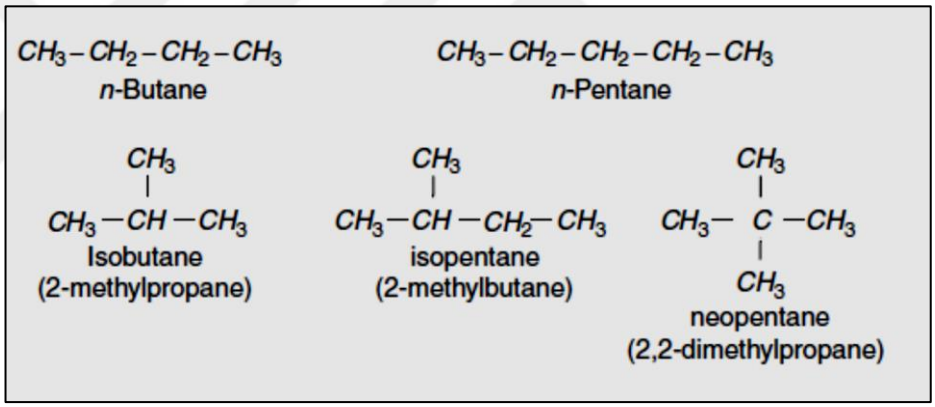

Figure 1.4 Examples of paraffin compounds (Fahim *et al.* 2009)

Naphthenic: Formula ($\mathbf{C_nH_{2n}}$) they saturated cyclic hydrocarbons. They consist of one ring or more. The crude oil rich with cyclic naphthenic consists of five or six carbon atoms. The boiling point is higher than paraffin which has the same carbon atoms. Naphthene is considered the main source for producing aromatics, and their conversion to aromatics is considered the fastest reaction and absorbs high heat (Oyekan 2018). Some examples form of cyclic naphthenic compounds are shown in Figure 1.5.

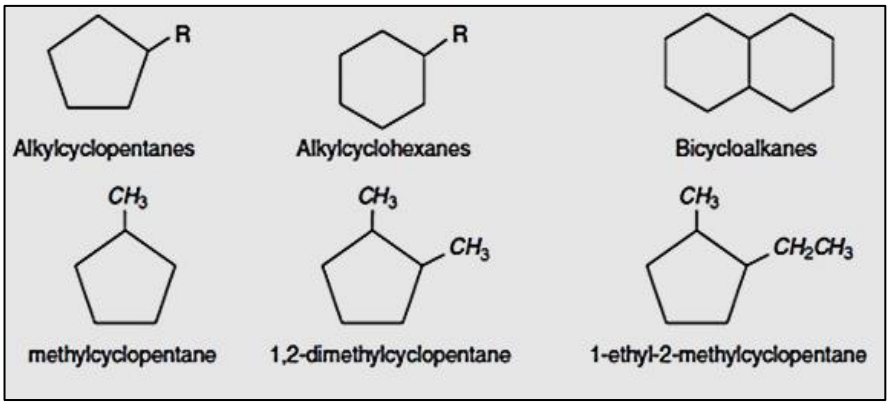

Figure 1.5 Examples of naphthenic rings (Fahim *et al.* 2009)

Aromatic: Formula ($\mathbf{C_nH_{2n-6}}$) unsaturated cyclic hydrocarbons. It consists of one ring or more and has a double bond. The boiling point is higher than that of paraffin and naphthenic with the same carbon atom (Antos *et al.* 1995). examples form of cyclic aromatic compounds are shown in Figure 1.6.

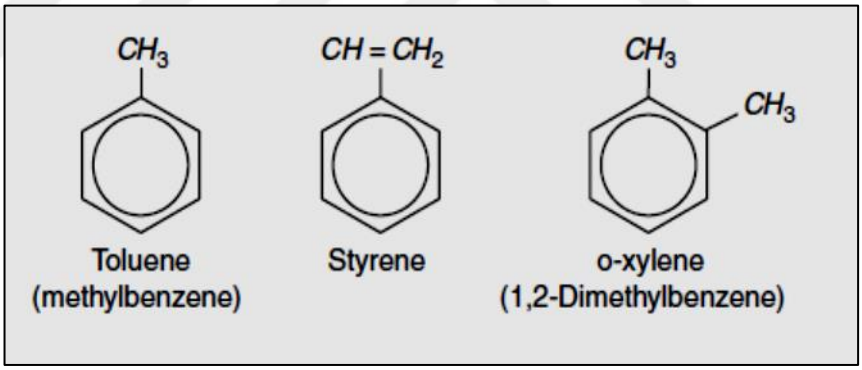

Figure 1.6 Example of aromatics rings (Oyekan 2018)

Olefin: Formula ($\mathbf{C_nH_{2n}}$) unsaturated hydrocarbons in the chain have different concentrations depending on the Heavy Naphtha source, and they must stay low (Antos *et al.* 1995). In Figure 1.7 are some forms of olefins compounds.

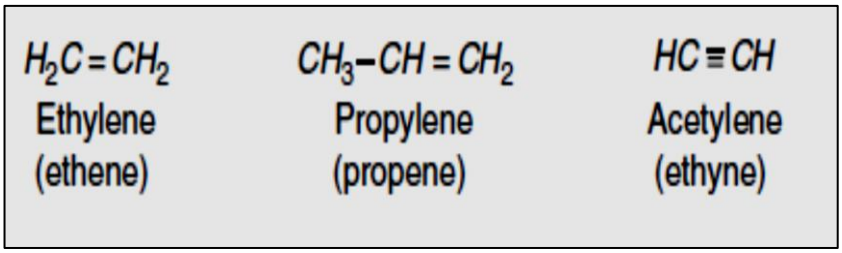

Figure 1.7 Examples of olefin chains (Oyekan 2018)

1.4.3 Heavy naphtha quality

The multiplicity of sources of crude oil in the world leads to differing chemical composition of Heavy Naphtha because of the different specifications of crude oil, so the specifications of crude oil also differ in terms of the hydrocarbon content of the main compounds Paraffins, Naphthene, and Aromatics. So, Heavy Naphtha is considered a complex mixture that contains hundreds of hydrocarbon compounds (paraffins, olefins, aromatics, and naphthenic); these compounds consist of carbon atoms ranging from (C_5 to C_{11}) with low octane numbers; in addition, they have different concentrations depending on the specifications of the crude oil (Ancheyta 2011).

The difference in the concentrations of hydrocarbon compounds, especially (Paraffins and Naphthene), affects the operating conditions of the naphtha reforming process depending on the specifications of the crude oil. As we have spoken previously, the key to the severity of the process is Heavy Naphtha composition; when the feedstock contains a high concentration of Paraffins, it must increase the severity by increasing the inlet temperature of reactors to achieve the desired octane number. This feedstock is called paraffinic; on the other hand, if Heavy Naphtha contains a high concentration of naphthene compounds, this will reduce the severity of the process because dehydrocyclization reaction will be little compared with reactions of naphthene has a high rate and give more aromatics components (Edgar 1983). Table 1.2 shows the difference between paraffinic and naphthenic feedstock.

Table 1.2 Heavy naphtha specification differences between two sources of crude oil (Oyekan 2018)

Parameter	Paraffinic Naphtha	Naphthenic Naphtha
Research Octane Number (RON)	50	66
Paraffin **Naphthene (vol. %)** **Aromatic**	66.6 23.4 8	32.6 55.5 11.9
N+2A	39.4	79.3
Distillation range (ASTM D86)	IBP: 92 50%: 123 (°C) FBP: 155	IBP: 88 50%: 123 (°C) FBP: 161
Average molecular weight	114	119
C_5^+ yield, vol. %	73.5	84.7

Table 1.2 shows a big difference between naphtha rich in naphthenic compounds and naphtha rich in paraffinic compounds, as the first has a higher-octane number than the second. The amount of output from the process using naphtha rich in naphthenes is higher than the other, and thus, we conclude that obtaining an octane number of reformate by using naphtha rich in naphthenes, it does not need high temperatures, unlike if naphtha rich in paraffins was used.

1.5 Purpose of Naphtha Catalytic Reforming

Heavy Naphtha catalytic reforming process works on rebuilding the molecular shape and changing concentrations of main compounds (paraffin, naphthene, and aromatics) to obtain a product with a high-octane number and small change in the number of carbon atoms, except reactions hydrocracking it makes a change in numbers of atoms. For example, dimethyl cyclopentane, methyl cyclopentane, and methyl-cyclohexane, give toluene by dehydrogenation and dehydrocyclization reactions of normal-heptane (Taskar and Riggs 1997).

So, in naphtha reforming, the concentration of aromatics Benzene, Toluene, and Xylene (BTX) compounds in reformate have a range of 40 -70 wt.%, which is a main source for gasoline pool and petrochemical industries, xylenes or toluene extracted, and the remaining is returned to crude oil storage to recirculate to naphtha reforming (Antos *et al.* 1995, Oyekan 2018).

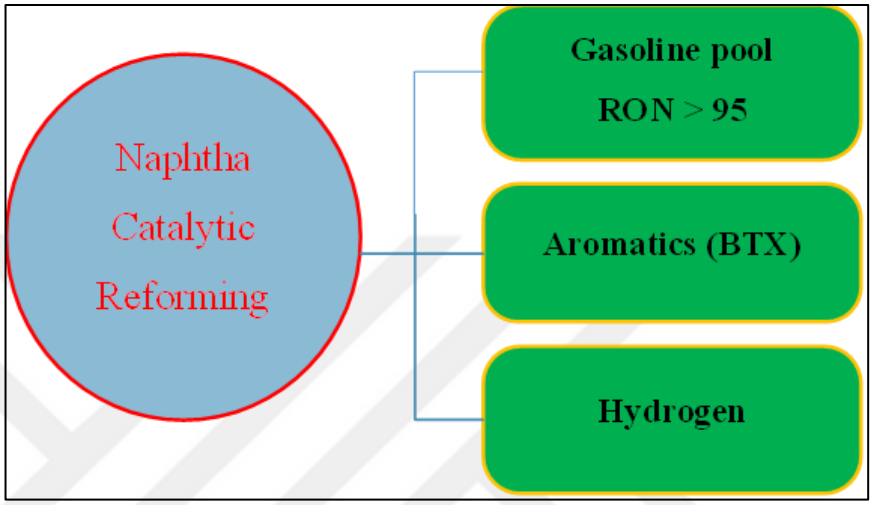

Figure 1.8 Objectives of naphtha catalytic reforming process

Figure 1.8 shows the objectives of the naphtha reforming process: (increasing the octane number of the gasoline product, increasing the aromatic compounds that can be used in other industries, and finally producing hydrogen that is used in other units).

1.6 Catalyst Used in Naphtha Reforming Process

The main part of the naphtha reforming unit is the reaction section because it contains the catalyst, which plays a fundamental and pivotal role in the process; as a result, the catalysts are continuously developed to ensure high performance of the operational process by developing work to change the structure of the catalyst in a simple way which has great returns in addition to high product selectivity therefore, catalysts are developed to be resistant to extreme operating conditions that cause deterioration in catalyst performance over time as a result of deactivation by poisoning and coking (Said-Aizpuru *et al.* 2020).

In 1949, UOP Company presented the first formulation of catalysts used in naphtha reformer, a monometallic platinum supported over chloride alumina (Pt/Al_2O_3–Cl) (R Seif Mohaddecy and S Sadighi 2014). In the year 1968, the process of developing the catalyst began when rhenium metal was added; it was observed that this addition increased the efficiency of the catalyst and the absorption of hydrogen by reducing the cocking deposition on the surface of the catalyst (Grau and Parera 1989).

In the year 1969, tin metal was added, and an increase in the selectivity of the catalyst for aromatic compounds was observed, and it prevented cock deposition on the catalyst; it can regenerate, and therefore it was used in the naphtha reforming units with continuous regeneration process (CCR) (Fioroni *et al.* 2022).

Additional metals have different properties and have a direct effect on the activity and stability of the catalyst; for example, rhenium is highly active in dehydrogenation and Dehydrocyclization reactions with more selectivity to increase (C^{5+}) and hydrogen Yield; add to that, rhenium makes the catalyst more Stable in reactors with a low-pressure design (Ciapetta and Wallace 1972).

The acidic function (chlorine) level of acidity of the catalyst support is required to promote some of the desired reactions (isomerization, Dehydrocyclization); the Chlorine content in the catalyst has a range 0.9 - 1.3 wt.% is considered the optimum to decrease coke deposit (Pieck *et al.* 1996).

The content of the main metals, such as (platinum, rhenium, germanium, and tin) are different and depend on the type of naphtha reforming process with a range from 0.2-0.8 wt. % from total catalyst weight; also, the catalysts may contain traces of some other metals (Ravi *et al.* 2017). Also, these properties differ according to the type of naphtha reforming process, but this difference is wide (Talaghat and Karimi 2020).

1.7 Reformate Properties

The final product of the heavy naphtha reforming process (Reformate) has two important characteristics, namely the octane number and aromatic content, in addition to the vapour pressure of the product. The final product's physical properties are initial boiling point = 33 ºC and final boiling point = 178 ºC in the naphtha reformer No. 800 process (Jones and Pujadó 2006). The characteristics of Reformate can be explained as follows.

1.7.1 Octane number

A very important property of automobile gasoline is resistance to knock detonation during service, high octane number mean allows a high compression ratio inside the engine, and thus we get an increase in engine performance and optimal economy in the consumption of the fuel (Antos and Aitani 2004, Antos *et al.* 1995). Fuel detonation in an engine depends on its composition and gives us indicators of engine power, economy, and efficiency. The octane number can defined as the volume percent of isooctane in blending with normal heptane that has the same performance as the naphtha being tested or defined as a measure of the anti-knock detonation quality of a hydrocarbon compound (Antos *et al.* 1995).

Octane number is measured in labs by using an engine containing one cylinder and operates at 600 rpm, this process is called Research Octane Number (RON), and it has the same engine circumstances as driving a car in a city; there are other tests to measure octane number called motor octane number (MON) of fuel correlates best with an engine performance test at 900 rpm, it computes performance of an engine in a road highway and under severity conditions like hill climbing (Oyekan 2018). In Table 1.3 below are properties and differences between RON and MON tests. Table 1.3 shows the difference in the test method, the operational terms and conditions that must be met in the octane number tester, and the two types (RON and MON).

Table 1.3 RON and MON test conditions (Eiman 2008)

Test engine condition	Research Octane	Motor Octane
Test Method	ASTM D2699-92(102)	ASTM D2700-92(104)
Engine	Cooperative Fuels Research (CFR)	Cooperative Fuels Research (CFR)
Engine RPM	600 RPM	900 RPM
Intake Air Temperature	Varies with Barometric Pressure (88kpa=19.4 °C,101.6kpa=52.2 °C)	38°C
Intake Air Humidity	3.56-7.12 g H_2O/kg dry air	3.56-7.12 g H_2O/kg dry air
Intake Mixture Temperature	Not Specified	149 °C
Coolant Temperature	100°C	100 °C
Oil Temperature	57°C	57 °C

Figure 1.9 Research octane number test engine.

In Figure 1.9, you can see the search engine for the octane number; it consists of an engine with a single cylinder head, where the size of the combustion chamber is changed when the fuel is pumped, for which the octane number is to be checked until the sound of the knock that occurs disappears. Then, the reading of the chamber volume is taken and compared with standard Tables with the room volume having the corresponding octane number, and the device manufacturer sets these Tables.

Many theoretical equations can use to calculate the octane number of the product (Reformate) after making a PIONA analysis to determine the composition of reformate (Paraffin, Naphthene, and Aromatic) and their concentrations, as each compound has an octane number. Table 1.4 some examples of different types of hydrocarbons and the octane number of these compounds.

Table 1.4 Research octane number (RON) for some hydrocarbon compounds (Antos and Aitani 2004)

Group	**Hydrocarbon**	**RON**	**Hydrocarbon**	**RON**
nparaffin	n-Butane	113	Heptane	0.0
	Pentane	62	Octane	-19.0
	Hexane	24.8	Nonane	-17.0
isoParaffin	isopentane	92.3	2-Methyl heptane	26.8
	isoheptane	42.4	2,2,3-Trimethylbutane	113
	3-Methylheptane	21.7	2,2,4-Trimethylpentane	100.0
	2Methylpentane	83	4-Methyl 1-Pentene	95.7
Naphthene	1, lDimethylcyclopentane	96	Cyclohexane	110
	1,3Dimethylcyclopentane	98	Methylcyclopentane	107
	1,l,3Trimethylcyclopentan	94	Ethylcyclopentane	75
Aromatic	Benzene	99	Isopropylbenzene	132
	Toluene	120	1 Methyl2ethylbenzene	125
	o-Xylene	120	l-Methyl-3-ethylbenzene	162

It has been proven, in a practical way, that the octane number of a mixture of hydrocarbons tested by engine (RON test) does not match the average of the octane number of the same mixture, which is calculated theoretically by summation of (concentration * octane) for all hydrocarbon compounds that this mixture consists of, as a result of the above another name for the octane number developed, which refers to the octane number of the hydrocarbon compound after mixing it with other compounds (Fioroni *et al.* 2022).

This name is the mixing octane number; in addition, the difference between the octane number of the mixture and the research octane number is due to the synergistic molecular effects between the hydrocarbon compounds, and the effect of this mixture differs between the hydrocarbons (Oyekan 2018). Table 1.5 shows examples of hydrocarbon compounds, the octane number of each compound in the normal state, and when mixed with other compounds.

Table 1.5 Blending octane number for some components (Oyekan 2018)

Compound	**Actual**	**Blending**
Butane	93	113
Pentane	62	62
Hexane	25	19
Cyclopentane	101	141
Methyl cyclopentane	91	107
Methanol	92	134–138
Ethanol	97	128–135
2,2-Dimethyl butane	92.8	89
2-Methyl-1-butene	102	146
Cyclopentane	101	141

1.7.2 Aromatic content

The aromatic content is one of the characteristics of the reformate produced from the naphtha reforming process because its increase means a high octane number; in addition to that, it is used in some petrochemical industries, in which toluene compounds or xylene are extracted, however, in the recent years, especially after the year 2000, the trend began to reduce the aromatic content in reformate while maintaining the same octane number, after the application of new standards related to air pollution and the lack of complete combustion of aromatic compounds, especially the benzene ring, which was found to be able to cause cancer (Antos *et al.* 1995).

The Eurozone began to impose certain limits on the concentrations of aromatics. As a result, international companies began to add industrial processes that reduce the concentrations of the benzene ring (Antos and Aitani 2004). One common method is splitting the product into light reformate with six or fewer carbon atoms. Then the isomerization process takes place on this product to reduce concentrations of the benzene ring, and the second process is to extract the benzene ring from reformate.

1.8 Reactions in Naphtha Catalytic Process

The reactions that occur inside reactors of the naphtha catalytic reforming process are multiple and different in nature due to the presence of large numbers of different compounds, and because of this difference, most researchers in the field of laboratory experiments and simulations have reached a set of main reactions,

1.8.1 Desire reactions:

- Dehydrogenation of Naphthene to aromatics.
- Dehydrocyclization of Paraffin to Naphthene and then to aromatics.
- Paraffin and Naphthene isomerization.

1.8.2 Undesired reactions:

- Cracking of Paraffin and Naphthene to light hydrocarbons (C_1, C_2, C_3, and C_4).
- Dealkylation of Aromatics, this reaction led to loss (C_1, C_2, C_3 and C_4).
- Cock formation.

1.9 Literature Review

The processes of modeling reactions conducted by researchers on Heavy Naphtha have been going on for sixty years; due to the complexities in the composition of the raw material and reactions that occur in the naphtha catalytic reforming process, it is difficult to get a mathematical model for the process. Therefore, Heavy Naphtha was divided into three hydrocarbon groups, paraffin, Naphthene, and aromatic, to facilitate the mathematical model's formulation (Ancheyta 2011).

So, each compound has its reactions, and building a detailed mathematical model for all the compounds and chemical reactions will be very complicated because it is difficult to know the behavior of each compound. For this, the researchers agree it would be appropriate to build a mathematical model for each group of carbon atoms based on their similar properties and behavior (Ancheyta 2011, Bommannan *et al.* 1989).

Researchers used many mathematical and computational programs. But, in recent years, computer programs used to simulate industrial processes, such as Aspen, Aspen Hysys, Unisim, PRO/II, and ProSim programs, where in some of these programs, there is a complete simulation of the naphtha reforming process like Aspen Hysys. In other programs, we need to build a simulation complete with all its details, like the PRO/II program. Each program has special features and a method of work that differs from the other, but they are close in calculating equations and their results.

Smith (1959) was the first researcher to work on developing a mathematical model. He divided naphtha into three basic compounds, paraffin, naphthenic, and aromatic, based on assumptions:

- Each lump has one compound with an average of that class's properties.
- There is no difference within the same category based on the number of atoms.(Bommannan *et al.* 1989, Chernyakova *et al.* 2015).

On the same rhythm, considering some speculations, Krane et al. (1959) proposed a more complex and comprehensive mathematical model to simulate the catalytic reforming process of naphtha; they assumption: Firstly, the reaction network consists of 20 pseudo-compounds with several carbon atoms from six to ten, secondly: all compounds in each group having the same number of carbon atom different properties on other (Rahimpour *et al.* 2013).

Conversely, Ramage et al. (1980, 1987) developed a detailed kinetic model based on extensive studies with pure components and a narrow-boiling fraction of naphthene at a pilot-plant reactor. For instance, the reaction differences between feedstocks make catalyst deactivation by coke formation, and This model predicts the reactions of 13 lumps, including hydrocracking, hydrogenation – dehydrogenation, cyclization, and isomerization. They assumed that the reactions are reversible between compounds with

the same number of carbon atoms and irreversible reactions between compounds that are unequal in the number of carbon atoms (Elizalde and Ancheyta 2015).

Dr. Zaidoon M. Shakor simulated the naphtha reforming process using the 24 hydrocarbon compounds (paraffin, naphthenes, and aromatics) using the hypothesis of 71 reactions, he compared the obtained results with laboratory results and reached the simulation process of operational conditions: Raising the reaction temperature increases the aromatics content, and concluded that the pressure and the ratio of hydrogen to hydrocarbon have little effect on the aromatics content in Reformate (Shakoor 2011).

Conversely, Taskar (1996), Taskar, and Riggs (1997) developed a complex and rigorous kinetic model comprising 35 pseudo-compounds through a network of 36 reactions. They used Hougen-Watson Langmuir-Hinshelwood-type reaction-rate expressions to improve the performance of a naphtha catalytic reformer plant depending on the data and variables of the operating conditions, where the model focused on improving feed temperature to reactors to obtain an optimal model for the extended life of the catalyst (Taskar and Riggs 1997).

A developed kinetic model by Padmavathi and Chaudhuri (1997) consisting of 26 pseudo-components to study the performance of four commercial plants different in performance by predicting temperature, feedstock, and octane number. In addition to the composition of the recycled gas, the model included equations to calculate the energy balance in combined feedstock and recycled gas entering the reactors (Vathi and Chaudhuri 1997).

R. Seif Mohaddecy and S. Sadighi. They developed a kinetic model for the naphtha reforming process using the ASPEN Hysys simulation program; they used nine pseudo compounds using four main reactions. They compared the results with the results of more complex models, and the results were 4.8% and 3.2%, respectively (Reza Seif Mohaddecy and Sepehr Sadighi 2014, Mohaddecy *et al.* 2008).

Aminu Z. Yusuf, Yakubu M. John, Benjamin O. Aderemi, Raj Patel, Iqbal M. Mujtaba. They worked on developing a kinetic model on a semi-regenerative naphtha reforming process at the KPRC refinery in Nigeria using (gPROMS) Model Builder (5.0.0). To study the effect of partial pressure of hydrogen and increasing the ratio of (H_2/HC) on the operational conditions and the quality of the product, where the results were a decrease in the aromatic content, an increase in the amount of Reformate, an increase in hydrogen production, and a decrease in the percentage of coke deposition (Yusuf *et al.* 2020).

Davood Iranshahi, Mohsen Karimi, Shahram Amiri, Mitra Jafari, Razieh Rafiei, and Mohammad Reza Rahimpour developed a kinetic model for the (CCR) and compared the results with actual results from a commercial plant. They developed a kinetic model to calculate the deactivation of the catalyst using 32 pseudo-compounds and 84 reactions; they used two phenomena of naphtha flow in reactors (axial and radial flow)to study the effect on other operating conditions, and the results were identical to the real results (Iranshahi *et al.* 2014).

Ignacio Elizalde and Jorge Ancheyta developed a kinetic model using the gPROMS program for the first time to find out the behavior of reactions in the case of stable and Unstable conditions in a commercial plant; the kinetic data and properties of the model were taken from the literature, and the results of the kinetic model were matched with the available results from the literature and then applied to the commercial plant to monitor the thermal behavior and concentrations of paraffin, naphthenes and aromatics in reactors in addition to studying hydrogen productivity and octane number with the observation that the compounds behave similarly in terms of reactions inside the reactors, it was found that the results match well with the data of the commercial plant (Elizalde and Ancheyta 2015).

S.Reza Seif Mohaddecy, Sepehr Sadighi, and Majid Bahmani conducted a study to optimize the distribution of the catalyst in the reactors of the naphtha reformer unit in the Tehran refinery using the Aspen Hysys program, as they relied on their study on the redistribution of the catalyst while keeping the operating conditions constant, where they reached The proposed distribution leads to an increase in the octane number and the

octane number per barrel by 0.8 and 0.2 per cent, respectively, while keeping the catalyst mass unchanged (Mohaddecy *et al.* 2008).

Aboalfazl Askari, Hajir Karimi, M. Reza Rahimi, and Mehdi Ghanbari prepared a simulation of the naphtha reforming process in the Isfahan refinery using the Aspen Hysys program. The results were confirmed after matching them with the actual results taken from the refinery, where they focused in their study on the effect of changing the feedstock composition on the rate of the production flow and the octane number; in addition to that, the effect of changing temperature and pressure on the same variables was studied. The result of the simulation was that when increasing the flow rate of the feed that was supplied with heavy Isomax naphtha by 20%, the flow rate and the octane number would increase, and they concluded that the increase in temperature and pressure did not affect output flow rate and octane number (Askari *et al.* 2012).

Researchers used the PRO/II program to simulate many industrial processes, including atmospheric distillation of crude oil, as it was used by K. Wanga, B. J. Zhanga, Q. L. Chena to conduct simulations on the crude oil unit through a complex simulation model of the atmospheric distillation process using Three towers, two furnaces, and a network of heat exchangers, using light crude oil and heavy crude oil, where they reached ideal operating conditions with retrofit solutions through two actual units. The modernization was evaluated by thermodynamics and economic analysis of the conditions of operations. The financial cost of the modernization operations required 102925$ and 177215$. As for the cost, the financial savings amount is 355,226$/year and 656,181$/year, with a shorter recovery rate of 0.29 and 0.27 per year, considering the characteristics of heavy and light crude oil (Wang *et al.* 2016).

Erick Yair Miranda-Galindo, Juan Gabriel Segovia-Hernandez, Salvador Hernandez, and Adrian Bonilla-Petriciolet carried out a multi-target optimization process on the gas oil hydrogenation unit to improve the operating conditions to reduce the annual economic cost, reduce sulfur emissions and carbon dioxide emissions through An interactive column was placed next to the main reactor, where five models of gas oil were used. By using a multi-objective optimization process with complex algorithms due to the

multiplicity of operational variables, they noticed competition in the three main objectives, which prompted them to use the Pareto solutions method to reach the required results. Reducing sulfur emissions will increase the economic cost and CO_2 emissions. However, optimal conditions can be determined to reduce the annual economic cost (Miranda-Galindo *et al.* 2014).

Omar S. Bayomie, Omar Y. Abdelaziz, and Mamdouh A. Gadalla conducted a regeneration study on a modern refinery that showed high energy efficiency by 93%, meaning that the savings rate is 7% for the current practical operational conditions, they proposed an energy recovery algorithm in modern refineries, which helps to save energy by more than the energy goals that have been identified, and the algorithm begins to simulate the process by matching it with the real factory data, for example, the flow was divided to reach the energy goals that were previously determined using Pinch analysis, then these goals are transferred to a lower level of the algorithm to make possible process modifications to reduce power consumption. The results showed that the refining unit could reach the levels needed to reduce energy consumption by dividing the electric current and saving energy consumption by 2.69 MW. The process also led to energy savings of 31.3%, which exceeds the current level of the station. In addition, an environmental assessment was conducted, and similar reductions were obtained in greenhouse gas, with carbon dioxide emissions reduced by 45.1%. Therefore, they concluded that the model could reduce energy consumption in Modern refineries by making good adjustments to achieve energy levels that exceed energy targets (Bayomie *et al.* 2019).

Kunru Yang, Shirun Liu, Chang He, Bingjian Zhang, Qinglin Chen, and Ming Pan have produced a linear programming model that is solved using a double-loop algorithm, and the goal is to reduce the practical energy use while retaining the same economic benefits. The results were compared with the data of the Aspen Plus program. And the actual data of the air and vacuum distillation units, where they designed a tool that helps engineers adjust the main parameters to achieve energy savings higher than the usual traditional methods, up to a saving of 1.06 MW without the need for retrofitting, which means reducing CO_2 emissions of up to 2800 tons annually (Yang *et al.* 2020).

D. Ibrahim, M. Jobson, J. Li, and G. Guillén-Gosálbez focused on developing new methodologies for designing new distillation systems that deal with one raw material for crude oil or raw materials. The proposed model, designed for the crude oil distillation process, used A strict model for each tray, and therefore they assumed in the design that the number of active trays in each section is a design degree of freedom. This model was built in two programs; the first is the Aspen Hysys program, in which the distillation model was built, and the second program is MatLab, in which the optimization process is conducted using a genetic algorithm, thus during process simulation, data can be exchanged and improved. In addition, alternative models were developed to address the deficiencies in the distillation process by using artificial neural networks (ANN) and the support vector machine (SVM) and using them in the optimization process. When designing the proposed new model, they took into account the raw materials of crude oil and their different specifications, in addition to introducing different models of Distillation columns for multiple crude oils and the application of a new approach to improve operational conditions and the goal, is to increase the net profit while maintaining the quality of production; they concluded that the results resulting from the new model compared to strict models reduces the computational time without difference in the accuracy of the solution and optimization using case studies (Ibrahim 2018, Ibrahim *et al.* 2018).

1.10 Aim of Thesis

This study aims to simulate the Heavy Naphtha reforming unit by the PRO/II program (v. 2022) to obtain the best operating conditions. Optimizing such conditions shows how the octane number can be improved, not to mention reducing the utility usage. Octane number, highest productivity, and prolonged operational life of the catalyst are crucial traits to consider from an engineering perspective. It is done in the catalytic reforming unit 800 at the North Refineries Company (NRC).

The first part deals with changing the parameters of the main reaction, which is dehydrogenation, such as the temperature, H_2 partial pressure, and required activation energy. Selectivity is another parameter to be considered and statistically recorded among

the three other reactions: isomerization, hydrocracking, and dehydrocyclization. The second part studies the effect of changing the recycled gas purity and flow rate. That shows how the control hydrogen/ hydrocarbon ratio can affect the overall results.

Simulations began in all scientific fields, including the oil industry, and because of scientific development, computer programs began to appear not long ago used to simulate oil operations. Among these programs is the AVEVA PRO/II program. The naphtha reforming unit, which is an important part of the oil industry, has many variables that affect the quality and quantity of the product; for this reason, this study has chosen conditions of the naphtha reforming process to increase the quality of the product (RON) by making optimization to find optimum operational conditions of the process, in addition, to study these variables and the surprising problems and how can for engineers solve these problems.

2. MATERIAL AND METHODS

The experiment used was a computer simulation process using the AVEVA PRO/II program. First, draw a flow chart of the operational process of unit 800, as shown in Figure 2.1. The compounds that form the heavy naphtha were selected and entered the molar composition based on PIONA analysis. After that, the data of all the equipment used, such as (reactors, exchangers, etc.), was entered. After that, enter reaction data into the program. After completing the data entry and running the program, the simulation results compared with the actual results and showed a good close.

Each study used laboratory devices to obtain the necessary data to complete the study or to compare the results with the actual results. This study used the following devices to complete the data entry into the simulation program and then compare the simulation results with the actual results: Reformate product composition (wt.% and mol.%), hydrogen yield%, RON, aromatic content, C^{5+}.

- Gas Chromatographic device use in PIONA analysis type Clarus 580 GC, Method type ASTM D6730 ...6729 DHA shown in Figure 2.2.

- Octane number test device type CFR Engine, model F1/F2 made in USA showing in Figure 1.9.

- Distillation test device type Kohler made in Germany showing in Figure 2.3.

- Computer used for operating AVEVA PRO/II program.

2.1 PRO/II Program

PRO/II program is a simulation program for industrial processes in the steady state and using process design and operational study, like all computer programs, is designed in a way that makes the program easy to use as it contains several windows with all the options required to simulate operations. Therefore, the program is easy to use for process engineers in the chemical industries and gas operations (Ghasem 2021).

AVEVA Group plc developed the simulation software PRO/II version 2022. The data used for this study was obtained from the Salah Al-din/2 refinery. They include detailed Process Flow diagrams of naphtha catalytic reforming, operating parameters for heavy naphtha (feed) and compositions, and operation conditions of process no. 800.

The PRO/II program has simple and easy-to-use windows that help complete the simulation process to get the results quickly. Can summarize the main windows as follows:

2.1.1 Building the process flow diagram

Drawing the process flow diagram is the first and essential step in any simulation, whether small or large. Provided that the drawing of the process flow diagram is virtually identical to the real diagram with some differences, which are preferable not to put in the flow diagram, such as control devices and valves, which do not affect the simulation (Kang 2005). Figure 2.1 shows the process flow diagram of a naphtha reformer unit consisting of three fixed bed reactors drawn and plotted using software AVEVA PRO\II.

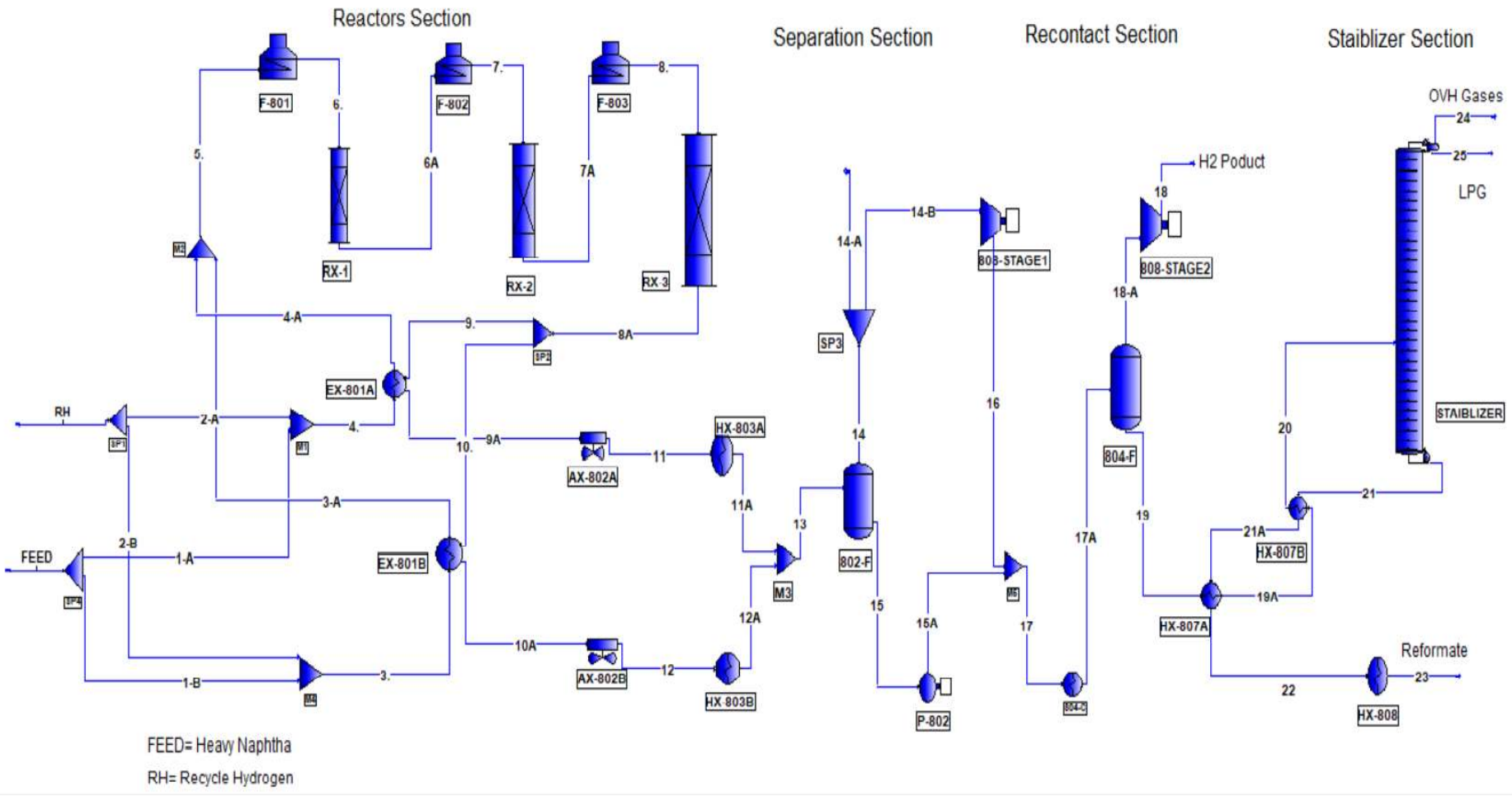

Figure 2.1 Building flowsheet of naphtha catalytic reformer by PRO/II

2.1.2 Setting the input units of measure

The simulations provided by the program require choosing the type of units of measure required to perform mathematical calculations, whether these units are (SI, metric, or English units), whose selection depends on the user's desire. Figure 2.2 shows many options for choosing a measurement unit to help the user perform the simulation easily and quickly.

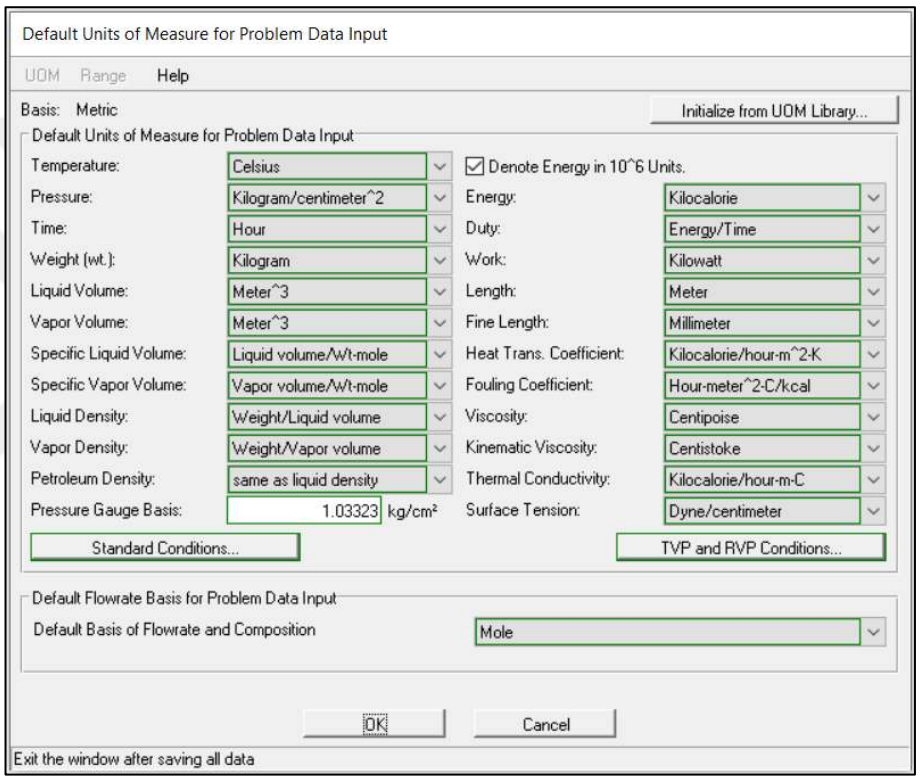

Figure 2.2 Input units of measure in PRO/II

2.1.3 Library choosing and defining the components

The PRO/II program contains many libraries such as (PROCESS library, SIMSCI library, DIPPR (Design Institute for Physical Property Research) library from the American Institute of Chemical Engineers and others, through which compounds to be entered into the simulation are selected, and a library has been selected SIMSCI because it is a fully

documented library that contains a complete bank of information on the physical properties of compounds.

The PRO/II program has libraries that enable the user to choose the compounds he needs effortlessly and without complication. These libraries contain data for more than 2000 compounds. Once he enters the compound selection window, the full compound name, chemical symbol, or access name can used, facilitating the search process for the required compound to put in the list component of the simulation process.

For example, you can retrieve methane information using commonly used names: C_1, CH_4, METH, and METHANE. Figure 2.3 shows the types of libraries contained in the program, the methods for selecting these libraries, and the method for choosing the name of a compound or the chemical formula of any compound.

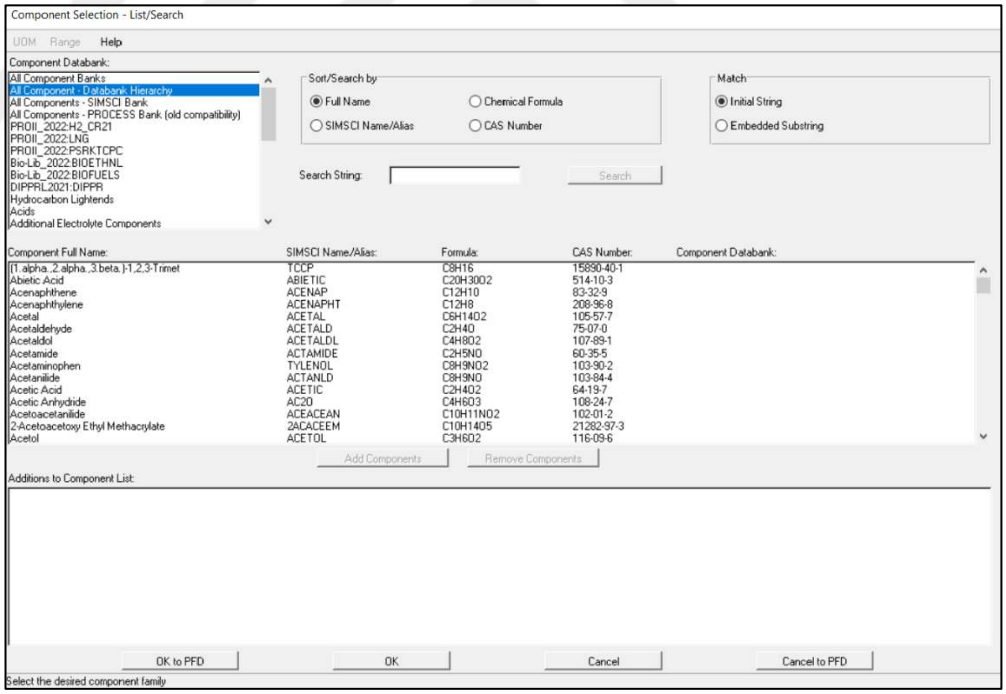

Figure 2.3 Component Selection window

2.1.4 Selecting equation of state

Choosing a thermodynamic method for the flow chart is a particularly major decision because if a thermodynamic method is chosen wrong, it does not help calculate the flow process's behaviour correctly, and it will lead to results that are not valid for simulation. Therefore, the improper choice of the thermodynamic model is considered the biggest cause of error in the simulation. Therefore, it is always good to compare the simulation data with the actual factory data (Kang 2005).

PRO/II contains all the equations and methods for calculating the physical properties of the simulation. For this reason, the equation of state (PENG-ROBINSON) was chosen to calculate thermodynamic properties based on the program references, which recommend using this method in this industrial simulation process.

Figure 2.4 shows the types of thermodynamic calculation methods in the PRO/ II program and how to choose the appropriate method.

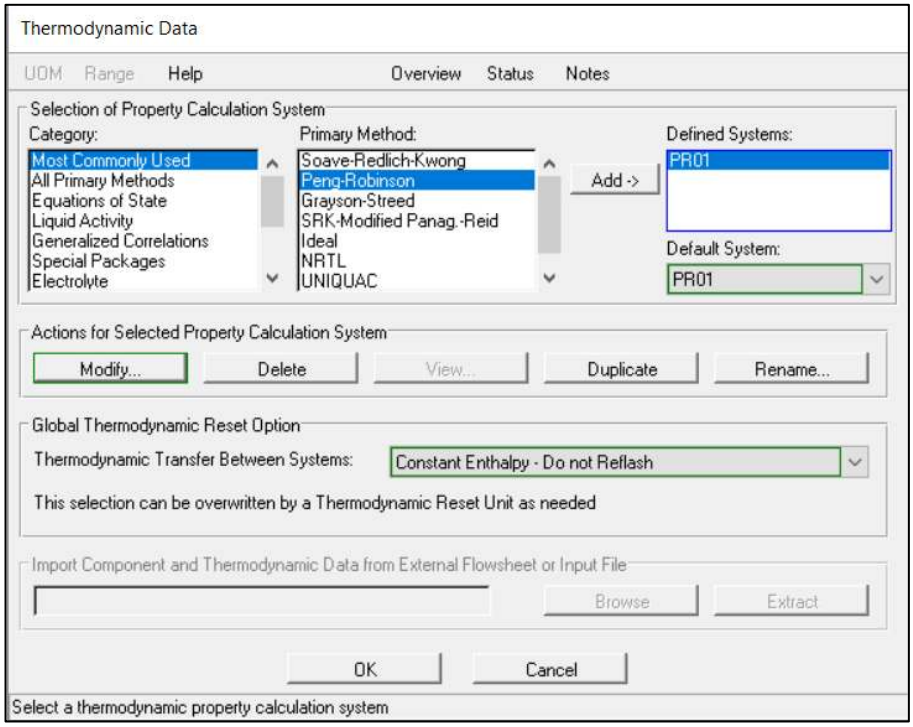

Figure 2.4 Selection property of thermodynamic window

2.1.5 Flowsheet optimizer main

The advantage of the PRO/II program is that it contains an optimization tool that helps users in the optimization process and saves time instead of using other known methods. The tool contains a window in which the desired optimization target is. It also contains the method for selecting variables and the scope of each variable as approved in any optimization process. The tool also contains a window for restrictions through which restrictions on the optimization process can entered. Figure 2.5 shows the optimization tool and the windows it contains.

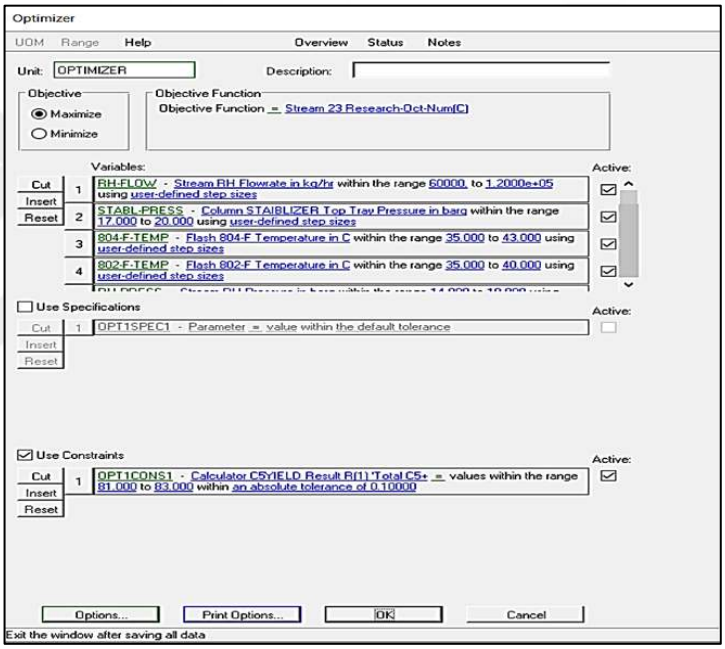

Figure 2.5 Optimization tool window

2.2 Heavy Naphtha Quality

Heavy Naphtha consists of the basic compound paraffin, which has several carbon atoms from (C_1 to C_{11}). The cyclic naphthenes consist of two main rings and the number of carbon atoms constituting them (5 and 6) atom carbon and aromatics, whose number of carbon atoms is from (C_5 to C_6). So, this complex structure of Heavy Naphtha is affected by two important characteristics: a range of distillation and chemical composition and its direct effect on the conditions of the Naphtha reforming process.

2.2.1 Distillation range

The initial boiling point, when it is low, shows the presence of a high percentage of light compounds, in addition to a higher percentage of hexane, which leads to increased severity of the operating conditions due to the difficulty in converting hexane into aromatic compounds, in addition, obtain a high quality of the product. When the initial boiling point is low, this leads to a lower aromatic content and a lower octane number.

On the other hand, when the initial boiling point is high, this shows a high naphthene and aromatic content in Heavy Naphtha, which reduces the severity of the operating condition to obtain a high-quality product. The main source of Heavy Naphtha feedstock for naphtha catalytic reforming number 800 in Salah Al-din\2 refinery from atmospheric distillation.

2.2.2 Chemical composition of heavy naphtha

The chemical composition of naphtha can be determined by GC analysis, which is important to determine the operation's aromatic content and level of severity. So, in any study about naphtha catalytic reforming, it is necessary to know the composition of Heavy Naphtha because this gives us a big idea about the specification of naphtha, especially the percent of compounds (paraffin, naphthene, and aromatic). So, it is considered an important factor for the naphtha reforming units. It determines the severity of the process's operating conditions, especially the feed entering the reactors (reaction temperature), and its effect on catalyst activity. Tables 2.1 and 2.2 show the weight, volume, and molar percent of the hydrocarbon groups (paraffin, iso-paraffins, naphthene, olefin, and aromatic) in addition to the weight percent of the hydrocarbon groups that have the same number of carbon atoms.

Table 2.1 PIONA analysis of heavy naphtha by GC analysis.

Groups	Mass %	Volume %	Mole %
Paraffin	31.5595	33.3521	32.3268
iso-paraffins	33.7850	35.2366	32.7644
Naphthene	19.6248	18.6248	19.8329
Olefins	0.2469	0.2562	0.2046
Aromatics	14.3904	12.1189	14.5355

Table 2.2 Hydrocarbon atom percent by wt. % of heavy naphtha

Atom Group	N-paraffins	Iso-paraffin	Olefin	Naphthene	Aromatics
C_1	0.00228	0.00000	0.00000	0.00000	0.00000
C_2	0.00000	0.00000	0.00000	0.00000	0.00000
C_3	0.00472	0.00000	0.00000	0.00000	0.00000
C_4	0.04340	0.00496	0.00000	0.00000	0.00000
C_5	1.21064	0.58104	0.00000	0.13555	0.00000
C_6	3.86382	3.21531	0.00000	1.64590	0.20662
C_7	8.70177	6.20940	0.00000	5.41524	2.35977
C_8	9.25905	10.52662	0.04245	6.62545	6.14333
C_9	6.39886	8.41408	0.03878	4.95092	4.75087
C_{10}	2.03174	4.51972	0.16568	1.11433	0.92981
C_{11}	0.04321	0.41881	0.00000	0.02587	0.00000
Total	31.55949	33.88994	0.24691	19.91326	14.39040

Figure 2.6 showed that, simplified image of GC device type Clarus 580 GC used for the analysis of PIONA.

Figure 2.6 GC device used for the analysis of PIONA.

The reformability index (N+2A) to express naphtha quality. When the reformability index is above 50, Heavy Naphtha is rich in naphthene and aromatic and needs low-severity operation conditions to get the desired level for (RON). On the other side, the reformability index is low, and it needs high-severity operation conditions. So, international companies differ in formulating the reformability index. For example, Axens Company uses the formula (A+0.85N) as the reformability index.

2.2.3 ASTM D86 method

This laboratory method covers all atmospheric distillation products. as it works to determine the properties of the range of boiling points based on a mass or volume basis for light naphtha, heavy naphtha, kerosene, aviation fuel, motor fuel, and furnace fuel, so this method is used for light distillates and is not used to test Products that contain a high percentage of crude oil residue (Santos *et al.* 2021).

The sample in one of five groups based on the composition of the sample, vapour pressure, or the initial or end boiling point; therefore, the arrangement of the device, the temperature of the condenser, and other variables determined by the group in which the sample located; the volume of the sample that distilled is 100 milliliter's, where the distillation performed under ambient pressure and conditions designed for sample fragmentation. The recording is according to the user's need for data such as temperatures, volumes of distilled quantities of the sample, and the sizes of lost quantities and residues. Heavy naphtha properties by ASTM D86 shown in Table 2.3, and the distillation boiling point device shown in Figure 2.7.

Table 2.3 Heavy naphtha properties by ASTM D86

DISTILLATION (VOL. %)	**TEMPERATURE (^{O}C)**
IBP	85
5 %	92
10 %	98
30 %	112
50 %	121
70 %	134
90 %	143
95 %	152
EBP	161
DENSITY AT 15.0 ^{O}C	730 – 745 kg/m^{3}
MOLECULAR WEIGHT	105
SULFUR	0.7 - 1.0 PPM wt.

Figure 2.7 Distillation boiling point device

2.2.4 Gas chromatographic analysis (GC)

In the oil field, gas chromatography is an important device of the most widely used methods due to its importance in determining the composition of the crude oil industry and other products. Due to its importance in measuring the product type and its suitability for the required standards, it normally used to analyze the gaseous like (N_2, H_2, CO, CO_2, and H_2S) and light hydrocarbon gaseous like (LPG+ Off gas) compositions. The GC devices designed to work on a temperature range between 70-400℃. Some of these devices operate at temperatures more than 600 ℃, and in some cases, the devices operate at -100℃ (Smolkova-Keulemansova and Feltl 1991).

2.3 Catalyst Specification

The used catalyst here type denoted (Pt-Re/Cl-Al_2O_3) consists of the dual function consists of (platinum and rhenium) as the metal function catalyzes the hydrogenation and dehydrogenation reactions loaded on (chlorinated-Al_2O_3) as the acidic function promotes the isomerization and dehydrocyclization reaction. The amount of the catalyst is (54405

kg) distributed into three fixed-bed reactors. The physical and chemical properties for catalyst are shown in Table 2.4.

Table 2.4 Catalyst specification used in naphtha reformer 800.

Parameter	Unit	Specification
Platinum	wt. %	0.3
Rhenium	wt. %	0.3
Chlorine	wt. %	0.6-1.1
Support	Al_2O_3	ALUMINA
Density	kg/m^3	610 - 700
Shape	-	CYLINDRICAL
Surface Area	m^2/g	≥ 180
Length	mm	4
Diameter	mm	1.6
Pore Volume	ml/gm	≥ 0.47

2.4 Methods

Every study needs steps and procedures to be complete, and in this study, a sample of heavy naphtha was started with the PIONA test, as shown in Table 2.5 below. On this basis, the data entered into the simulation program in addition to entering the reaction data and operation variable conditions and finally starting the simulation process. After obtaining the results, they compared them with the actual results taken from the database of unit 800, and then after completing the matching of the results, they were compared to find the optimum operation conditions.

2.4.1 Heavy naphtha feed stream building

The simulation begins with selecting hydrocarbon compounds and entering the values of the molar, weight, or volume ratios of these compounds, from which heavy naphtha is formed and used as a feedstock for catalytic reforming units. In the following Table 2.5 mention these compounds and the values of their molar percent.

Table 2.5 PIONA analysis (mol %)

Component	MOL%	Component	MOL%	Component	MOL%
METHANE	0.0000	23DMOCT	0.6000	PXYLENE	1.6500
ETHANE	0.0000	24DMOCT	0.4000	MXYLENE	1.6000
PROPANE	0.0000	26DMOCT	0.7000	OXYLENE	1.5000
I-BUTANE	0.0094	25DMOCT	0.5000	EBENZENE	1.6000
BUTANE	0.0850	5MNON	0.6000	124MBENZ	1.0500
IPENTANE	0.8800	DECANE	1.6200	M3EZ	1.1000
PENTANE	1.8300	3MDECANE	0.1000	135MBENZ	0.9000
2MP	1.2800	MEDECAN2	0.0500	123MBENZ	0.7000
3MP	0.9800	23DMC9	0.0700	PRBENZEN	0.3300
23MB	1.0900	NC11	0.0300	INDANE	0.2500
22MB	0.8500	CP	0.2100	1234TMBZ	0.2500
HEXANE	4.9100	MCP	1.2000	SBBENZEN	0.0000
2MHX	0.5000	CH	0.9500	TBBENZEN	0.0000
3MHXAN	0.5900	CHP	0.9000	12DM3EBZ	0.0500
22MP	0.6000	11MCYPNT	0.8000	2EPXYL	0.0800
23MP	0.7000	ECP	0.8900	NAPHTHLN	0.0400
24DMP	0.9000	MCH	0.8500	1235TMBZ	0.0500
33DMP	0.9000	1C2C	0.7600	14EZ	0.0500
223MB	1.3000	1C3M	0.7800	13DEBZ	0.0250
3EPENT	1.3000	1T2C	0.6000	IBBENZEN	0.0360
HEPTANE	9.5100	1T3M	0.5000	1M2PRBZ	0.0420
22DMHX	0.6000	113C	1.2500	1M3PRBZ	0.0900
33DMHX	0.2000	COCT	1.1000	1M4PRBZ	0.0500
2MHP	0.4000	1C2H	0.8000	1MNP	0.0000
4MHP	0.6000	1T2H	0.9000	2MNP	0.0000
3MHP	0.6500	ECYHXN	0.8000	PISOPRST	0.0000
223P	0.7500	CT4C	0.3000	PNBZ	0.0000
224P	1.3000	CTCP	0.3200	4TBUTSTY	0.0000
233P	1.1000	TC4C	0.3000	HXBNZN	0.0000
234P	0.9000	11CH	0.2500	MDIPBN	0.0000
25HX	1.2000	1T3H	0.3000	CYPENTEN	0.0150
2M3E	1.1000	PRCP	0.2000	3M1BUTEN	0.0300
3M3EPN	1.3000	IPCH	1.1000	3M1PNTEN	0.0400
OCTANE	8.8800	PCH	1.1500	3MCPEN	0.0300
4MO	1.3000	BCYP	1.1000	33M1BUTE	0.0500
2MO	1.1000	1T35TMCH	0.9400	2E1PNTEN	0.0200
3MO	1.1000	IBCH	0.0000	1HEPTENE	0.0400
224MHX	0.9000	BCH	0.2806	2E1HEXEN	0.0020
235MHX	1.3000	CYCDECAN	0.3700	1OCTENE	0.0020
233MHX	1.5000	HXCPEN	0.0180	C4OCTENE	0.0200
NONANE	5.5200	BENZENE	0.2890	T4OCTENE	0.0100
22DMOCT	0.7000	TOLUENE	2.8060		

2.4.2 Process type

Naphtha-reforming unit no.800 is the basis of our study. It is one of the fixed-bed world's catalyst reactors and the most widespread type. The Naphtha catalytic process (800) in Salah Al-din\2 refineries consist of four sections: In Figure 2.8, the sections of the naphtha catalytic reformer unit 800 have been explained. It consists of four main sections, and each of these sections is complementary to the earlier section, but each section has properties because the operating conditions differ from the other sections, and each section will be explained with the operational conditions. Table 2.6 shows the sections' names with each section's operational conditions.

Table 2.6 Naphtha reformer 800 sections.

Sections	**Parameters**
Reactors Section	T, P, LHSV And H_2/HC Ratio
Low Pressure Separation Section	802-F Separator, T And P
High Pressure Separation Section	804-F Separator, T And P
Stabilization Section	Reflux Ratio, Heat Duty of Re-Boiler and Condenser

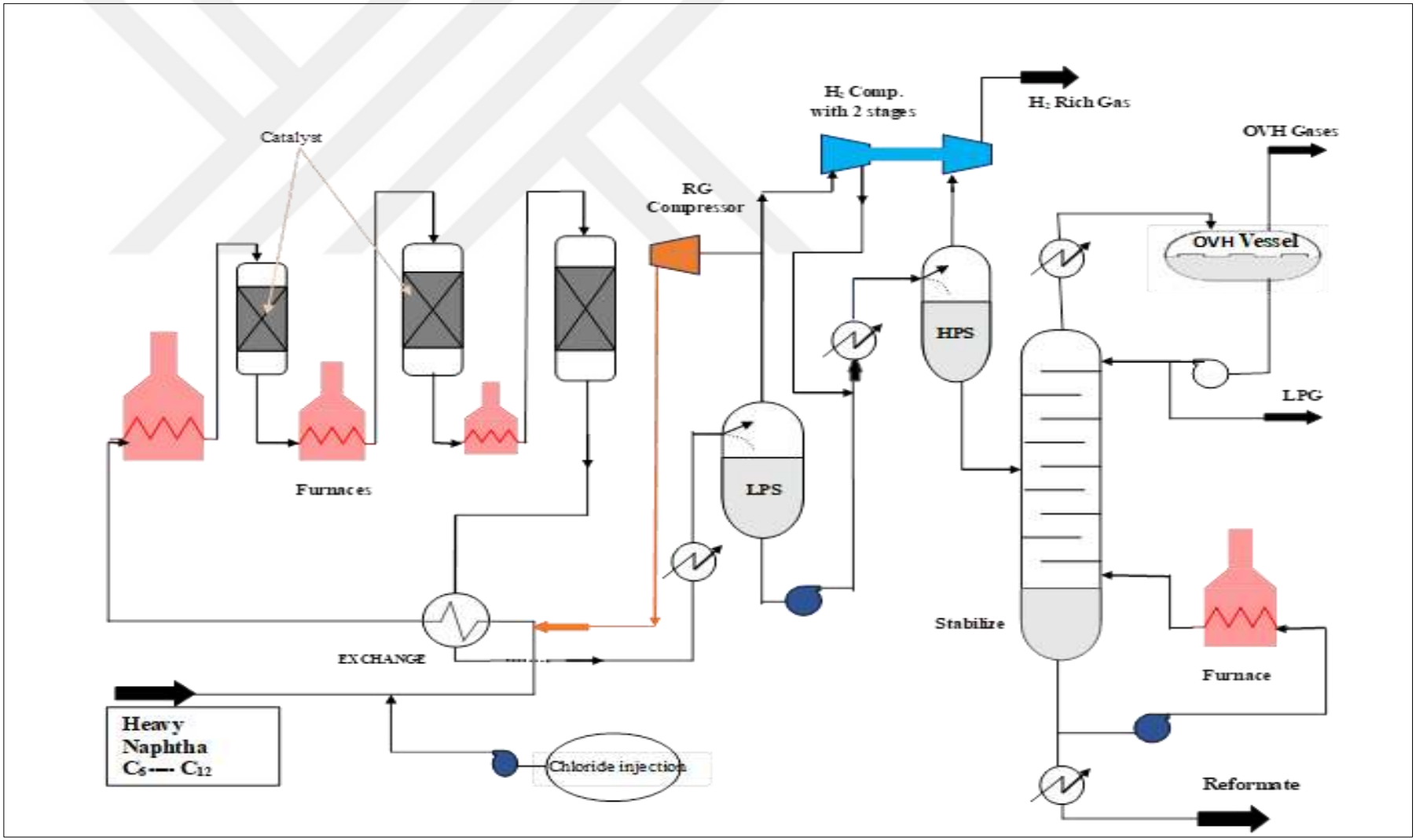

Figure 2.8 Naphtha catalytic reformer unit 800 process flow diagram

2.4.3 Process description

The Reformer Unit 800 in Salah Al-Din/2 refinery Baiji, Iraq, consists of four main sections, which is: The first section of the reactors, which consists of three reactors that contain the catalyst; secondly, the low-pressure section; third, the high-pressure section and the fourth section of the stabilization tower.

- **Reactors Section**

Feed (Heavy Naphtha) enters vessel 801-F and pumped to the reaction section, but before entering, the stream is divided into two streams, the same in quantity, and each stream mixed with recycled gas coming from the separation section by a centrifugal compressor rich with hydrogen has range 60-90 (mol %).

The combined feed of two streams, which consists of (Heavy Naphtha+ RG) enters two heat exchangers, 801-CA and CB, to the tubes of the exchanger to preheat the combined streams (CF), and at the same time, the outlet stream from reactor 803-D it is cooling. The streams out from the heat exchanger rejoin again with a temperature of about 440 oC and enter furnace 801-B to raise the heat of the feed to the desired temperature level.

Afterwards, the combined stream enters the first reactor 801-D, filled with catalyst, and because the high endothermic reactions occur, the CF out from the reactor is reheated again by second furnace 802-B and enters the second reactor 802-D. Again, because of the endothermic reactions, the CF stream is reheated in furnace 803-B and, after out, enters third reactor 803-D.

The main parameters in reactors section it:

- Pressure inside reactors.
- Temperature required for reactants to start reactions in reactors to reach the desired final product.
- Hydrogen gas moles/hydrocarbon moles ratio or (partial pressure).
- Heavy naphtha feedstock quantity (LHSV).

Reactors in naphtha catalytic reformer 800, design type fixed bed with radial direction. The lengths, diameters, and quantity of catalysts in each reactor are shown in Table 2.7.

Table 2.7 Reactor specification and catalyst distribution

PARAMETER	**UNIT**	**REACTOR 1**	**REACTOR 2**	**REACTOR 3**
LENGTH	m	4.3	5.72	6.7
DIAMETER	m	1.9	2.4	3.1
REACTOR VOLUME	m^3	23.2494	40.2627	73.0615
CATALYST VOLUME	m^3	12.418	26.027	50.742
CATALYST WEIGHT	kg	7575	15877	30953
CATALYST DISTRIBUTION	wt. %	13.93	29.18	56.89

- **Low pressure separation section (LPS)**

After CF comes out from the reactor, 803-D divides into two streams and enters the shell of heat exchanger 801-CA, CB, then to air cooler 802-CA, CB, and water cooler 803-CA, CB. Then, it enters the separation vessel 802-F (Low-Pressure Separator), with two-phase (liquid + gas) inside the vessel. Liquid out from vessel and pump by 802-J to high-pressure section, the gases out from the top with two streams, the first stream RG to reactor section by centrifugal compressor 807-J, the second stream is hydrogen as product to the first stage for reciprocating compressor 808-J in high-pressure section.

The parameters in this section it:

- Separation temperature in vessel 802-F.
- Pressure of separation vessel 802-F.

- **High pressure separation section (HPS)**

The gases (H_2 + HC) compressed by the first stage for compressor 808-J and liquid pumped by 802-J; they mix in one stream before entering water cooler 804-C and then entering separation vessel 804-F (High-Pressure Separator). The liquid out from the bottom transfers to the stabilization section by pressure difference because the pressure in the stabilizer is less from the high-pressure section, and the gases out from the top of the vessel enter the second stage of compressor 808-J and push to other units (HDS, HDT).

The High-Pressure section mainly aims to separate more LPG from hydrogen and increase hydrogen purity to push it to other units. Second, the pressure in the unit (800) is less than from others; for this need, a compressor like (808) raises the pressure of pushed gases (Yusuf *et al.* 2019).

The parameters in this section it:

- Separation temperature in vessel.
- Pressure inside vessel.

➢ **Stabilization section**

The main and important goal of the stabilization tower is to keep the vapor pressure of the reformate at a constant level because storing the product with high vapor pressure will lead to problems in the storage tanks as well as the car's tank, especially during the summer season, it done by removing liquefied petroleum gases (LPG) and keeping a constant percentage in the product.

The tower has 32 trays from top to bottom and consists of two sections: the upper section starts from 1 – 14 trays and is smaller than the lower section, which starts from 15 – 32 trays. Liquid from the HPS section enters heat exchanger 807-CA, CB in the tubes to preheat with the hot final product (reformate), then enters stabilizer tower 801-E in the middle between 14 and 15 trays. This region is called the flash zone because the pressure difference will release (LPG) to the top and liquid down. The liquid in the bottom of the tower circulates by pump 804-J to furnace 804-B to raise its temperature and return to the bottom at the upper point to release more LPG and stabilize the RVP of reformate.

The LPG release from the top of tower enters air cooler 805-C and then water cooler 806-C, then enters the vessel 805-F; in this vessel, some gases condensate like ($C_3 + C_4$) they pushed by pump 803-J again to the top of the tower enter at tray (5) as a reflux to maintain the temperature of the top. The excess quantity of LPG is pushed to the (LPG) recovery unit. The other gases, like ($C_1 + C_2$), are pushed from vessel 805-F by pressure to the LPG recovery unit. The final product from the tower enters the shell of heat exchanger 807-CA, CB, then air cooler 812-C and water cooler 808-C and after that, to storage vessels.

Finally, the vapour pressure is measured by the Reed method, and because of this, the term (RVP) is used in calculating vapour pressure, which stands for Reid vapour pressure measurement.

The parameters in this section it:

- Reboiler duty (bottom temperature).
- Condenser duty (vessel 805-F temperature).
- Reflux ratio of (LPG) at top of tower.

2.5 Process Variable

Four variables influence the naphtha catalytic reforming process as it affects the performance and product quality. These parameters affect all naphtha catalytic reformers: Reactor inlet Temperature, Reactor inlet Pressure, Space Velocity, and H_2/HC Ratio.

- **Reactor inlet temperature (RiT)**

Most of the reactions in the naphtha reforming units are endothermic reactions, so they require high temperatures to give the desired results, but raising the temperature has limitations, such that increasing the temperature will increase the rate of hydrogen cracking reactions, and this causes a decrease in the amount of production, in addition to that it causes sedimentation Carbon on the surface of the catalyst and reduces its efficiency.

The terms (WAIT= weighted average inlet temperature) and (WABT= weighted average bed temperature) are the two main parameters in industrial units. They used to express the reforming reactor's average temperature as a measure of temperature distribution inside each reactor and the mathematical expression in equations 2.1 and 2.2 below.

$$WAIT = \sum_{i=1}^{n}(wfi * Ti) \quad (2.1)$$

Where:

wf = The ratio of the weight of the catalyst in each reactor to the total weight of the catalyst.

T_i = inlet temperature for each reactor.

n= number of reactors.

$$WABT = \sum_{i=1}^{n}(wf * \left(\frac{Ti+T0}{2}\right) \quad (2.2)$$

Where:

wf= The ratio of the weight of the catalyst in each reactor to the total weight of the catalyst.

T_i= inlet temperature to each reactor.

T_o= outlet temperature from each reactor.

n= number of reactors.

These terms are used to express the rate of heat distribution over all reactors and the difference between them is that WAIT depends on the entry temperature into the reactor, while WABT depends on the rate of heat along the catalyst layer in the reactor.

- **Pressure**

The pressure inside the reactors is considered one of the important operating conditions, as the decrease in pressure leads to an increase in the production of reformate and production of hydrogen. Hydrocracking reactions cause carbon deposition on the catalyst's surface, reducing efficiency. The pressure inside the reactors is constant in the naphtha reforming units, and its value is from 3- 35 barg depending on the reactor design.

- **Feed quantity or space velocity**

In all naphtha reforming processes, the rate of product and the octane number can be controlled by controlling the amount of naphtha feedstock with temperature of the reactors. Therefore, increasing the severity of the process is either by raising the temperature of the reactors or decreasing the space velocity (feed quantity) to obtain a constant octane number.

The terms (LHSV) and (WHSV) express the space velocity by volume or weight of feedstock; space velocity can be expressed in equations 2.3 and 2.4 below.

$$\text{WHSV} = \frac{Weight\ flowrate\ of\ feed\ (kg/hr)}{Weight\ of\ catalyst\ (kg)} = hr^{-1} \tag{2.3}$$

$$\text{LHSV} = \frac{Volumetric\ flowrate\ of\ feed\ at\ 15\ oC\ (m3/\ hr)}{Volume\ of\ catalyst\ (m3)} = hr^{-1} \tag{2.4}$$

- **Hydrogen/hydrocarbon ratio (H_2/HC)**

The ratio of hydrogen to hydrocarbons in naphtha reforming is molar, i.e. (the ratio of moles of hydrogen in the recycling gas/moles of naphtha feedstock), as increasing this ratio will lead to an increase in Partial pressure of hydrogen helps to remove the carbon deposited on the surface of the catalyst. Thus, the general effect is to increase the life of the catalyst. This ratio can be described using the following expression in equation 2.5 below:

$$\frac{\text{H}_2}{\text{HC}} = \frac{\text{Hydrogen moles in recycle gas}}{\text{Heavy Naphtha feedstock moles}} \tag{2.5}$$

2.6 Normal Operation Conditions for Unit 800

In simulations used in industrial processes, we need to know the operating conditions of a unit to start the simulation process based on which the results range from the actual results. Normal operation conditions for naphtha catalytic reforming no. 800 shown in Table 2.8.

Table 2.8 Normal operation conditions for unit 800

PARAMETER	**OPERATION CONDITION**	
UNIT CAPACITY (Feed Quantity)	80	m^3/hr.
LHSV	0.887	hr^{-1}
Rx: Temperature, Pressure	475 ^{O}C	14.5 barg
LPS: Temperature, Pressure	42 ^{O}C	12.5 barg
HPS: Temperature, Pressure	45 ^{O}C	22.5 barg
STABILIZATION TOWER	TOP: 110 ^{O}C BOTTOM: 240 ^{O}C	17.5 barg

2.7 Model

Reactions can help study the mechanism inside the reactors, which can be understood by building a kinetic model. In addition, kinetics helps to study the effect of catalysts on these mechanisms. From this point of view, the kinetic model used in the simulation was built using the Arrhenius equation in structure, which is in the program's structure (AVEVA PRO/II). Feedstock (heavy naphtha) stream Build depends on GC analysis; therefore, the simulation is done without changing feed quality and character.

2.7.1 Assumptions

Simulations are mathematical calculations that need some hypotheses through which we can facilitate the computational process of the simulation process. These hypotheses considered a bridge to facilitate access to results that are identical to the actual results, and therefore, these hypotheses considered correct. and among these hypotheses that have been assumed are as follows:

- It was assumed that the mechanism of occurrence of the reactions depends on the behavior of each compound and not assume that the lumps of compounds (paraffin's, naphthene, and aromatics).
    - Fixed bed adiabatic reactor-type axial flow direction.
    - Steady state for mass and energy balance equation.
    - Reactions are in the same phase (homogenous reactions), the vapour phase.
    - The Ping-Robinson equation is used for vapour/liquid Thermodynamic calculation.
    - First-order pseudo reaction concerning hydrocarbons and kinetic data taken from literature (Ancheyta 2011).

2.7.2 Kinetic model

The study is developing a model to simulate the operating conditions of naphtha reformer 800 using a program PRO/II simulation. This development includes simulating the reactions inside the reactors and studying how they affect operation conditions on these reactions. It is normal in any series of complex chemical reactions because of the multiplicity of types and characteristics of the reacting compounds, the occurrence of

reactions that give undesirable results, as is the case with the desired reactions, so it is necessary to work on providing the best conditions that increase the desirable reactions and reduce the reactions that give undesirable results.

The main goal of the reactions in the naphtha reforming reactors is to increase the aromatics and branched paraffins that have a high-octane number. As a result, the following reactions were chosen to be the basis of the simulation process, with an illustration for each reaction.

2.7.2.1 Dehydrogenation of naphthenes to aromatics

Converting naphthenes into aromatics is considered the most important reaction that occurs inside the reactors due to its importance in increasing the concentration of aromatics with a high-octane number in addition to hydrogen production. One of the characteristics of these reactions is that they are fast, and the conversion rate of naphthenes in them reaches more than 95%, but they are endothermic, and we notice this decrease in the first reactor, which is the smallest in size, which requires compensation for the lack of heat using furnaces. An example of this reaction is shown in Figure 2.9.

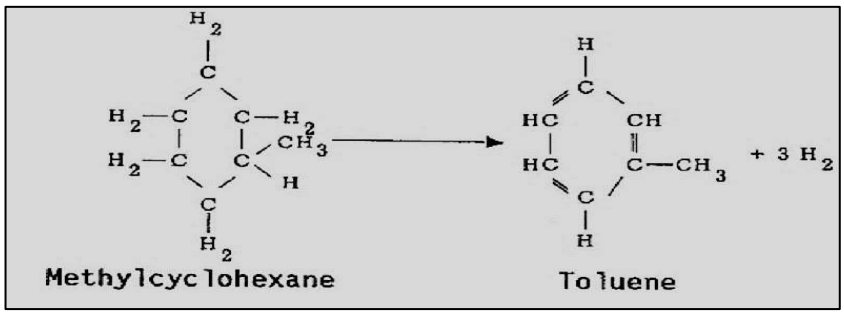

Figure 2.9 Simple Figure for naphthene dehydrogenation reaction (Gary *et al.* 2007)

2.7.2.2 Dehydrocyclization of paraffins to aromatic

Converting paraffins into aromatic compounds is the second most important reaction in the reactors of catalytic reforming units due to their importance in increasing the concentration of aromatic compounds and thus obtaining a high-octane number. These reactions are slow and need a longer residence time in the reactor because they go through steps, and as a result, they are endothermic. The reactions of converting branched paraffins into aromatic compounds are faster than the reactions of normal paraffins; in addition to that, the higher the number of carbon atoms, the higher the conversion rate; for example, the process of converting iso-hexane is more difficult than iso-octane. These reactions increase the concentration of aromatics and give at the same time hydrogen, which is redundant and can be used in other units. The reaction example is shown in Figure 2.10.

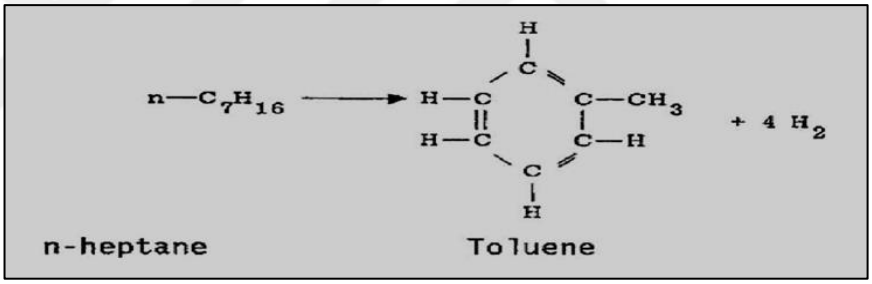

Figure 2.10 Simple figure for paraffin dehydrocyclization reaction (Gary *et al.* 2007)

2.7.2.3 Isomerization reactions

Isomerization reactions are important reactions that occur for paraffin compounds with a continuous chain, as well as in naphthenic compounds with a five-ring ring, where ordinary paraffins with a low octane number are converted into branched paraffins with a high-octane number, and these reactions are slow and heat-emitting. Hexagonal rings with a higher-octane number are also heat-emitting and faster than the isomerization reactions of paraffins. In the catalytic reforming units, the selectivity of the isomerization reactions of naphthenes is higher than that of paraffins, but the gain in paraffins is higher than 30, while in naphthenes, it almost does not exceed 10. The reaction example is shown in Figure 2.11.

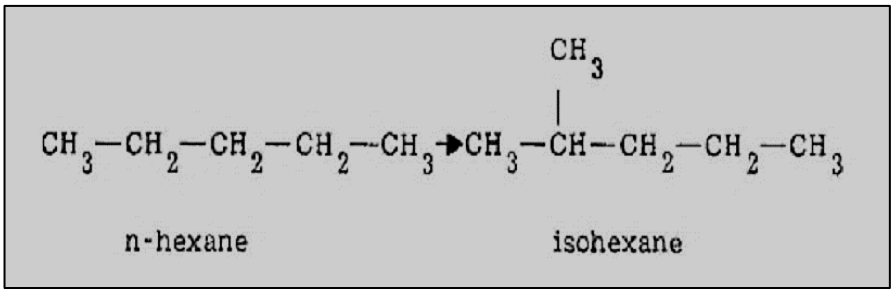

Figure 2.11 Simple figure for isomerization reaction (Gary *et al.* 2007)

2.7.2.4 Hydrocracking reactions

Hydrocracking reactions are considered undesirable because they lead to the loss of the final product and turn it into light gases with a low economic cost. These reactions are slow and need a longer time for them to occur, and they emit heat. As a result, the last reactor in the catalytic reform units has a small temperature difference due to the time required for these reactions to occur. The incidence of these reactions in normal paraffins is higher than that of branched paraffins and naphthenes, but these reactions help reduce coke deposition on the surface of the catalyst, which leads to the deactivation of the catalyst due to hot temperatures (high hardness of the process). An example of these reactions is shown in Figure 2.12 below.

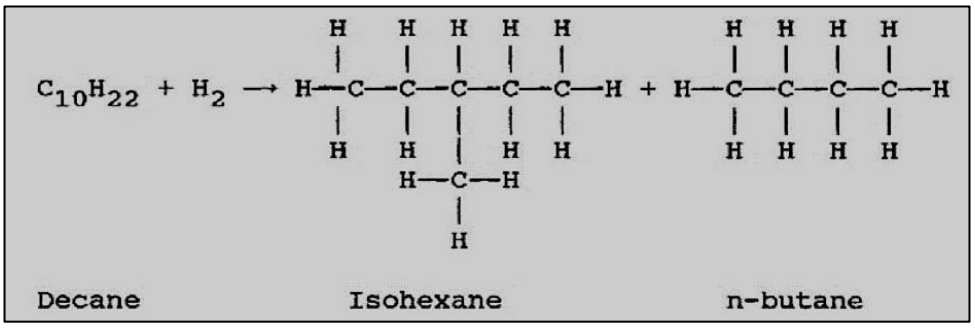

Figure 2.12 Example of paraffin hydrocracking reactions (Gary *et al.* 2007)

3. RESULTS AND DISCUSSION

This section will analyze the results of the simulation process of the operating conditions of the Naphtha Reformer Unit (800), which was conducted by AVEVA Pro/ii software, and compare them with the operational conditions to obtain ideal operating conditions for the Reformer Unit (800) within the actual data and normal operation conditions of the unit.

Equipment (reactors, furnaces, heat exchangers, compressors, separating vessels, pumps, and towers) are designed in commercial, industrial units within design operational limits and conditions that cannot be exceeded because this causes failure or malfunction of this equipment or in most cases can lead to a decrease in their efficiency and thus directly affect the quantity and quality of the product.

The simulation was conducted by changing the operational variables and their impact on the progress of the production process to reach a high-quality product in terms of (octane number, aromatic content, and hydrogen yield).

The simulation was conducted by changing the operational variables and their impact on the progress of the production process to reach a high-quality product in terms of (octane number, aromatic content, C^{5+} yield, and hydrogen yield).

3.1 Simulation of Variable Parameters Effect on Reaction Section

The reactors section is considered the most important and the first in the naphtha reforming units because it has the catalyst, which is the basis for determining the product's quality, specifications, and quantity (Reformate). In addition, the catalyst is extremely sensitive to any change in all the previously mentioned operational conditions. Therefore, the effect of changing the operating conditions on the catalyst was studied as follows:

3.1.1 Reactors inlet temperature (RiT)

Through the simulations that were conducted, we note that the increase in the temperature of the feed entering the reactors leads to an increase in the rate of all reactions, which we notice affects the quality and quantity of the product leaving the unit as follows:

- **Temperature influence on aromatic content**

Conclude from Figure 3.1 below when increasing the temperature of the feedstock entering the reactors (increasing the reaction temperature) leads to an increase in the rate of the reactions of converting naphthenic compounds into aromatic compounds, and this leads to a rise in the concentration of aromatic compounds. Because these reactions are fast and highly endothermic, this leads to a decrease in the heat leaving (increased delta temperature), especially in the first reactor.

In addition, as reactions of converting paraffinic compounds to cyclic naphthenic compounds and then their conversion to aromatics, these reactions are also endothermic. However, they are slow, so the possibility of these reactions occurring in the second reactor and more converting in the third reactor is due to the availability of residence time inside the reactor because of the large volume of the reactor. During the simulation process, it was seen that the branched paraffins are converted more than the normal paraffins into naphthenic compounds.

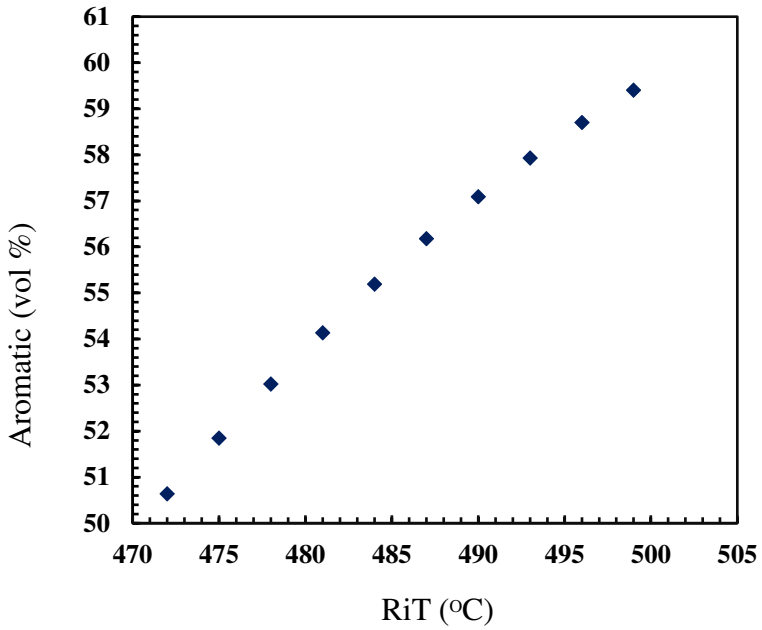

Figure 3.1 RiT vs. Aromatic content (vol. %)

It is clear from Figure 3.1 that the results of the simulation process are positive and that whenever the temperature rises, we will get a higher aromatic content, which is a positive result.

- **Temperature effect (RiT) on RON**

The main objective of the naphtha reforming units is to raise the octane number of heavy naphtha; conclude from Figure 3.2 below that if it is required to obtain a high octane number, then the reaction temperature must be increased inside the reactors, which will lead to an increase in the conversion of naphthenic compounds to aromatics, in addition to the transformation of paraffin chains into cyclic and then into aromatic This leads to an increase in the concentration of these compounds that have a high octane number, which leads to an increase in the octane number of the final product (Reformate). Aromatic compounds have a customized feature: when mixed, their octane number will differ from the pre-mixing, either in the direction of increase or decrease.

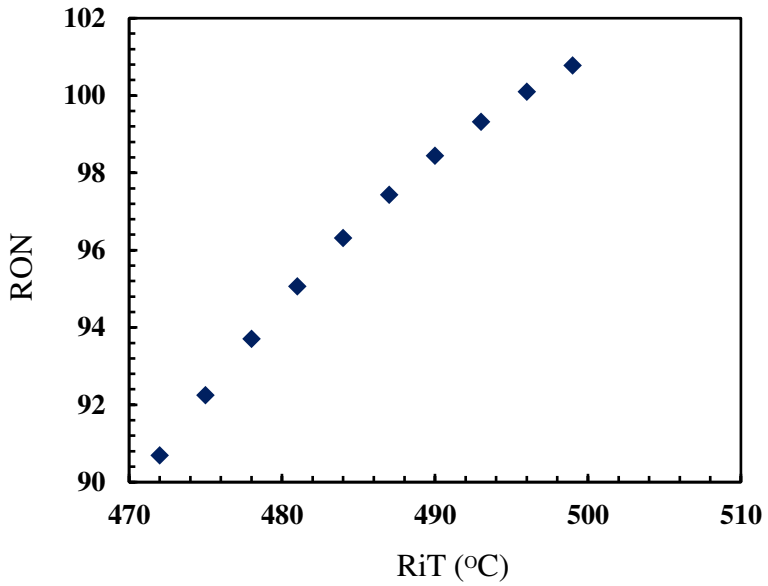

Figure 3.2 RiT vs. RON in reformate product

It is clear from Figure 3.2 that an increase in the octane number is directly proportional to the rise in temperature, which is considered a positive result in the simulation process.

- **Temperature effect (RiT) on C^{5+} yield (wt. %)**

The cracking reactions are heat-emitting, but they are slow rate and therefore notice its effect in the second and third reactors because of the availability of more residence time. The simulation showed that the regular paraffin chains are more susceptible to these reactions than the rest of the hydrocarbon compounds. The liquefied petroleum compounds that occur because of cracking reactions have a low economic cost, in addition to causing an increase in the vapour pressure of the product. Therefore, they need special storage operations and cause problems inside the engines. The temperature effect is shown in Figure 3.3 below:

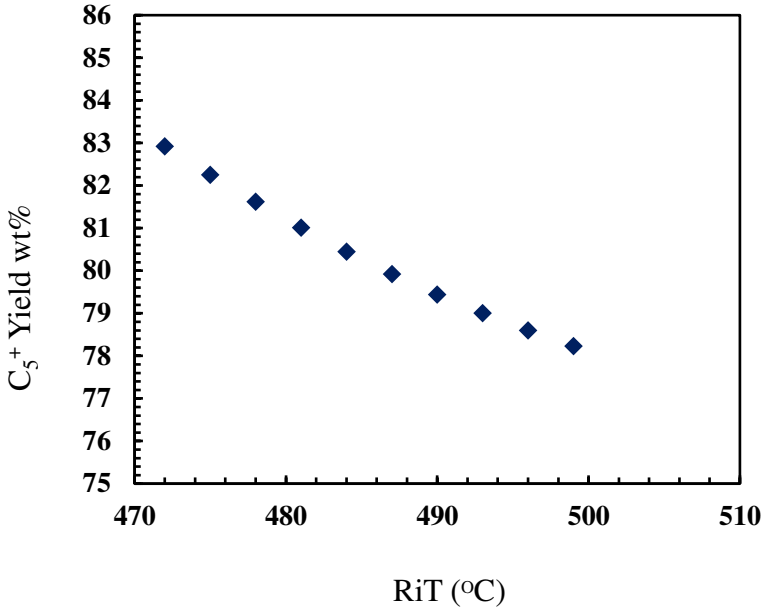

Figure 3.3 RiT vs. C^{5+} yield in (wt. %)

Concluding from that, increasing the temperature of the reactions will lead to minimizing the quantity of the product as well as a decrease in the quality of the product, i.e. (reducing compounds with several carbon atoms of 5 or more), and this is a result of the increase in the hydrocracking reactions and the conversion of hydrocarbons into light petroleum compounds.

- **Temperature effect on H_2 yield (wt. %)**

We conclude from the Figure below that an increase in the temperature of the reactions will lead to an increase in the production of hydrogen, which is used in desulfurization and hydrocracking units. Due to reactions, aromatic production by naphthene dehydrogenation releases 4 moles of hydrogen and gives more excess hydrogen.

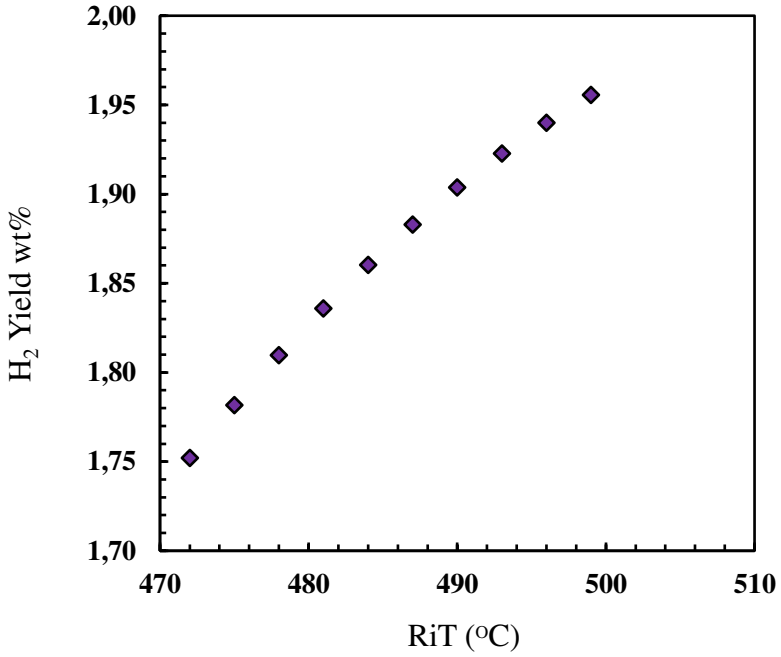

Figure 3.4 RiT vs. H_2 yield (wt. %)

The production of hydrogen in the reactors will increase this considered good and lead to a reduction of coke deposit on the catalyst's surface, thus keeping its efficiency and increasing the cycle life of the catalyst.

3.1.2 Pressure

Pressure is one of the important operating conditions that have a direct impact on the progress of the operational process through a direct impact on the efficiency of all equipment, taking into account that each piece of equipment has fixed limits that cannot be exceeded pressure, and from this point of view, in the process of repairing naphtha, the pressure in the part of the reactors is more; as a result, other equipment has fixed pressure limits, and as a result of this, a study was conducted to find out the effect of pressure inside the reactors employing the simulation program, and the following conclusions were reached:

- **Pressure effect on aromatic content**

The increase in partial pressure of all hydrocarbon compounds increases the kinetics of all reactions in the positive direction of the reactions that increase the concentration of aromatics, as shown in Figure 3.5 below.

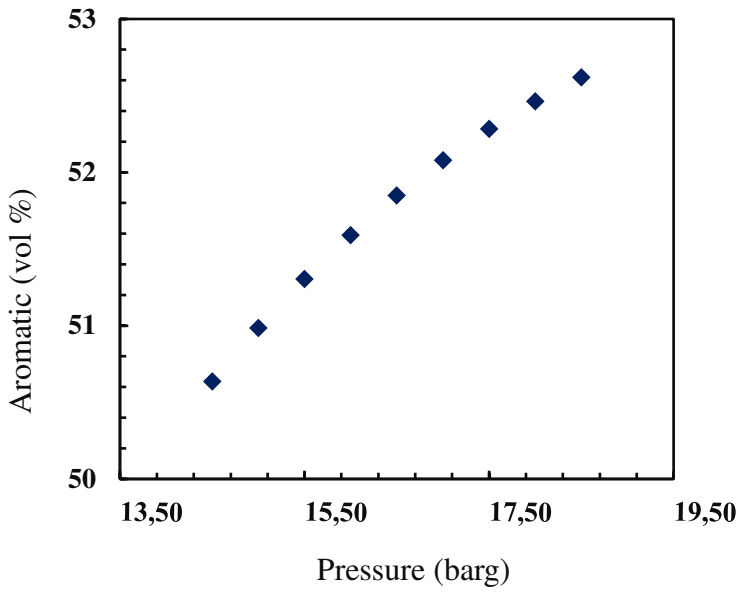

Figure 3.5 Pressure at reaction section on aromatic content (vol %)

Concluding from Figure 3.5 that, aromatic content increased with the pressure inside the reactor, this is considered a positive case.

- **Pressure effect on RON**

Concluding from Figure 3.6 below, because of the increase in the aromatic content, it is normal to notice a rise in the value of the octane number with the rise in pressure inside the reactors, and this indicator is positive.

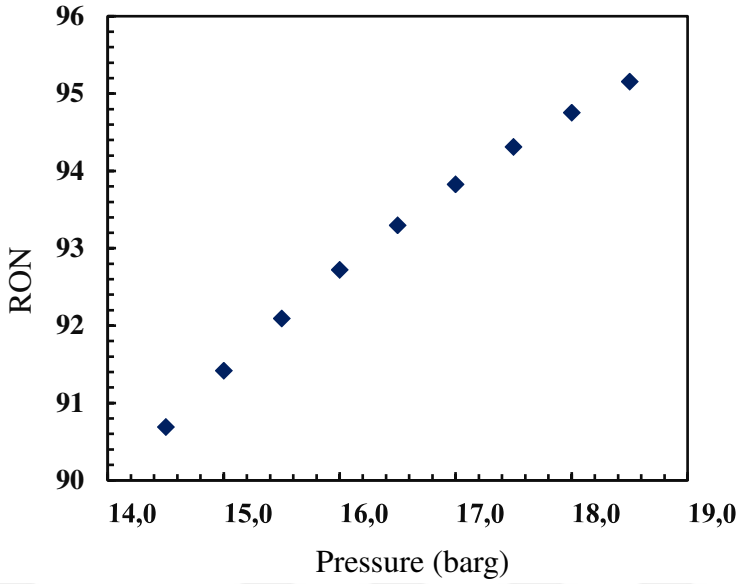

Figure 3.6 Effect of pressure at reaction section on RON in reformate

This case considers reliable results from the simulation process and can be used to predict the effect of increasing the pressure in reactors.

- **Pressure effect on C_5^+ yield (wt. %)**

From Figure 3.7 at the bottom, we conclude that increasing the pressure, especially inside the reactors, will lead to an increase in the rates of hydrogen cracking reactions due to the increase in the partial pressure of hydrogen, which leads to a decrease in the amount of the product (reformate) and an increase in light hydrocarbon compounds, and this result is considered undesirable.

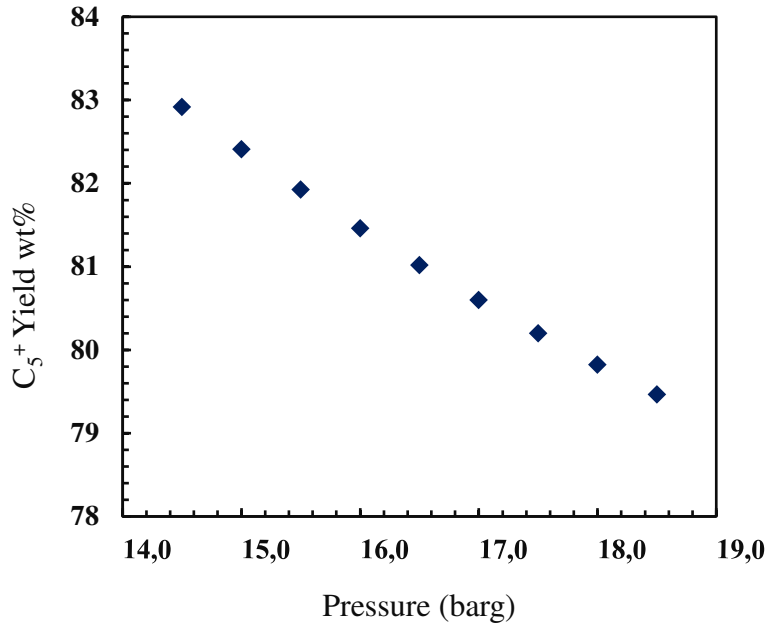

Figure 3.7 Influence of pressure at reaction section on C_5^+ yield by (wt. %)

This case could be better and lead to a loss of product yield, so any increase in pressure must be careful and limited.

- **Pressure effect on H_2 yield (wt. %)**

Increasing the pressure, as we mentioned earlier, will raise the partial pressure of hydrogen, leading to an increase in the rates of hydrogen cracking reactions, which are faster than the reactions of converting paraffins into cyclic compounds that consume hydrogen. Therefore, we will notice a decrease in the purity of the hydrogen produced and the purity of hydrogen in the recycled gas shown in Figure 3.8 below.

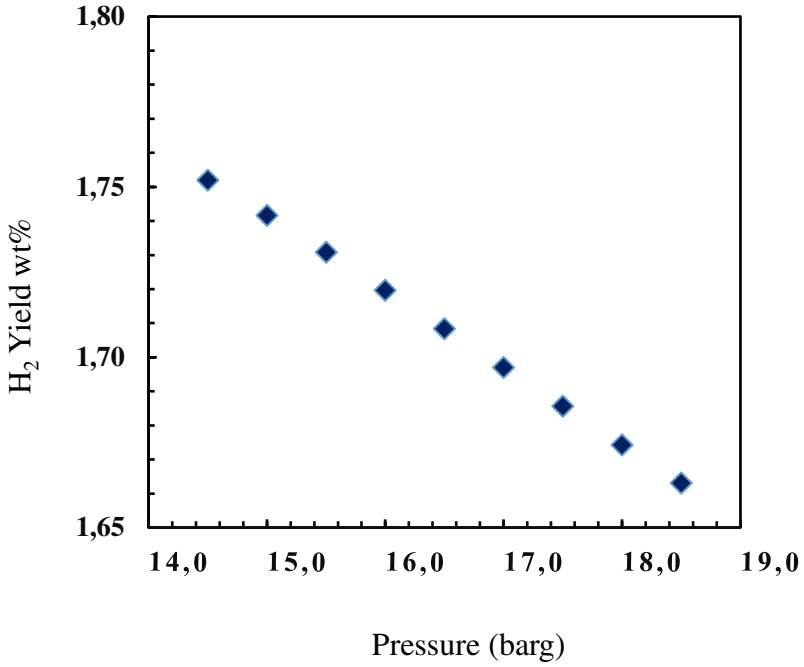

Figure 3.8 Pressure vs. H_2 Yield (wt. %)

This case is not good, so the pressure in reactors must be decreased to prevent hydrogen product loss.

3.1.3 Recycle gas quantity (RG).

Injecting hydrogen-rich recycled gas into the feedstock stream is especially important because it homogeneously distributes the feedstock (heavy naphtha) within furnaces, heat exchangers, and reactors and regulates heat transfer as it passes through equipment and lines. Therefore, the main goal of the reinjection of hydrogen-containing gas is to prevent the coking of heavy naphtha on the catalyst's surface and inside the furnace tubes because of the hot temperatures. Gas recycling with heavy naphtha directly impacts the reaction kinetics in the reactors section. Through simulation, the following results were reached:

- **Recycle gas effect on aromatic content**

Figure 3.9 at the bottom show increasing the amount of recycled gas will lead to an increase in the value of the H_2/HC ratio, and this means an increase in the partial pressure of hydrogen, as it will lead to a decrease in the rate of reactions to convert paraffinic compounds into cyclic (naphthenic) compounds.

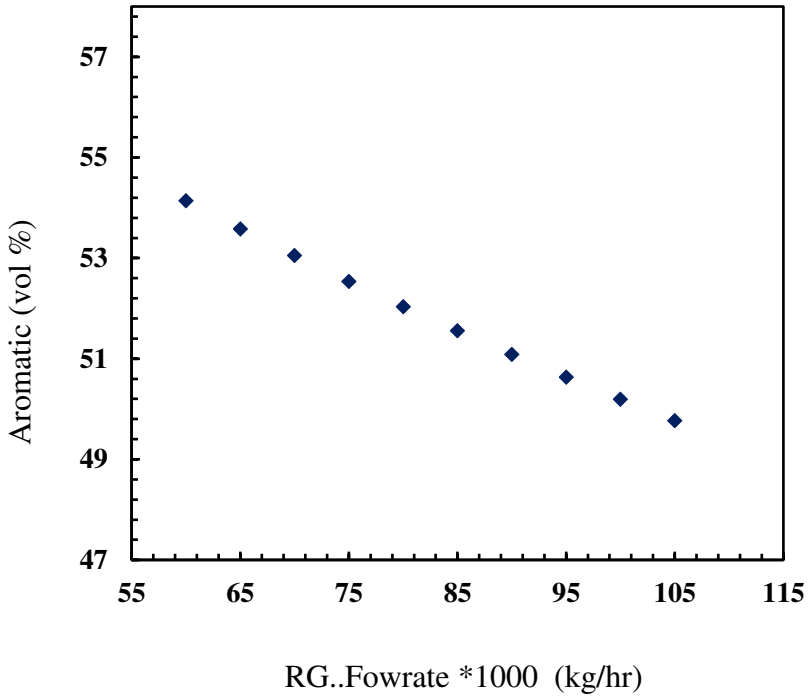

Figure 3.9 RG quantity influence on aromatic content (vol %)

This case considers good because the RG quantity must be decreasing to prevent any loss of aromatic content in the reformate; at the same time, a decreased RG quantity means a decreased speed of the compressor, which will decrease steam consumption and save the efficiency of the compressor.

- **Recycle gas quantity effect on RON.**

Increasing the amount of hydrogen injected (recycle gas) with the feedstock affects the decrease in the value of the octane number due to the decrease in the percentage of aromatic compounds in the product, which we have explained the reason for the decrease in its percentage, but this decrease is rather simple and not severe, as shown in Figure 3.10 below:

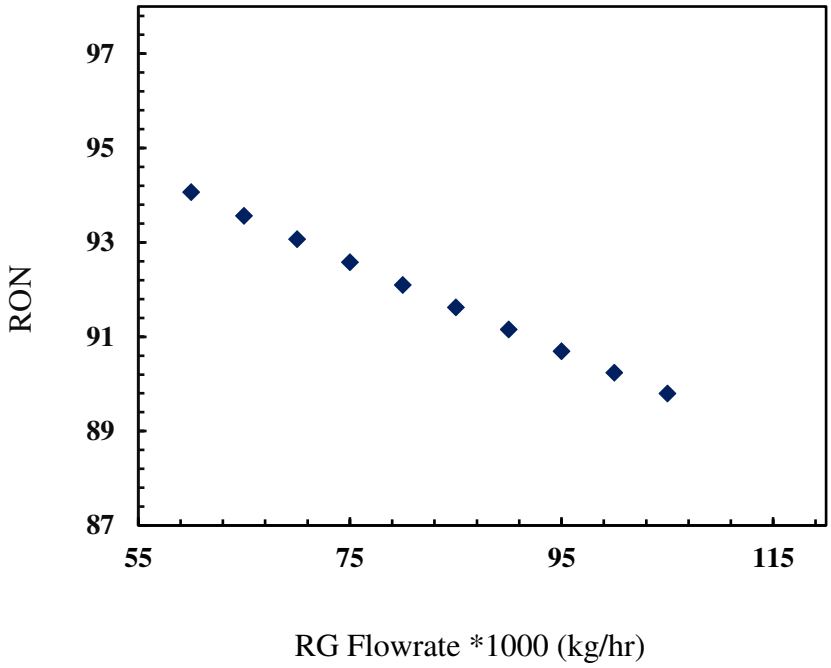

Figure 3.10 RG quantity effect on RON in reformate

Again, recycling gas quantity must be decreased to get more research on octane number and save compressor and steam consumption efficiency. Decrease recycling gas compressor speed will lead to decrease pressure in reactors.

- **Recycle gas effect on C_5^+ yield (wt. %)**

From Figure 3.11 below, through simulation, we notice that raising the value of the H_2/ HC ratio has a limited effect, which causes a slight increase in the desired production

quantity, and this is due to the decrease in the rate of reactions of the paraffin chains to naphthenic compounds.

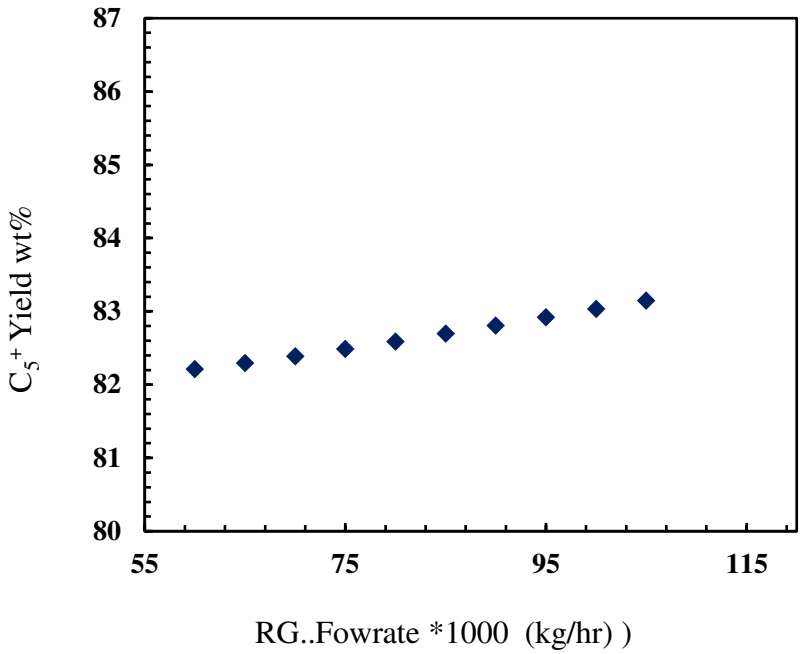

Figure 3.11 RG vs. C_5^+ yield (wt. %)

This case is considered good but effect not too much, so it may not need to increase recycling gas quantity and lead to an increase in a load of heat consumption in furnaces.

- **Recycle gas quantity (RG) effect on H_2 yield (wt. %)**

From Figure 3.12, notice that raising the H_2/HC ratio by increasing the amount of recycled gas will decrease the amount of hydrogen produced, also due to the low kinetics of the conversion reactions of the paraffin chains to naphthenic compounds and then to aromatic compounds.

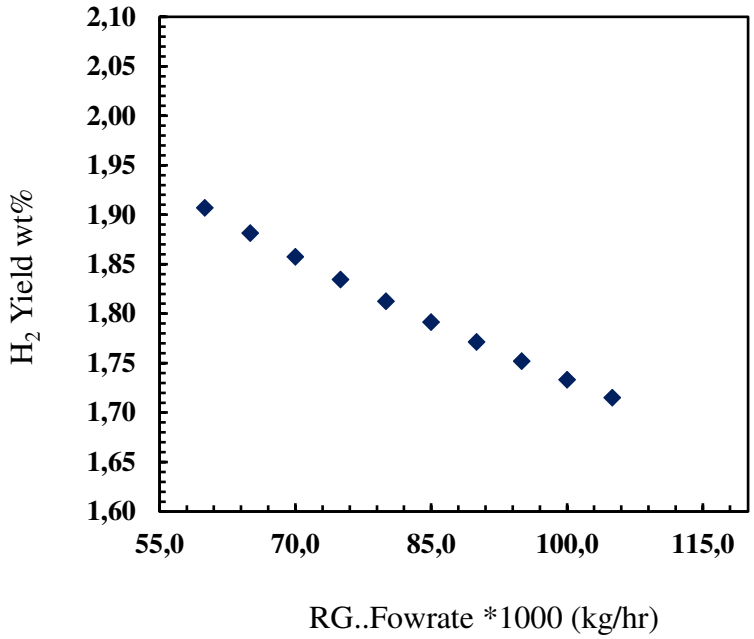

Figure 3.12 RG quantity vs. H_2 yield by (wt. %)

It is considered a negative case because it increases pressure in reactors and leads to hydrogen consumption in cracking reactions.

3.1.4 Feed flowrate (space velocity)

The severity of the operational process can be defined as the high temperature of reactions inside reactors compared to a constant quantity of feed. In other words, if the temperature increases while keeping the amount of feedstock the same, the severity of the operational process increases. The impact severity of operating conditions is clear in reactors conditions. Increasing the severity of the process reduces the life of the catalyst, so every increase in the temperature of the reactors must be matched by an increase in the feedstock. The effect of increasing the amount of feedstock on the quantity and quality of reformate produced from the naphtha reforming unit was studied as follows:

- **Feed effect on aromatic content (vol %)**

From Figure 3.13 at the bottom, we conclude that increasing the amount of feedstock entering the reactors at a constant reaction temperature leads to a decrease in the aromatic content in the final product. The insufficient heat needed to increase the kinetics of the reactions that increase the aromatic content because of the increase in compound concentrations leads to a decrease in the aromatics content compared to other compounds.

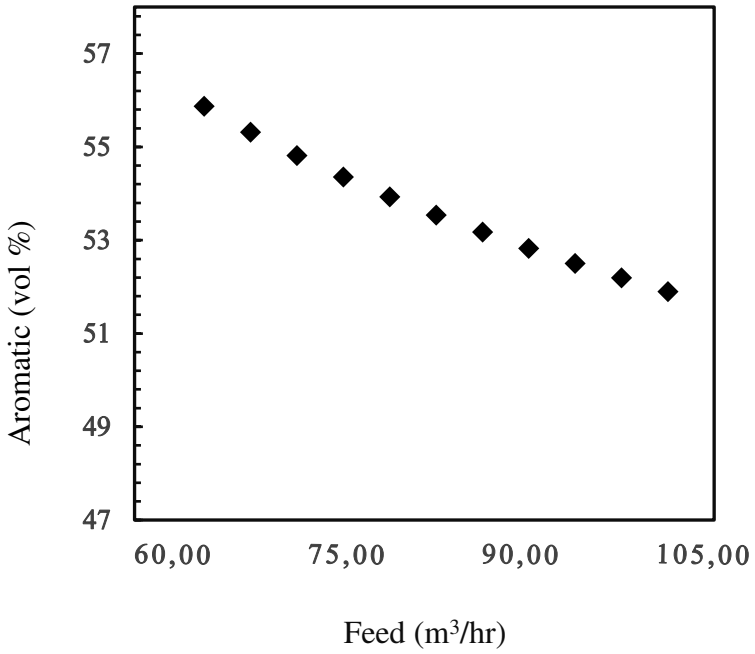

Figure 3.13 Feed flow influence on aromatic content by (vol %)

In nature, the case when increasing feed quantity at constant temperature will decrease aromatic content, so this case is not good. To solve this problem, the temperature of reactors must increase or decrease feed quantity.

- **Feed flowrate effect on RON**

As a result of the decrease in the aromatic content, the octane number will naturally decrease, and this decrease has an inverse relationship with the increase in the amount of feedstock at a constant temperature in the reactors, as shown in Figure 3.14.

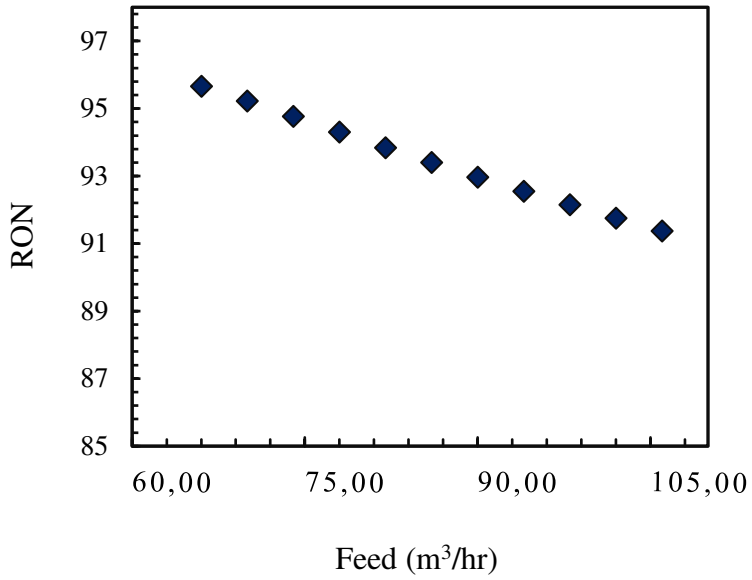

Figure 3.14 Feed flowrate vs. RON of reformate at constant temperature

Any increase in feed quantity will decrease RON in reformate products at a constant temperature, so we must increase feed temperature (more heat in furnaces) to reach the proper level of RON.

- **Feed flowrate effect on C_5^+ yield (wt. %)**

Increasing the amount of feed entering the reactors leads to an increase in the content of the desired compounds in the final product, and this is due to a decrease in the hydrocracking reactions for all hydrocarbon compounds (paraffins and naphthenes) as shown in the Figure 3.15.

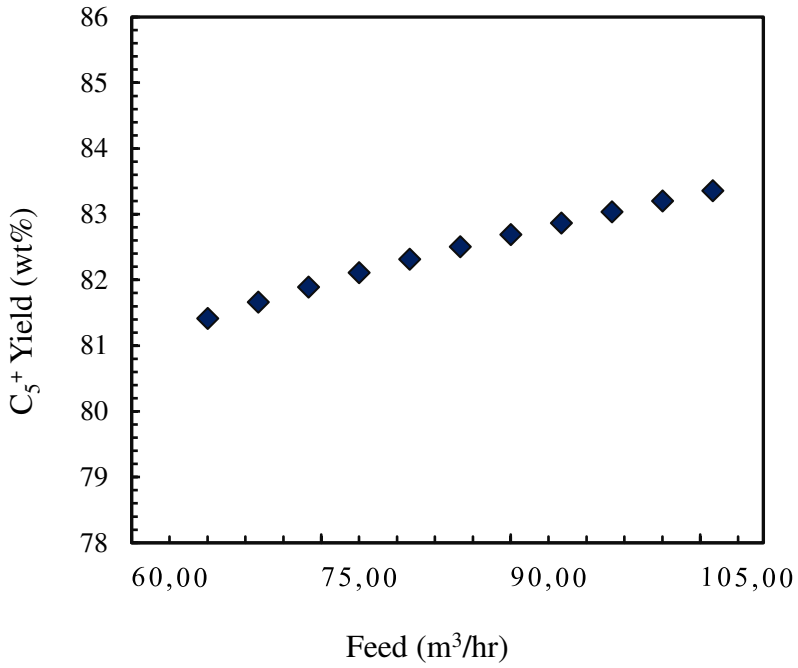

Figure 3.15 Feed flow vs. C_5^+ yield by (wt. %)

Normally any increase in feed quantity will lead to an increase desired product so that the simulation can predict the percentage of that increase.

- **Feed effect on H_2 yield (wt.%)**

The amount of hydrogen produced from the unit is affected by the increase in the amount of feed, as this increase affects the rate of dehydrogenation reactions from naphthene compounds, which have a direct effect on the amount of hydrogen produced, in addition, down rate converting paraffins to naphthenes by dehydrocyclization reactions which release hydrogen because the temperature in reactors not enough as shown in the Figure 3.16.

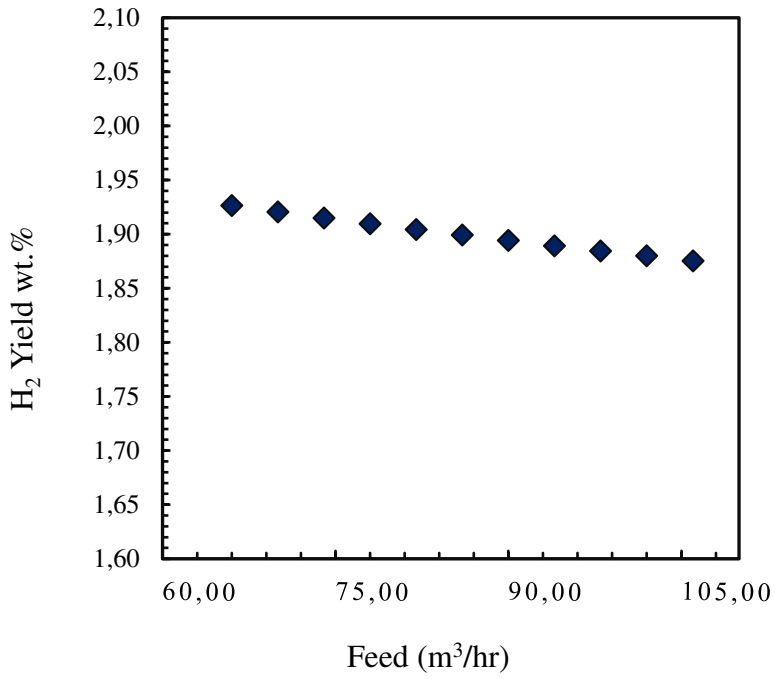

Figure 3.16 Feed flowrate vs. H_2 yield by (wt. %)

When increasing quantity of feed increases at a constant temperature, hydrogen produced will decrease because it needs more heat to reach the desired product.

3.2 Optimization

The optimization tool in the program was used to perform the optimization process on the operating conditions of the naphtha reforming process to obtain a high-octane number, and this process was done by entering the operational variables required for optimization to the tool; in addition to that the required constraints were entered for the optimization results to be realistic. Actual, simulation and optimization data are given in Table 3.1 and different simulation and optimization results are given Figure 3.17.

Feed= 80 m^3/hr,

Reactors inlet Temperature (RiT)= 472 ºC

Table 3.1 Actual, simulation and optimization data results

Parameters	**units**	**Actual**	**Simulation**	**Optimization**
Hydrogen rich gas injection (quantity)	kg/hr	90000	90000	60000
Low Pressure Separation (temperature)	ºC	39	40	40
Stabilizer Pressure	barg	17	18	17
High-Pressure separation Temperature	ºC	42.5	43	43
RON		**90.5**	**90.8**	**93.7**

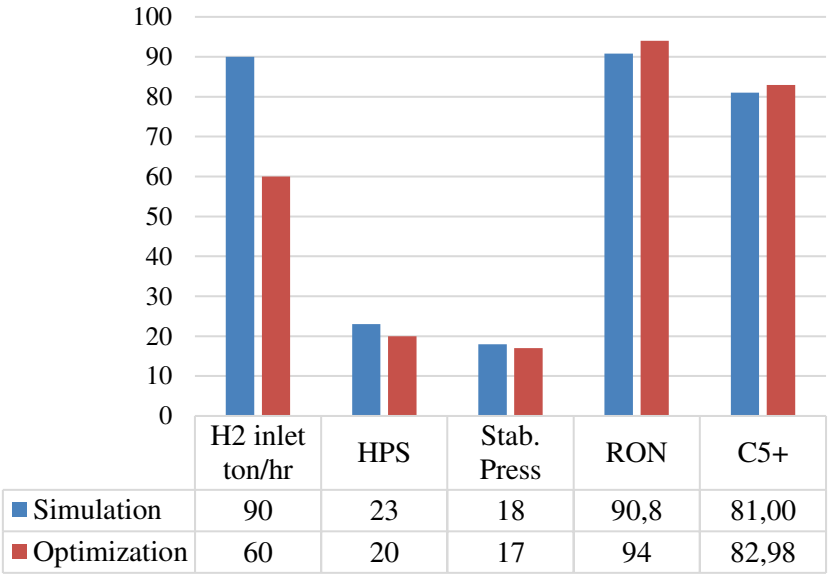

Figure 3.17 The different between simulation and optimization results.

4. CONCLUSION AND RECOMMENDATION

In this study, a simulation of the heavy naphtha reforming process was done by using the AVEVA PRO/II program. The model proposed agrees very well with the actual data from the naphtha reforming unit in the Salah Al-din\2 refinery. It can be used in this model to select optimum operating conditions. In addition, it can be used to predict reformate octane number and desired product yield (C^{5+}) at any time. Other products include hydrogen product yield and LPG liquid from naphtha reforming unit 800.

The temperature of the reactors is within the permissible limits depending on the octane number required for the final product. Therefore, it was concluded that when there is a need to raise the octane number one degree, it needs to raise the reactor inlet temperature (RiT) by 2.6 ºC. The pressure inside the reactors must be high, so it must be raised to the permissible limits of the reactor design 18 barg. The amount of recycled gas is as low as possible because this will give reliable results regarding the octane number. In addition, it will reduce the amount of fuel gas used in the furnace.

The optimization was made on the operational conditions of the naphtha reforming process to obtain a high octane of the product at a constant temperature for the naphtha entering the reactors, in addition to constraining the optimization by introducing a range for C_5^+, not less than 80% relative to the amount of naphtha entering the reactors. The optimization results were an increase in the octane number from 90.6 to 93.7 and the optimum amount of gas entering with naphtha from 90 tons/hr to 60 tons/hr.

One of the benefits resulting from the improvement process is the decrease in the amount of energy consumed in the naphtha reforming unit, according to the following Table 4.1 below.

Table 4.1 Energy amount different between simulation and optimization.

	Unit	**Simulation**	**Optimization**	**Recovery %**
Duty	M*KJ/hr	333.213	271.6759	18.467 %
Work	KW	1769.1649	1365.1054	22.838 %

This difference in the amount of energy results from reducing the return gas, which requires more energy to reach the required heat from the furnaces. In addition, the decrease in the amount of working energy is located specifically in the turbine compressor because of reducing the amount of return gas, and this reduces the required energy consumption and thus reduces the amount of steam consumption used to operate the turbine compressor 807JT.

REFERENCES

Anabtawi, J., Redwan, D., Al-Jarallah, A., and Aitani, A. 1991. Advances in the chemistry of catalytic reforming of naphtha. Fuel science & technology international, 9(1): 1-23.

Ancheyta, J. 2011. Modeling and simulation of catalytic reactors for petroleum refining. 511 page, John Wiley and Sons.

Antos, G. J., and Aitani, A. M. 2004. Modeling Catalytic Naphtha Reforming. In Catalytic Naphtha Reforming, Revised and Expanded pp. 519-561, CRC Press.

Antos, G. J., Aitani, A. M., and Parera, J. M. 1995. Catalytic naphtha reforming: science and technology. 529 page, Marcel Dekker Inc.

Askari, A., Karimi, H., Rahimi, M. R., and Ghanbari, M. 2012. Simulation and modeling of catalytic reforming process. Petroleum & Coal, 54(1): 76-84.

Babaqi, B. S., Takriff, M. S., Kamarudin, S. K., Othman, N. A., and Ba-Abbad, M. M. 2016. Comparison of catalytic reforming processes for process integration opportunities: Brief Review. Int. J. Appl. Eng. Res, 11: 9984-9989.

Bayomie, O. S., Abdelaziz, O. Y., and Gadalla, M. A. 2019. Exceeding Pinch limits by process configuration of an existing modern crude oil distillation unit–A case study from refining industry. Journal of Cleaner Production, 231: 1050-1058.

Behin, J., and Kavianpour, H. R. 2009. A comparative study for the simulation of industrial naphtha reforming reactors with considering pressure drop on catalyst. Pet. Coal, 51(3): 208-215.

Bommannan, D., Srivastava, R., and Saraf, D. 1989. Modelling of catalytic naphtha reformers. The Canadian Journal of Chemical Engineering, 67(3): 405-411.

Chernyakova, E. S., Koksharov, A. G., Ivanchina, E. D., and Yakupova, I. V. 2015. Heavy naphtha fractions 85-155 C recycling in the catalytic reforming industrial unit. Procedia Chemistry, 15: 378-383.

Ciapetta, F., and Wallace, D. 1972. Catalytic naphtha reforming. Catalysis Reviews, 5(1): 67-158.

Edgar, M. D. 1983. Catalytic reforming of naphtha in petroleum refineries. In Applied Industrial Catalysis pp. 123-148, Elsevier.

Eiman, A. 2008. Improvement of gasoline octane number by blending gasoline with selective components MSc. Thesis, University of Technology, 99 page, Republic of Iraq.

Elizalde, I., and Ancheyta, J. 2015. Dynamic modeling and simulation of a naphtha catalytic reforming reactor. Applied Mathematical Modelling, 39(2): 764-775.

Fahim, M. A., Al-Sahhaf, T. A., and Elkilani, A. 2009. Fundamentals of petroleum refining. 485 page, Elsevier.

Fioroni, G. M., Rahimi, M. J., Westbrook, C. K., Wagnon, S. W., Pitz, W. J., Kim, S., and McCormick, R. L. 2022. Chemical kinetic basis of synergistic blending for research octane number. Fuel, 307: 121865.

Gary, J. H., Handwerk, J. H., Kaiser, M. J., and Geddes, D. 2007. Petroleum refining: technology and economics. 442 page, CRC press.

Ghasem, N. 2021. Computer methods in chemical engineering. 474 page, CRC Press.

Grau, J. M., and Parera, J. M. 1989. Naphtha reforming capacity of catalysts with different metallic functions. Industrial & engineering chemistry research, 28(11): 1596-1600.

Ibrahim, D. 2018. Optimal Design of Flexible Heat-integrated Crude Oil Distillation Systems. 24 page, The University of Manchester (United Kingdom).

Ibrahim, D., Jobson, M., Li, J., and Guillén-Gosálbez, G. 2018. Optimization-based design of crude oil distillation units using surrogate column models and a support vector machine. Chemical Engineering Research and Design, 134: 212-225.

Iranshahi, D., Karimi, M., Amiri, S., Jafari, M., Rafiei, R., and Rahimpour, M. R. 2014. Modeling of naphtha reforming unit applying detailed description of kinetic in continuous catalytic regeneration process. Chemical Engineering Research and Design, 92(9): 1704-1727.

Jones, D. S., and Pujadó, P. P. 2006. Handbook of petroleum processing. 1900 page, Springer Science & Business Media.

Kang, J. S. 2005. Integration of provision-PRO/II computer simulation into laboratory experiments. 78 page, The Cooper Union for the Advancement of Science and Art.

Meyers, R. A. 2016. Handbook of petroleum refining processes. 832 page, McGraw-Hill Education.

Miranda-Galindo, E. Y., Segovia-Hernández, J. G., Hernández, S., and Bonilla-Petriciolet, A. n. 2014. Multiobjective optimization of a hydrodesulfurization process of diesel using distillation with side reactor. Industrial & engineering chemistry research, 53(42): 16425-16435.

Mohaddecy, R. S., and Sadighi, S. 2014. Developing a steady-state kinetic model for industrial scale semi-regenerative catalytic naphtha reforming process. Kemija u industriji: Časopis kemičara i kemijskih inženjera Hrvatske, 63(5-6): 149-154.

Mohaddecy, R. S., and Sadighi, S. 2014. Modeling catalytic naphtha reforming process using discrete lumping approach. 309-320.

Mohaddecy, S. R. S., Sadighi, S., and Bahmani, M. 2008. Optimization of catalyst distribution in the catalytic naphtha reformer of Tehran Refinery. Petroleum & Coal, 50(2): 60-68.

Oyekan, S. O. 2018. Catalytic Naphtha Reforming Process. 360 page, CRC Press.

Pieck, C., Sad, M., and Parera, J. 1996. Chlorination of Pt–Re/Al2O3 during naphtha reforming. Journal of Chemical Technology & Biotechnology: International Research in Process, Environmental AND Clean Technology, 67(1): 61-66.

Rahimpour, M. R., Jafari, M., and Iranshahi, D. 2013. Progress in catalytic naphtha reforming process: A review. Applied energy, 109: 79-93.

Ravi, R., Vinu, R., and Gummadi, S. N. 2017. Coulson and Richardson's Chemical Engineering: Volume 3A: Chemical and Biochemical Reactors and Reaction Engineering. 596 page, Butterworth-Heinemann.

Said-Aizpuru, O., Allain, F., Diehl, F., Farrusseng, D., Joly, J.-F., and Dandeu, A. 2020. A naphtha reforming process development methodology based on the identification of catalytic reactivity descriptors. New Journal of Chemistry, 44(18): 7243-7260.

Santos, R. N., Lima, E. R., and Paredes, M. L. 2021. ASTM D86 distillation curve: Experimental analysis and premises for literature modeling. Fuel, 284: 118958.

Shakoor, Z. M. 2011. Catalytic reforming of heavy naphtha, analysis and simulation. Diyala Journal of Engineering Sciences, 4(2): 86-104.

Shakor, Z. M., AbdulRazak, A. A., and Sukkar, K. A. 2020. A detailed reaction kinetic model of heavy naphtha reforming. Arabian Journal for Science and Engineering, 45(9): 7361-7370.

Smolkova-Keulemansova, E., and Feltl, L. 1991. Analysis of substances in the gaseous phase. 479 page, Elsevier.

Talaghat, M., and Karimi, M. 2020. Operation parameters effect on yield and octane number for monometallic, bimetallic and trimetallic catalysts in naphtha reforming process. Energy Sources, Part A: Recovery, Utilization, and Environmental Effects, 42(2): 176-193.

Taskar, U., and Riggs, J. B. 1997. Modeling and optimization of a semiregenerative catalytic naphtha reformer. AIChE Journal, 43(3): 740-753.

Vathi, G. P., and Chaudhuri, K. K. 1997. Modelling and simulation of commercial catalytic naphtha reformers. The Canadian Journal of Chemical Engineering, 75(5): 930-937.

Wang, K., Zhang, B., and Chen, Q. 2016. Optimization of a crude oil distillation unit based on total-process simulation. In Computer Aided Chemical Engineering Vol. 38, pp. 2163-2168, Elsevier.

Yang, K., Liu, S., He, C., Zhang, B., Chen, Q., and Pan, M. 2020. Improving energy saving of crude oil distillation units with optimal operations. Journal of Cleaner Production, 263: 121340.

Yusuf, A. Z., Aderemi, B., Patel, R., and Mujtaba, I. M. 2019. Study of industrial naphtha catalytic reforming reactions via modelling and simulation. Processes, 7(4): 192.

Yusuf, A. Z., John, Y. M., Aderemi, B. O., Patel, R., and Mujtaba, I. M. 2020. Effect of hydrogen partial pressure on catalytic reforming process of naphtha. Computers & Chemical Engineering, 143: 107090.

APPENDICES

APPENDIX 1. Optimization results data for main streams

Stream No.		**1**	**2**	**18**	**24**	**25**	**23**
Stream Description		**Feed**	**H_2- RG**	**H_2 product**	**OVH Gases**	**LPG**	**Reformate**
Temperature	^{O}C	50	60	68.0	35.8	35.8	43
Pressure	barg	27	16.0721	32	16.5	16.5	7.7
Liquid Act. Rate (vol)	m3/hr	92.92	-	-	-	6.35	72.299
Total Std. Liq. Rate [at 1 atm, 15.56 C]	m3/hr	90	222.8	29.7	3.41	6	70.2
Flowrate	kg-mol/hr	607.60	5205.18	738.84	44.45	65.42	564.58
Total Mass Rate	kg/hr	66510.	60000	7072.013	1484.5	3092.24	54861.44
Paraffin Content (Total)	-	70.428	99.39	99.49752	99.994	99.96	42.65148
Paraffin Content (ISO)	-	26.103	8.04	5.74	8.74	22.29	28.69
Naphthene Content	-	16.621	0.061	0.036	-	-	1.339
Aromatics (Total)	-	12.756	0.506	0.42	-	-	55.43
Research Octane Number (RON)		44.031	12.92	8.89	14.19	38.208	95.74
RVP (default)	psi	1.9813	-	-	784.24	183.84	8.04
Liquid Std. Density	kg/m3	739.00	-	-	-	515.37	780.66
Total Std. Vap. Rate [at 1 atm, 0 C]	m3/hr	13618.	116669	16560.41	996.48	1466.44	12654.56

APPENDIX 2. Actual and simulation Distillation data for Feed and Reformate streams

Stream Name	**FEED**		**REFORMATE**	
ASTM D86	Actual	simulation	Actual	simulation
1%	87	65.95	33	16.20
5%	96	85.99	51	48.85
10%	100	92.61	62	59.34
30%	110	107.17	92	93.30
50%	119	123.69	111	110.83
70%	130	134.24	131	131.60
90%	143	148.54	154	157.46
95%	148	157.84	165	162.75
98%	155	162.66	176	170.86

APPENDIX 3. Bi- Product streams data out from unit 800

Stream Name		**18**		**24**		**25**	
Description		**H_2 product**		**OVH Gases**		**LPG**	
		Actual	Simulation	Actual	Simulation	Actual	Simulation
Temperature	^oC	80	66.89	37	38.36	36.5	38.36
Pressure	barg	31.5	32.00	17.5	17.50	17.5	17.50
Liquid Act. Rate (vol)	m^3/hr	-	-	-	-	7	6.41
Total Std. Liq. Rate [at 1 atm, 15.56 C]	m^3/hr		-		-	-	6.00
Flowrate	kg-mol/hr	-	498.76	-	39.21	-	65.37
Total Mass Rate	kg/hr	4710	4628.46	1000	1301.32	3100	3097.38
Liquid Std. Density	kg/m^3	-	-		-	530	516.23
Vapor Std. Density	kg/m^3	0.373	0.385	1.387	1.48	-	-

APPENDIX 4. Actual and simulation data for reformate composition (mol%)

Group	paraffins		iso-paraffins		Naphthene		Aromatics		Olefins		sum	
	Actual	Simulation	Actual	Simulation	Actual	Simulation	Actual	Simulation	Actual	Simulation	Actual	Simulation
C_1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
C_2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
C_3	0.2710	0.6919	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.2710	0.6919
C_4	3.3607	3.9804	1.9918	3.3737	0.0000	0.0000	0.0000	0.0000	0.0227	0.0000	5.3752	7.3541
C_5	4.5450	4.9136	5.8828	4.5368	0.2074	0.1614	0.0000	0.0000	0.0966	0.0848	10.7317	9.6965
C_6	3.7223	2.8600	8.8975	7.6378	0.2997	0.2764	2.6614	2.7183	0.1119	0.1474	15.6928	13.6399
C_7	2.5639	2.6177	8.9565	8.3750	0.5403	0.6035	12.2946	12.1802	0.1692	0.2295	24.5245	24.0059
C_8	1.0165	0.9681	4.3142	3.8630	0.6308	0.5883	19.3078	20.6680	0.0000	0.0059	25.2693	26.0932
C_9	0.2089	0.2577	0.8010	0.6354	0.0915	0.1039	12.7643	13.5952	0.0000	0.0000	13.8657	14.5922
C_{10}	0.0223	0.0104	0.0878	0.0786	0.0000	0.0030	3.4790	3.5540	0.0000	0.0000	3.5890	3.6461
C_{11}	0.0300	0.0000	0.0000	0.0000	0.0000	0.0000	0.5126	0.2802	0.0074	0.0000	0.5500	0.2802

APPENDIX 5. Actual and simulation data for reformate composition (wt.%)

Group	Paraffin		Iso-Paraffin		Naphthene		Aromatic		Olefin	
	Actual	Simulation	Actual	Simulation	Actual	Simulation	Actual	Simulation	Actual	Simulation
C_1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
C_2	0.00000	0.00001	0.00000	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
C_3	0.12228	0.11413	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
C_4	1.99876	2.02144	1.18459	1.49809	0.00000	0.00000	0.00000	0.00000	0.01304	0.00000
C_5	3.35545	4.23262	4.34310	3.71096	0.14886	0.13949	0.00000	0.00000	0.06925	0.14028
C_6	3.28233	3.12620	7.84587	7.02174	0.25811	0.36861	2.12721	2.53175	0.09630	0.33787
C_7	2.62886	3.08472	9.18337	8.62407	0.54280	0.68941	11.59187	12.44166	0.17002	0.00709
C_8	1.18816	1.28371	5.04267	4.81583	0.72433	0.72376	20.97498	22.35439	0.00000	0.08432
C_9	0.27417	0.36685	1.05119	0.88011	0.11819	0.14361	15.69855	14.93214	0.00000	0.00000
C_{10}	0.03244	0.01700	0.12778	0.10427	0.00000	0.00407	4.74220	3.88476	0.00000	0.00000
C_{11}	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.77254	0.29304	0.01161	0.00000

APPENDIX 6. Data of temperature effect on aromatic content in the product

RIT (C)	472	475	478	481	484	487	490	493	496	499
AROMATIC VOL%	50.64	51.85	53.02	54.14	55.19	56.18	57.09	57.93	58.70	59.40

APPENDIX 7. Data of temperature effect on RON

RIT (C)	472	475	478	481	484	487	490	493	496	499
RON	90.69	92.24	93.71	95.06	96.31	97.43	98.44	99.32	100.1	100.7

APPENDIX 8. Data of temperature effect on C_5^+ yield

RIT (C)	472	475	478	481	484	487	490	493	496	499
C_5^+ YIELD WT%	82.92	82.25	81.62	81.01	80.45	79.92	79.44	79.00	78.60	78.23

APPENDIX 9. Data of temperature effect on H_2 yield production

RIT (C)	472	475	478	481	484	487	490	493	496	499
H_2 YIELD WT%	1.75	1.78	1.81	1.84	1.86	1.88	1.90	1.92	1.94	1.96

APPENDIX 10. Data of pressure effect on aromatic content

PRESSURE (barg)	14.50	15.00	15.50	16.00	16.50	17.00	17.50	18.00	18.50
AROMATIC VOL%	50.64	50.99	51.30	51.59	51.85	52.08	52.28	52.46	52.62

APPENDIX 11. Data of pressure effect on RON in reformate

Pressure (barg)	14.50	15.00	15.50	16.00	16.50	17.00	17.50	18.00	18.50
RON	90.7	91.4	92.1	92.7	93.3	93.8	94.3	94.8	95.2

APPENDIX 12. Data of pressure effect on C_5^+ yield (wt.%)

PRESSURE (barg)	14.50	15.00	15.50	16.00	16.50	17.00	17.50	18.00	18.50
C_5^+ YIELD WT%	82.92	82.41	81.92	81.46	81.02	80.60	80.20	79.82	79.46

APPENDIX 13. Data of pressure effect on H_2 product

Pressure (barg)	14.50	15.00	15.50	16.00	16.50	17.00	17.50	18.00	18.50
H_2 Yield wt.%	1.75	1.74	1.73	1.72	1.71	1.70	1.69	1.67	1.66

APPENDIX 14. Data recycling gas quantity affects aromatic content

RG *1000 (kg/hr)	60	65	70	75	80	85	90	95	100	105
Aromatic vol%	54.14	53.58	53.05	52.54	52.04	51.56	51.09	50.64	50.20	49.77

APPENDIX 15. Recycle gas quantity effect on RON in reformate

RG *1000 (kg/hr)	60	65	70	75	80	85	90	95	100	105
RON	94.07	93.56	93.07	92.58	92.09	91.62	91.15	90.69	90.24	89.80

APPENDIX 16. Data of recycle gas quantity influence on C_5^+ Yield%

RG*1000 (kg/hr)	60	65	70	75	80	85	90	95	100	105
C_5^+ Yield wt.%	82.2	82.3	82.3	82.4	82.5	82.6	82.8	82.9	83.0	83.1

APPENDIX 17. Data of recycled gas quantity effect on H_2 production

RG Flowrate (kg/hr)	60	65	70	75	80	85	90	95	100	105
H_2 Yield wt.%	1.91	1.88	1.86	1.83	1.81	1.79	1.77	1.75	1.73	1.72

APPENDIX 18. Data of feed influences aromatic content in the product

Feed (m^3/hr)	66	70	74	78	82	86	90	94	98	102	106
Aromatic vol%	56	55	55	54	54	54	53	53	52	52	52

APPENDIX 19. Data of feed flow rate effect on RON

Feed (m^3/hr)	66	70	74	78	82	86	90	94	98	102	106
RON	95.7	95.2	94.8	94.3	93.8	93.4	93.0	92.5	92.1	91.8	91.4

APPENDIX 20. Data of feed effect on C_5^+ yield (wt. %)

Feed (m^3/hr)	66	70	74	78	82	86	90	94	98	102	106
C_5^+ Yield wt.%	81.4	81.7	81.9	82.1	82.3	82.5	82.7	82.9	83.0	83.2	83.4

APPENDIX 21. Data of feed flow effect on H_2 production

Feed (m^3/hr)	66	70	74	78	82	86	90	94	98	102	106
H_2 Yield wt.%	1.93	1.92	1.91	1.91	1.90	1.90	1.89	1.89	1.88	1.88	1.88

APPENDIX 22. Permission to Use the Data from factory

CURRICULUM VITAE

Personal Information

Name and Surname : Ali Salim JUMAAH

Education

MSc	Çankırı Karatekin University Graduate School of Natural and Applied Sciences Department of Chemical Engineering	2019-2023
Undergraduate	Tikrit University College of Engineering Department of Chemical Engineering	1999-2003

Work Experience

Year	Institution	Position
2004-2007	Northern Fertilizer Company	Process Engineer
2007-2023	North Refineries Company	