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Optimization of the Operating Conditions of Rectification Column C101/ C102 at Hassi R'Mel Plant.

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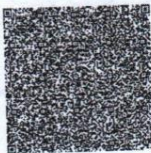
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Abstract

The natural gas sector is one of the most important energy sectors worldwide, and Algeria plays a significant role in this industry through the Hassi R'Mel gas complex. In this context, the purpose of this thesis was to evaluate and optimize the performance of the debutanizer column (C102). The study begins with the industrial context and the essential theoretical concepts related to natural gas processing and rectification. An Aspen HYSYS simulation model was then developed and validated using design operating conditions before being applied to the current operating case. This analysis enabled the identification of the key parameters affecting product quality, particularly the influence of the reflux rate on condensate Reid Vapor Pressure (RVP). To further improve process performance, the Particle Swarm Optimization (PSO) algorithm was applied to determine the optimal operating conditions while ensuring compliance with the required product specifications.

ملخص

يعد قطاع الغاز الطبيعي أحد أهم قطاعات الطاقة في العالم وتلعب الجزائر دوراً مهماً في هذا المجال بفضل مجمع حاسي الرمل للغاز الطبيعي في هذا السياق كان الهدف من هذه الدراسة تقييم وتحسين أداء عمود نزع البيوتان Debutanizer C102 بدأت الدراسة بعرض السياق الصناعي والمفاهيم النظرية الأساسية المتعلقة بمعالجة الغاز الطبيعي وعمليات التقطير بعد ذلك تم تطوير نموذج محاكاة باستخدام برنامج Aspen HYSYS والتحقق من صحته بالاعتماد على معطيات التصميم ثم تم تطبيقه على ظروف التشغيل الحالية وقد سمح هذا التحليل بتحديد أهم المتغيرات المؤثرة على جودة المنتجات خاصة تأثير معدل الراجع Reflux Rate على ضغط بخار ريد للمتكثفات RVP وتحسين أداء العملية بشكل أكبر تم تطبيق خوارزمية Optimization Particle Swarm لتحديد ظروف التشغيل المثلى مع ضمان مطابقة المنتجات للمواصفات المطلوبة.

Résumé

Le secteur du gaz naturel est l'un des secteurs énergétiques les plus importants au monde, et l'Algérie joue un rôle significatif dans cette industrie grâce au complexe gazier de Hassi R'Mel. Dans ce contexte, l'objectif de ce mémoire était d'évaluer et d'optimiser les performances de la colonne de débutanisation (C102). L'étude commence par présenter le contexte industriel et les concepts théoriques essentiels liés au traitement et à la rectification du gaz naturel. Un modèle de simulation Aspen HYSYS a ensuite été développé et validé à l'aide des conditions de fonctionnement de conception avant d'être appliqué au cas d'exploitation actuel. Cette analyse a permis d'identifier les paramètres clés affectant la qualité du produit, en particulier l'influence du taux de reflux sur la pression de vapeur Reid (RVP) du condensat. Afin d'améliorer encore les performances du procédé, l'algorithme d'optimisation par essaim de particules (PSO) a été appliqué pour déterminer les conditions de fonctionnement optimales tout en garantissant le respect des spécifications requises pour le produit.

Dedication

We dedicate this work

To our beloved parents, whose unconditional love, endless support, sacrifices, and encouragement have been the foundation of our success. No words can truly express our gratitude and appreciation for everything they have done for us.

To our brothers and sisters, for their love, understanding, and constant encouragement.

To our families, whose faith in us has always inspired us to move forward and achieve our goals.

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Abbreviations liste

NGL: natural gas liquid;

LPG: liquified petroleum gas;

PSO: particles swarm optimization.

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General introduction

Introduction

Natural gas has been known since ancient times, with the earliest evidence dating back to 6000–5000 BC in Baku, Azerbaijan. Around 500 BC, the Chinese used natural gas in salt production, while Ancient Persia utilized it for domestic purposes. Later, the Ancient Greeks built the Temple of Apollo at Delphi above a natural gas seep. Despite these early uses, the modern natural gas industry emerged in 1816 with the establishment of the first gas utility, while the first successful natural gas well was drilled by William Hart in 1821 [1].

Hassi R'Mel, Algeria's largest natural gas field, was discovered in 1956 alongside the Hassi Messaoud oil field and has since been operated by the state-owned company Sonatrach. Natural gas production began in 1961, and in 1964 Algeria became the world's first exporter of liquefied natural gas (LNG). Today, Algerian natural gas is exported to several countries through an extensive pipeline network [2].

To address the contemporary operational challenges of this vital field, the core of this thesis focuses on the simulation, performance analysis, and algorithmic optimization of the gas stabilization process. Specifically, this work establishes a validated digital model of the Hassi R'Mel debutanizer column using Aspen HYSYS, evaluates its current operating limitations, and applies a custom Particle Swarm Optimization (PSO) algorithm to determine the ideal parameters for maximizing product quality and energy efficiency.

This thesis begins with the industrial context and theoretical foundations. The first chapter presents the Hassi R'Mel gas field, including its geographical location, history, and main installations. It then provides an overview of natural gas, covering its composition, properties, extraction methods, and processing stages. The chapter also describes rectification columns, their operating principles, key operating parameters, and hydraulic limitations. Finally, it examines the impact of feed fluctuations on process performance, product quality, and energy consumption.

The second chapter focuses on the validation of operating parameters using Aspen HYSYS. It presents the simulation and validation of the debutanizer model by comparing design data with simulation results. The chapter then analyzes the current operating conditions and product quality before identifying the reflux rate as a critical parameter affecting condensate quality and suitable for further optimization.

The final chapter focuses on optimization using the PSO algorithm. It presents the fundamental principles of PSO and applies the algorithm to optimize the operating parameters of the debutanizer column while maintaining the required product quality specifications. The end of this work is a conclusion and some perspectives.

Chapter I

Industrial context and theoretical foundation

I.1. Generalities about natural gas

The natural gas since its discovery it has been a major industrial sector, in order to process it right, we need to know its composition, how it's formed, its properties and how to treat it well.

I.1.1. Definition and composition of natural gas

Natural gas is a hydrocarbon mixture obtained from a reservoir underground. The largest component is methane (CH_4) but it contains also other hydrocarbons such as ethane (C_2H_6), propane (C_3H_8), isobutene and noramalbutene etc., these light paraffins are gaseous under atmospheric conditions [6]. It contains also some of non-hydrocarbons, such as: nitrogen (N_2), hydrogen sulphide (H_2S) along with carbon dioxide (CO_2), traces of helium (He), carboxyl sulphide (COS) and various mercaptans along with water [3].

The figure I.2 represents the composition of natural gas.

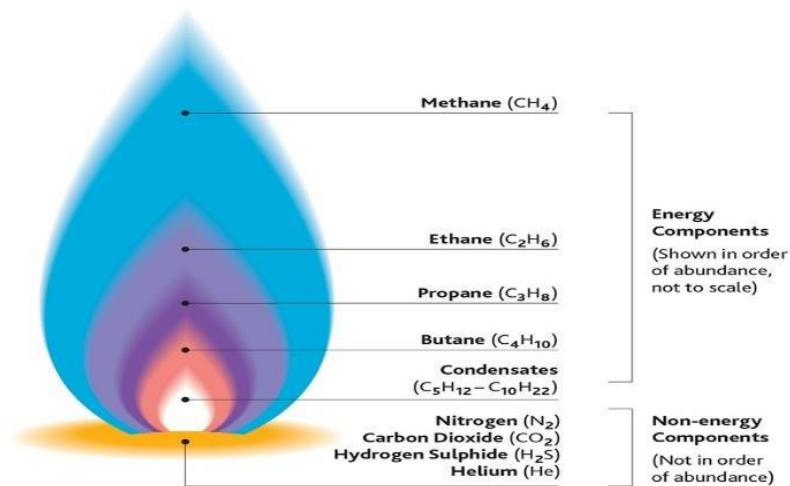


Figure I.2 Components of natural gas [2].

The table I.1 represents the composition and its percentage in the natural gas

Compound	Symbol	Percent in Natural Gas
Methane	CH_4	60-90
Ethane	C_2H_6	0-20
Propane	C_3H_8	0-20
Butane	C_4H_{10}	0-20
Carbon Dioxide	CO_2	0-8
Oxygen	O_2	0-0.2
Nitrogen	N_2	0-5
Hydrogen Sulfide	H_2S	0-5
Rare Gases	A, He	0-2

Table I.1 the composition and it's percentage in the natural gas [1].

I.1.2. Formation of the natural gas

The natural gas is formed by the high pressure applied by the mud and the sediment on the organic matter (ex: the remains of plants or animals) under the ground for a very long time (millions of years). Its formation also requires high temperatures, which can be found deep down the earth's crust [4]. The figure I.3 explains the natural gas formation.

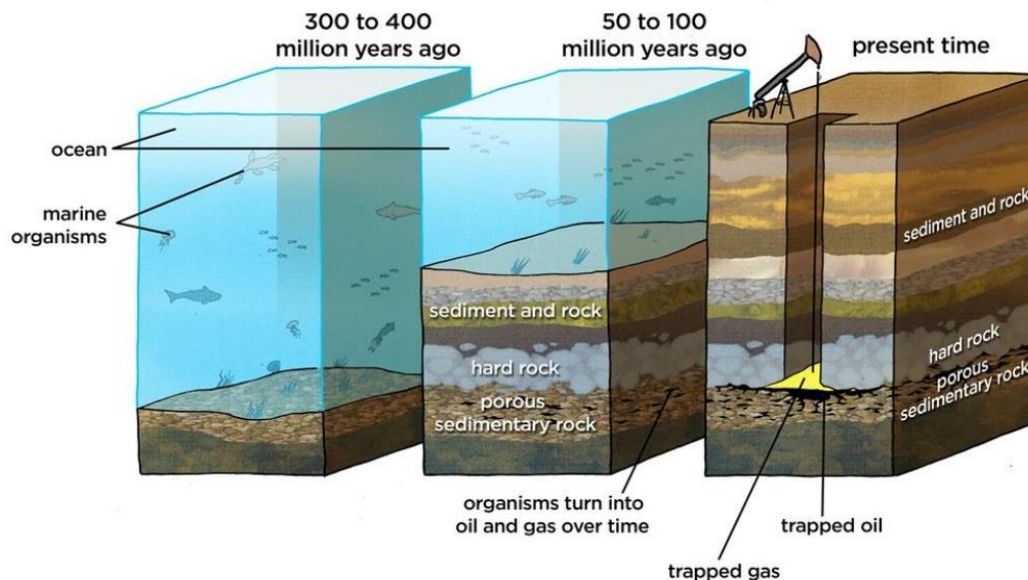


Figure I.3 Natural gas formation [3].

I.1.3. Natural gas properties

The raw natural gas has several properties, physical, chemical and thermodynamic properties, which are the following:

a) Physical properties

The raw natural gas is colorless, odorless, tasteless, and highly flammable, however some of the associated gases specifically hydrogen sulfide has a special and penetrating smell and a few parts per million are sufficient to impart a decided odor to natural gas [5].

b) Chemical and thermodynamic properties

There are too many, but these are the most important ones:

➤ Molecular weight

The molecular weight of a gas is defined by its mass per mole. Its value can be expressed in the following units: lbm/lbmole, g/mole, or kg/kgmol. It's can be calculated using the specific gravity by the following equation [6]:

$$\mathbf{MW}_{\text{gas}} = (\mathbf{G}_{\text{gas}}) (\mathbf{MW}_{\text{air}}) \quad (1)$$

Where:

$\mathbf{MW}_{\text{gas}}$: is the molecular weight of the natural gas

$\mathbf{MW}_{\text{air}}$) : is the molecular weight of air

$\mathbf{G}_{\text{gas}}$: is the specific gravity of the natural gas

➤ **Specific gravity of gas**

Specific gravity is defined by the ratio of the density of the gas to the density of air at the same temperature and pressure [7].

$$\mathbf{SpGr}_{\text{gas}} = \frac{\rho_{\text{gas}}}{\rho_{\text{air}}} \quad (2)$$

Where :

$\mathbf{SpGr}_{\text{gas}}$: is the specific gravity of a gas;

ρ_{gas} : is the density of the gas at a certain temperature and pressure;

ρ_{air} : is the density of air at the same temperature and pressure.

➤ **Compressibility factor of gas**

The compressibility factor of a gas (Z) at a certain temperature and pressure is the degree of its divergence from ideal gas law behavior [5].

- $Z = 1$; the gas behaves as ideal gas, which occurs at high temperature and low pressure;
- $Z < 1$; the gas deviate from the ideal gas behavior, it happens when the pressure is high and the temperature is low.

Modified Ideal Gas Law:

$$\mathbf{PV} = \mathbf{ZnRT} \quad (3)$$

Where:

$\mathbf{P}$: Absolute pressure

$\mathbf{V}$: volume

$\mathbf{Z}$: Compressibility factor

$\mathbf{n}$: Number of moles

$\mathbf{R}$: The constant of ideal gas

$\mathbf{T}$: Absolute temperature (°R)

➤ **Gas density**

The gas's density it's measured by its mass per unit volume, usually expressed in kg/m^3 for S.I units, it is a crucial parameter for gas pipe flow calculations. The density is affected by the pressure

and temperature it increases with high pressure and decreases with high temperature [5]

➤ **.viscosity of gas**

The viscosity is the measurement of the resistance of a fluid to flow, it is a very important parameter to calculate in pipe flow. There are two types of viscosity, one is the dynamic viscosity (μ) its unit is [Pa-s] or centipoise (cp); the other one is kinematic viscosity, its unit is m²/s or centistokes, we can calculate one viscosity of a fluid knowing the other one and its density, using the following equation [5]:

$$\nu = \mu / \rho \quad (4)$$

A convenient equation for calculating the viscosity of natural gas is that of Lee, Gonzalez and Eakin:

$$\mu_g = 10^{-4} K_v \exp \left[x_v \left(\frac{\rho_g}{62.4} \right)^{y_v} \right] \quad (5)$$

Where K_v , x_v and y_v are empirical intermediates that can be calculated as such:

$$k_v = \frac{(9.4 + 0.02 MW_g) T^{1.5}}{209 + 19 MW_g + T} \quad (6)$$

$$y_v = 2.4 - 0.2 x_v \quad (7)$$

$$x_v = 3.5 + \frac{986}{T} + 0.01 MW_g \quad (8)$$

In these expressions, T is the natural gas temperature in °R, ρ_g is the density of the gas in lbm/ft³, MW_g is the molecular weight of the gas, and μ_g is the dynamic viscosity of the gas in centipoise (cp).

➤ **Gas formation volume factor**

The formation volume factor of gas is the ratio of the volume of gas at the reservoir temperature and pressure to the volume at the standard or surface temperature and pressure (P_{sc} and T_{sc}). It is symbolized B_g and is often expressed in either cubic feet of reservoir volume per standard cubic foot of gas or barrels of reservoir volume per standard cubic foot of gas. This parameter is crucial for estimating reserves, designing production facilities, it is calculated as follows [7]:

$$B_g = \frac{\text{volume of gas at reservoir conditions}}{\text{volume of gas at surface conditions}} \quad (9)$$

But for real gas we calculate it as such:

$$B_g = \frac{\frac{znRT}{P}}{\frac{z_{sc}nRT_{sc}}{P_{sc}}} = \frac{P_{sc}}{T_{sc}} \frac{zT}{P} \quad (10)$$

Where:

z_{sc} : Z-factor at standard conditions = 1.0

P_{sc}, T_{sc} : standard pressure and temperature

P, T : reservoir temperature and pressure respectivel

P_{sc}, T_{sc} : standard pressure and temperature

P, T : reservoir temperature and pressure respectively.

➤ Isothermal compressibility

The isothermal gas compressibility, which it's symbol is C_g , is an important concept that will be used largely in determining the compressible properties of the reservoir, it's calculated as [7]:

$$C_g = -\frac{1}{V_g} \left(\frac{\partial V}{\partial p} \right)_T \quad (11)$$

Where V and P are volume and pressure, respectively, and T is the absolute temperature. For ideal gas:

$$C_g = \frac{1}{P} \quad (12)$$

Whereas, for non-ideal gas, compressibility is:

$$C_g = \frac{1}{P} - \frac{1}{Z} \left(\frac{\partial Z}{\partial p} \right)_T \quad (13)$$

Where

Z is the compressibility factor.

➤ Pseudo critical properties

For a gas with known composition the pseudocritical properties are determined from the critical properties using the mixing rule, where [8]:

- P_{Pc} , T_{Pc} : are the pseudo critical pressure and pseudo critical temperature respectively;
- P_{ci} , T_{ci} : are critical pressure and critical temperature of component i , respectively;
- y_i : the molar fraction of the component i .

$$T_{Pc} = \sum_{i=1}^{Nc} y_i \cdot T_{ci} \quad (14)$$

$$P_{Pc} = \sum_{i=1}^{Nc} y_i \cdot P_{ci} \quad (15)$$

I.2.4. Natural gas extraction and process

Natural-gas processing is a complex industrial process designed to clean raw natural gas by separating impurities and various non-methane hydrocarbons and fluids to produce what is known as pipeline quality dry natural gas.

a) Extraction

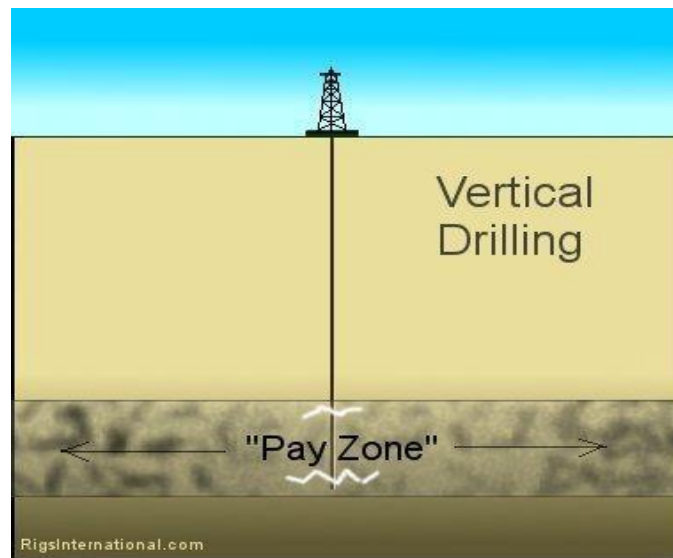
The first step is preparing the step, in order to make sure that the land is ready for the following steps, it starts with clearing the site, make access roads, and build the infrastructure.

These steps are very important to make sure that the extraction process of natural gas is smooth and safe. Most methods used are vertical drilling, horizontal drilling, hydraulic fracturing/ fracturing and acidizing [9].

➤ Vertical drilling

It has been used for a very long time, it drills straight down, reaching 300 to 800 meters of depth. This method is great at pinpointing shallow gas deposits. This method was used until the 1980s, it's still crucial to get the natural gas until now it lets us use old wells again, by providing a direct way to get gas. This method is simple and well-trusted by many [10],[11].

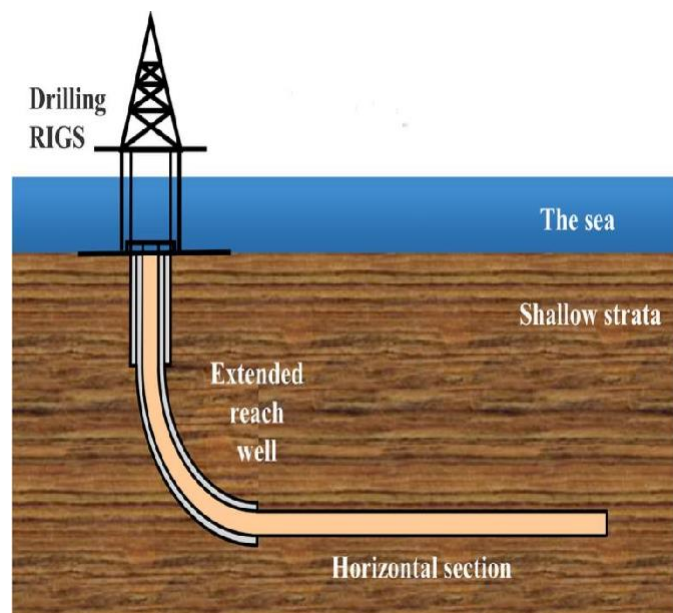
The figure **I.4** illustrates the vertical drilling method.



FigureI.4 Vertical drilling method [4].

➤ **Horizontal drilling**

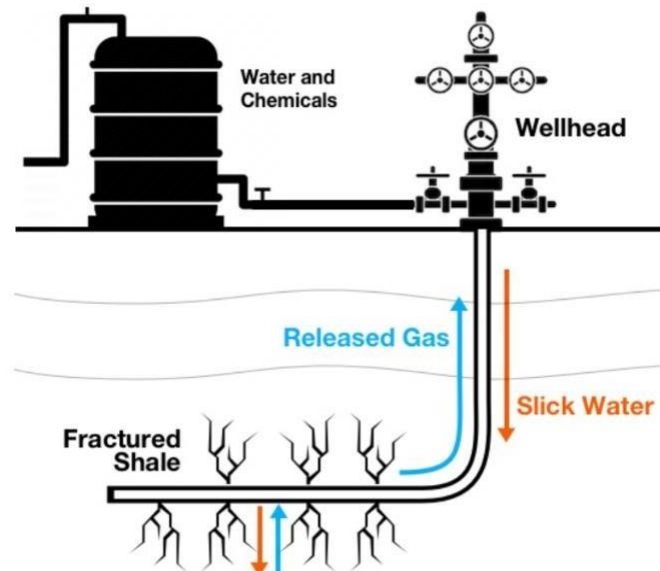
Horizontal drilling has significantly changed the way natural gas is extracted by allowing wells to curve horizontally after reaching a certain depth underground. This technique makes it possible to access larger gas reserves from a single drilling location, which increases production while reducing the number of drilling sites needed. In addition, modern technological advancements enable companies to reach deeper and more complex gas deposits with greater precision and efficiency [12]. The figure I.5 shows the horizontal drilling method.



FigureI.5 Horizontal drilling method [5].

➤ Hydraulic fracturing \ fracking

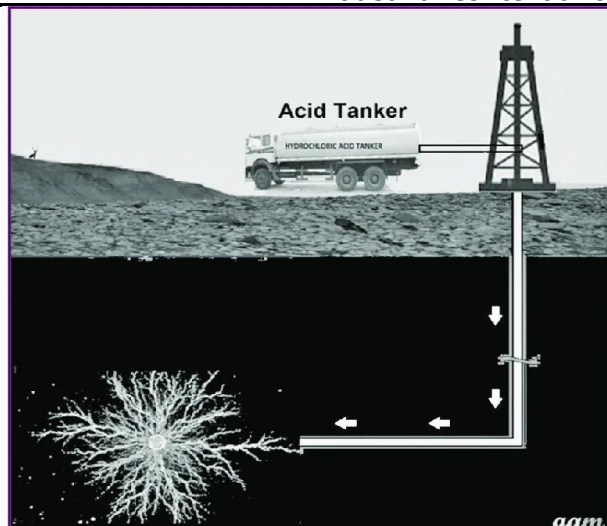
Hydraulic fracturing is a leading process in the extraction process, known also as fracking. It is based on breaking underground rocks by the high-pressure fluids which form openings that let stuck natural gas flow out and be collected. Hydraulic fracturing has boosted the efficiency of getting natural gas, especially from hard-to-reach areas [13]. The figure I.6 represents the hydraulic fracking metho



FigureI.6 Hydraulic fracking [6].

➤ Acidizing

Acidizing is a process that is generally used in aging wells that are in the lasts stages of production, it is based on the stimulation of a reservoir formation by injecting a solution of a reactive acid to increase the permeability of the rocks and improve the production of a well. In sandstone formations, the acids help enlarge the pores (Matrix acidizing), while in carbonate formations, the acids dissolve parts of the rock matrix and creates fractures (fracture acidizing) [14]. The figure I.7 represents the acidizing method.



FigureI.7 Acidizing method [7]

b) Process

The industrial process aims to eliminate the impurities contained in the extracted gas. The result is a dry gas (the main component is the methane CH_4), that is appropriate to transport and to consume. In order to get that the extracted gas undergoes a series of industrial operations; which are the following [15]:

➤ Separation of liquids and solids

Usually, the raw gas contained solids and some heavy liquids (such as sand, oil...) the first step is to perform a physical separation in order to get rid of them.

➤ Dehydration

This operation's main purpose is to eliminate the water vapor present in the substance obtained from the previous step t, two types of adsorption units can be use at this stage glycol adsorption units or molecular sieve adsorption unit, at this point this operation had prevent a hydrate formation eventually the pipeline corrosion.

➤ Removal of acid gasses

At this stage the purpose is to remove CO_2 and H_2S to avoid pipeline corrosion and fulfill the standards. Different methods are applied such as amine absorption. Some plants include sulfur compound removal if it is seen as necessary.

➤ Eliminating mercury and nitrogen

Some cases a presence of mercury and nitrogen can be noticed, in order to eliminate them we use activated carbon beds or specific sieves for the mercury, as for the nitrogen, a cryogenic distillation or adsorption are employed. The aim of this process is to increase the calorific value of the natural gas and decrease its volume, necessary for transportation.

➤ Recovery of Natural Gas Liquids (NGLs)

To separate the natural gas liquids (NGLs) or the condensates, the gained natural gas will be cooled and compressed. The condensates must receive a fractionation process for further utilization.

➤ Cryogenic processing

In purpose of liquefying separating heavy components, the cryogenic heat exchangers and the turbo-expanders are utilized to cool the gas to very low temperatures (cryogenic).

➤ Compression, storage and transportation

The last step is basically to compress the dry natural gas at high pressure in order to transport it. However, if is liquefied, it is stored in underground or in cryogenic tanks. The figure I.8 resumes the natural gas process.

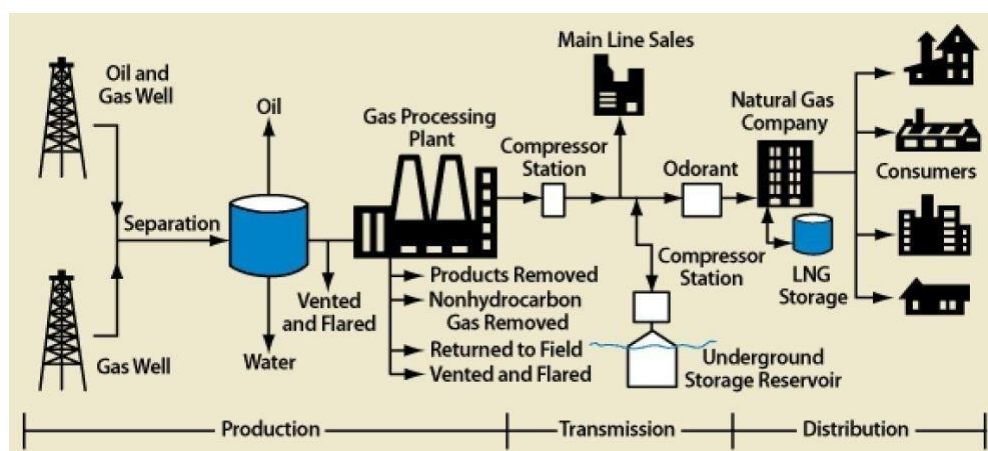


Figure I.8 Natural gas process [8].

I.3. Description of the rectification columns

The chemical industry in general and the refining specifically aim to get a pure liquid, several methods are involved but the most used one is the rectification [16], [17]:

I.3.1. Definition of rectification

The rectification operation is an operation used to purify a liquid by repeatedly distilling it, in order to get rid of water and impurities. This process guarantees to the operator a higher purity than the simple distillation, for this reason it is largely used in the petrochemical industries.

I.3.2. Principle of rectification

Rectification is a purification method that depends on repeated or fractional distillation. It usually takes place in tall cylindrical columns containing multiple plates that hold liquid. The contact between liquid and vapor occurs when the vapor goes upwards and the liquid goes downwards on each

plate. This interaction causes partial condensation of the vapor and partial evaporation of the liquid. There is a condenser at the top of the column which liquefies a part of the rising steam and send it back to the column as reflux. This repeating process of heat and mass transfer guarantee much higher product purity than simple distillation.

The Figure I.9 shows the principle of rectification.

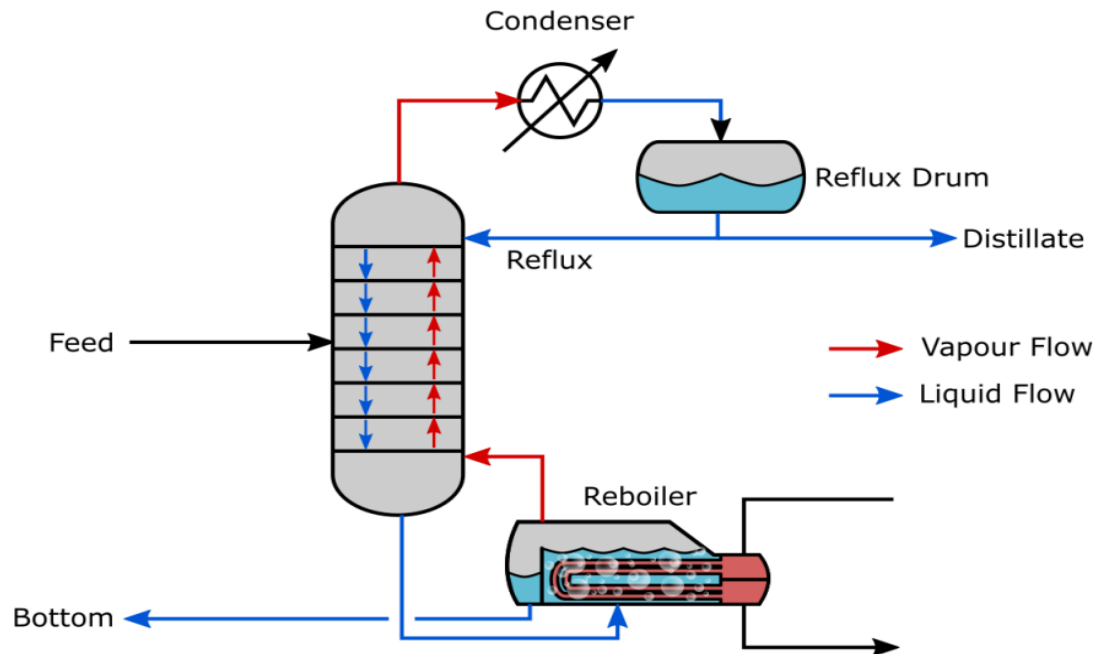


Figure I.9 Principle of rectification [9].

I.3.1. Key parameters

When a rectification process is ongoing the operator must pay attention to some operational parameters which are as follows:

a) Temperature

Temperature determines the driving force for heat and mass transfer between the rectifying and stripping sections. The lowest temperature difference (ΔT) between the two sections is a crucial design parameter that affects heat integration, required heat transfer surface area, and overall energy savings. When ΔT is properly selected (typically 2–5 K), the column can ensure high product purity while maintaining effective internal heat transfer [18].

b) Pressure

the pressure if it is too high, it affects the relative volatility of the component and mass transfer which will reduces the sharpness of the rectification and may need more theoretical plates, however a high pressure can accelerate the mass transfer, that's why it is crucial to maintain the rectification on optimal pressure which accelerate the mass transfer without adding more theoretical plates [19].

c) Feed stage location

It is very important to find the optimal position for the feed position that ensure the maximum separation capacity can be obtained on the same operating conditions, depending on the tower's structure, the material properties and the distillation requirements, the optimal plate can be in the top, middle or the bottom of the column, in industry to get more realistic results usually the feed port is situated between two trays [20].

d) Number of theoretical stages

It represents the stages needed so that the gas and liquid have sufficient contact time to reach the equilibrium phase; in reality the contact time between the two phases can never be perfect so for that the actual stages are more than the theoretical ones, these are determined first, and then the actual number of plates is estimated [20].

e) Reflux ration

The flux ratio is the ratio between the liquid turned to the rectification tower and the product flow taken from the tower, it is both economically and operationally crucial to find the optimal, because if it is too high it will increase the heating steam consumption and cooling water which leads to increase the operating costs besides it also affects the column dimension and increase the equipment costs [21].

f) Effect of Distillate to Feed Ratio

The distillate-to-feed ratio measures the amount of distillate produce the tower. If this ration is kept constant during the dynamic simulation, it will much easier to the operator to control the purity both on top and the bottom of the tower [20].

1.3.2. Hydraulic limitations

There are too many of hydraulic limitation that may occurs during the rectification process which are [22]:

a) Flooding

It occurs when excessive vapor flow that entrains the liquid up the column, and back up the down comer liquid, this cause the liquid to be stocked on the plate above, this phenomenon reduced severely the capacity of the rectification, it can be detected by an increase in the differential pressure of the column and a decrease in the separation efficiency.

b) Foaming

It occurs when the liquid expands resulting from the passage of vapor, whereas it guarantees a high interfacial contact, excessive foaming usually results in liquid buildup on trays. Whether foaming is driven by physical properties of the liquid mixtures, or due to tray designs and condition,

it will always reduce the separation efficiency

c) Weeping/Dumping

This phenomenon is caused by low vapor flow where the vapor pressure is insufficient to hold up the liquid on the tray. Therefore, liquid starts to leak through perforations (weeping). In some cases, extreme weeping will result in the liquid on all trays will crash (dump) through to the base of the column (via a domino effect). A sharp pressure drop in the column and reduced separation efficiency can lead us to dictate these phenomena.

d) Entrainment

Entrainment is a phenomenon where the liquid carried by vapor up to the tray above resulting from high vapor flow rates. A lower volatile material is carried up to high volatile material which highly affect the purity of the distillate. Excessive entrainment can lead to flooding.

I.4. Impact of feed fluctuations on the columns

Fluctuations in the feed rate and composition remarkably affect the efficiency of a rectification column. These disturbances change the internal equilibrium of the column and result in operational inefficiencies [21]:

I.4.1. Temperature profile

Modification in the feed disturb the thermal equilibrium in the column. In particular, variations in feed composition can cause an increase in reflux flow rate beyond actual separation needs. This excessive reflux leads to a decrease in the temperature of sensitive stages, altering the normal temperature gradient along the column. Therefore, the temperature profile becomes unstable, negatively affecting separation efficiency.

I.4.2. Differential Pressure

Feed modification can induce hydraulic disturbances within the column. Alterations in vapor and liquid flow rates (caused by the excess reflux or feed variation) may lead to variations in differential pressure along the column. Eventually this can result in operational problems as poor vapor-liquid contact or even risks of flooding or weeping, thereby decreasing column efficiency.

I.4.3. Product purity

An alteration in feed composition, specifically a decrease in heavy components, directly affects the separation process. This leads to a reduction in production yield and can cause the final products to diverge from needed specifications. Continuous adjustments are necessary to maintain purity, indicating reduced process stability and reliability.

I.4.4. Energy consumption

Feed modifications often cause an extreme energy consumption, especially in the reboiler. Due to the decrease in temperature due to an excessive reflux, the control system compensates by increasing the hot oil flow to the reboiler. This induces unnecessary energy usage to maintain product quality, making the process less energy-efficient.

The table **I.2** will resume the impact of the feed variation on rectification columns.

Impact Type	Specific Consequence	Operational Cause	Mitigation Strategy
Loss of Separation Performance	Significant degradation of separation efficiency and loss of sensitivity within the deproteinized column.	Deviations in the mole fractions of light components (N ₂ , C ₁ , and C ₂) and heavy components (C ₃ , C ₄ , C ₅ , C ₆ +) compared to design specifications.	Optimization of the reflux flow rate to restore separation efficiency and ensure product quality meets specifications.
Energy Consumption	Increased energy consumption due to elevated reboiling requirements.	Overestimation of the reflux flow rate, which lowers the temperature of sensitive stages and forces the reboiler to increase heat duty.	Identification of optimal operating parameters and reduction of the reflux flow rate to save energy while maintaining product purity.
Production Capacity	Reduction in the propane production flow rate.	Changes in feedstock composition and the operational shutdown of the LPG reinjection unit (pumps and drum).	Reduction of the reflux flow rate to an optimal value (e.g., 810 tones/day) to maximize production while maintaining a minimum purity of 95%.

Operating Parameter Disturbance	Abnormal temperature and flow profiles across the column stages.	Sudden increase in liquid flow relative to the vapor phase in the stripping section caused by feedstock entering in a liquid state.	Real-time monitoring of feedstock variations and adjustment of the cascade control loop between stage temperature and reflux flow.
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Table **I.2** Impact of the feed variation on rectification columns [2].**Conclusion**

This chapter provided an overview of natural gas, including its formation, composition, and key physical, chemical, and thermodynamic properties, along with a brief look at its extraction and treatment. It also examined rectification as a major process in natural gas processing, outlining its principles, key parameters, and the impact of feed variations on yield. The next chapter will focus on analyzing the productivity of rectification columns under fluctuating feed conditions.

Chapter II

Validation of operating parameters

Nowadays industries can enhance efficiency, safety and sustainability of any process due to simulations, which saved them a lot of time and money [23]. Many simulating programs exist such as, DWSIM, CHIMCAD and HYSYS. In this chapter, we will see the simulation of the design case and current case in HYSYS.

II.1. Definition of HYSYS

HYSYS is a widely used simulator developed by Aspen Technology; it is largely used in modeling and optimization chemical and petrochemical industries. It brings together process modeling with energy, safety conditions, and economic analysis to assist in decision-making across the entire lifecycle of industrial operations [24].

II.1.1. Definition of thermodynamic package

Thermodynamic packages refer to different sets of mathematics equation, correlations, sets of data, chemical and physical properties with different thermodynamic models which we can apply in a simulation depending on the component and working conditions in order to perform all the necessary calculation correctly, there are so many packages such as UNIFAQ, NRTL, UNIQUAC and Peng-Robinson [25].

II.1.2. Simulation process

The simulation parameters were selected based on the original design data of the C102 debutanizer provided by the Hassi R'Mel gas processing complex. These design data include the feed composition, feed conditions (temperature, pressure, and flow rate), column dimensions, feed tray location, and operating conditions. Using these industrial design values ensures that the HYSYS model accurately represents the real operating conditions of the debutanizer.

Figure **II.1** presents the Aspen HYSYS simulation flowsheet of the C102 debutanizer. In the industrial LPG recovery unit, C102 is located downstream of the deethanizer column (C101). The bottom product of C101 feeds C102, where propane is recovered as the overhead product (LPG), while the heavier hydrocarbons leave the bottom as stabilized condensate.

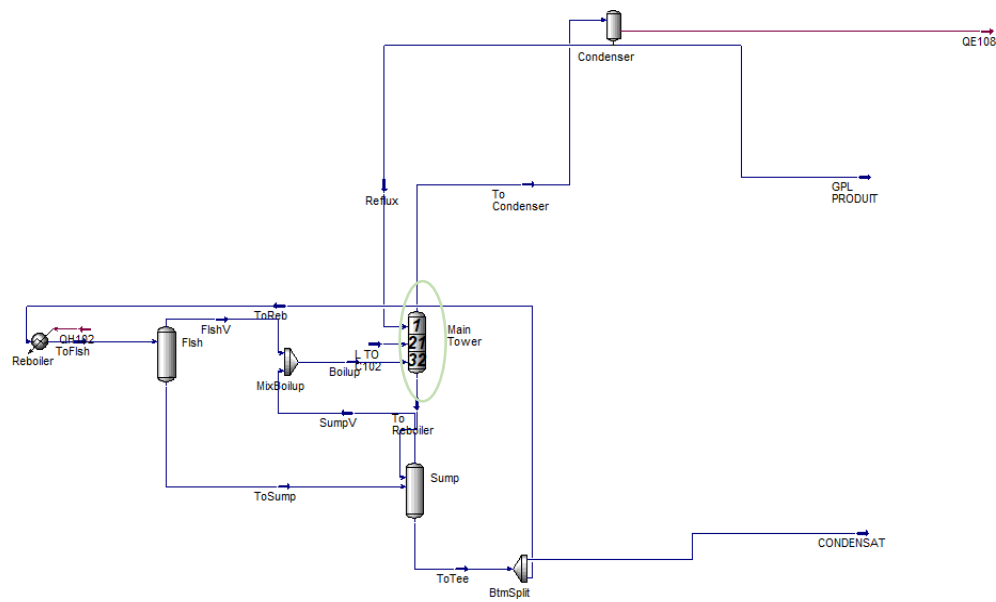


Figure II.1 simulation chart of the debutanizer C102 with Aspen HYSYS.

1. Define the feed composition and operating conditions according to the design data. The feed stream is specified with a molar flow rate of 2219.05 kmol/h, a temperature of 159.1°C, and a pressure of 15.03 kg/cm².

Figure II.2 shows the windows of feed parameters controlling.

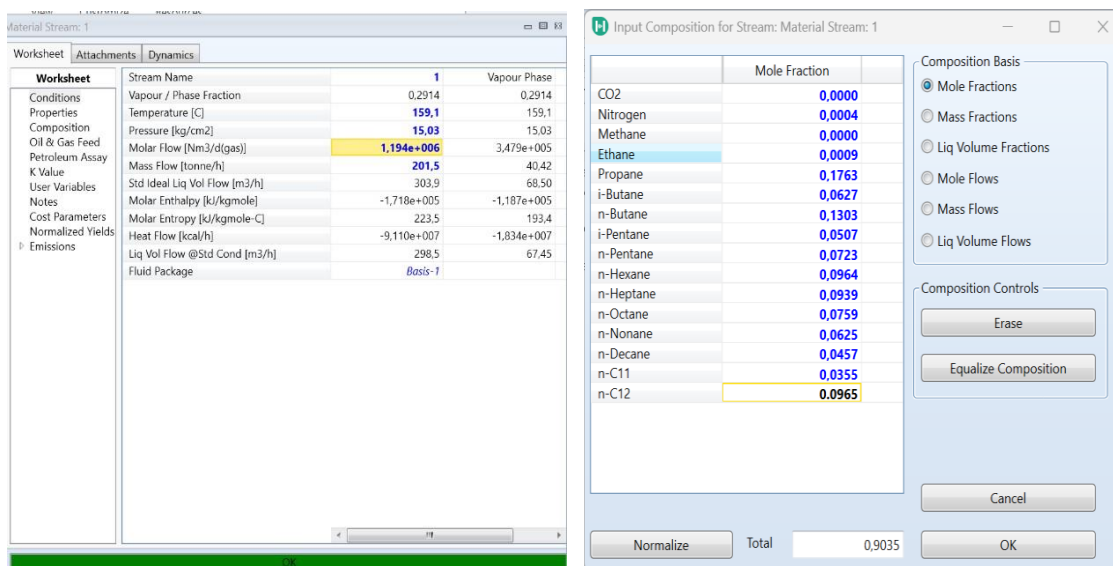


Figure II.2 Windows of feed parameters controlling.

2. Define the column dimensions by specifying a diameter of 2.5 m, 32 theoretical trays, a tray spacing of 0.6 m, an overall tray efficiency of 70%, and selecting tray 21 as the feed stage.

Figure II.3 illustrates the column design window.

Tower Sizing	
Tower	Main Tower
Uniform Section	☒
Internal Type	Sieve
Diameter [m]	2,500
Tray/Packed Space [m]	0,6000
Tray/Packed Volume [m3]	2,945
Disable Heat Loss Calcs	☐
Heat Model	None
Rating Calculations	☐
Hold Up [m3]	0,2454
Weeping Factor	1,000
Tray Sizing Analysis for Costing	Internals-1@Main

For more detailed and tray by tray information see the individual tower in the Column/Environment...

Delete Column Environment... Run Reset Converged

Figure II.3 Column design window.

Figure II.4 represents the feed position window.

Tower: Main Tower

Design Rating Worksheet Performance Dynamics

Design

Connections
Side Draws
Parameters
Pressures
User Variables
Notes

Name: Main Tower

Liquid Inlet: **Reflux**

Vapour Outlet: **To Condenser**

Vapour Inlet: **Boilup**

Liquid Outlet: **To Reboiler**

Optional Feeds

Stream	Stage
L TO C102	21_Main Tower

<< Stream >>

Delete

Figure II.4 Feed position window.

3. Enter the operating parameters required for column convergence, including a reboiler temperature of 254°C, a top reflux flow rate of 109.16 t/h, and a bottom reflux flow rate of 217.45 t/h.

Figure II.5 shows the representing window of these parameters

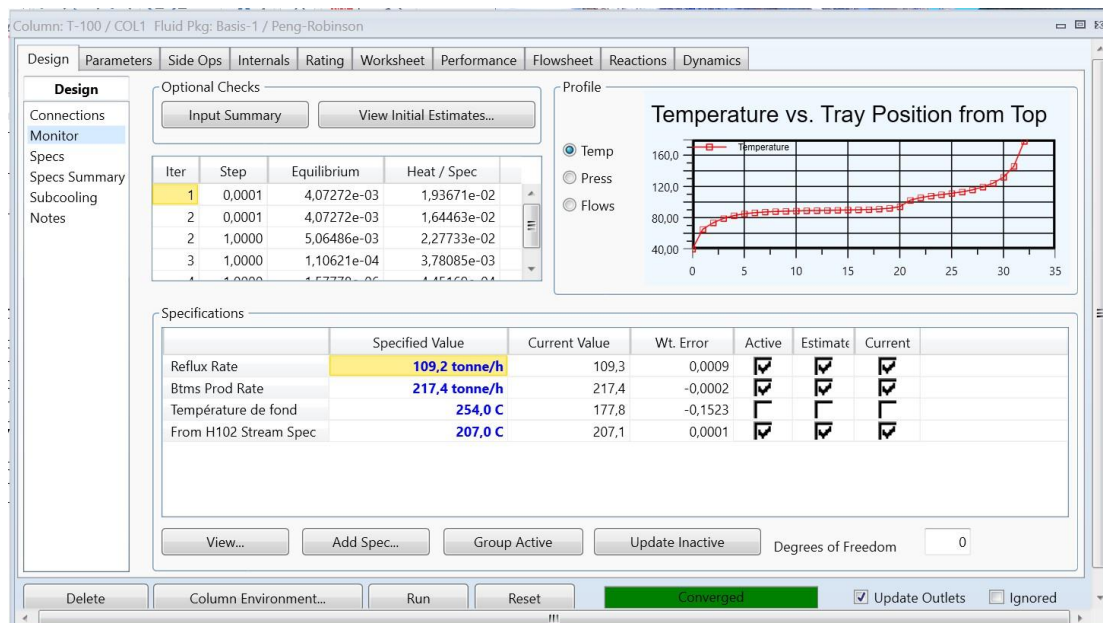


Figure II.5 window of operating parameters

III.2. Simulation of design case

In this part, we will simulate the design parameters in order to verify the HYSYS reliability.

II.2.1. Display of design case

The following table represent the design parameters:

a) Composition design

Table II.1 presents the feed composition used in the design simulation. The feed mainly consists of propane (C3), butanes (iC4 and nC4), pentanes, and heavier hydrocarbons, while nitrogen, carbon dioxide, and methane are present only in very small quantities. This composition corresponds to the design operating conditions of the C102 debutanizer.

Feed Component	Molar flow (Kmol/h)	Molar Fractions	Mass flow (Kg/h)	Mass Fraction
N ₂	0,79	0,0004	22,1303	0,0001
CO ₂	0,01	0,0000	0,4401	0,0000
CH ₄	0,01	0,0000	0,1604	0,0000

C₂H₆	2,06	0,0009	61,9440	0,0003
C₃H₈	391,12	0,1763	17247,2187	0,0856
iC₄H₁₀	139,09	0,0627	8084,4672	0,0401
nC₄H₁₀	289,08	0,1303	16802,4861	0,0834
iC₅H₁₂	112,60	0,0507	8124,2027	0,0403
nC₅H₁₂	160,50	0,0723	11580,2357	0,0575
C₆H₁₄	213,99	0,0964	18441,2093	0,0915
C₇H₁₆	208,31	0,0939	20873,7039	0,1036
C₈H₁₈	168,49	0,0759	19246,9501	0,0955
C₉H₂₀	138,79	0,0625	17801,0670	0,0883
C₁₀H₂₂	101,36	0,0457	14422,0083	0,0716
C₁₁H₂₄	78,82	0,0355	12320,5909	0,0611
C₁₂H₂₆	214,03	0,0965	36457,6571	0,1809
Total	2219,05	1,0000	201486,4720	0,9998

Table II.1 Feed composition.

a) Design feed condition

The table II.2 shows the feed design conditions.

Specifications	Values
Molar flow (Kmol/h)	2219,05
Mass flow (Kg/h)	201490
Pressure (Kg/cm²)	15,03
Temperature (°C)	159,1

Table II.2 Feed design conditions.

b) Debutanizer dimension design

The table II.3 summarizes the main design characteristics of the C102 debutanizer used in the Aspen HYSYS simulation.

Sizing	Value
Diameter (m)	2,5
Trays number (tray)	32
Trays spacing (m)	0,6
Feed tray position (tray)	21
Overall efficiency (%)	70

Table II.3 Debutanizer design dimension.

b) Design condition of the debutanizer

The table II.4 represents the operating conditions of debutanizer.

Parameters	Value
Reboiler temperature (°C)	254
Top reflux rate (t/h)	109,160
Bottom reflux rate (t/h)	217,450

Table II.4 Operating conditions of debutanizer.

II.2.2. Simulation of design case

After simulation, we will compare between the result we get and the design ones, the comparison will be shown in the following tables:

The table II.5 shows the tower's design and simulated design parameters

Parameters	Design	Simulated design	Relative deviation (%)
Top temperature (°C)	72,10	69,53	3,564493759
Bottom temperature (°C)	212,0	211	0,471698113

LPG temperature (°C)	57,60	58,26	1,145833333
LPG flow rate (t/h)	37,060	37,0625	0,006745818
Condensates temperature (°C)	212,0	211	0,471698113
Condensate flow rate (t/h)	164,43000	164,42	0,006081615
Condensate heat duty QC (kcal/h)	$1,1 \times 10^7$	$1,4 \times 10^7$	0,272727273
Reboiler heat duty QR (kcal/h)	$1,21 \times 10^7$	$1,4 \times 10^7$	0,166666667

Table II.5 Tower's design and simulated design parameters.

The table II.6 represents the design and simulated design composition for LPG and condensate.

Component	Design case		Simulated case	
	LPG	CONDENSATE	LPG	CONDENSATE
N₂	0,001077	0	0,001077	0
CO₂	0,000013	0	0,0000136	0
CH₄	0,000013	0	0,0000136	0
C₂H₆	0,002810	0	0,002807	0
C₃H₈	0,532954	0,000255	0,533164	0,0001
iC₄H₁₀	0,172641	0,008466	0,180698	0,0044
nC₄H₁₀	0,289563	0,051672	0,282220	0,0553
iC₅H₁₂	0,000818	0,075375	0	0,0758
nC₅H₁₂	0,000191	0,107927	0	0,1081
C₆H₁₄	0	0,144013	0	0,1440
C₇H₁₆	0	0,140191	0	0,1402
C₈H₁₈	0	0,113392	0	0,1134
C₉H₂₀	0	0,093404	0	0,0934

C₁₀H₂₂	0	0,068214	0	0,0682
C₁₁H₂₄	0	0,053045	0	0,0531
C₁₂H₂₆	0	0,144040	0	0,1441
TOTAL	1,000080	0,999994	0,9999596	1,0001

Table II.6 Design and simulated design composition for LPG and condensate.

The table II.7 shows the LPG and condensates design and simulated design specification.

Parameters	Design	Simulated design
C₂- LPG %	0,2823	0,28176
C₅⁺ LPG %	0,1008	0,282220
RVP Condensate (Kg/cm²)	0,5097	0,5023

Table II.7 LPG, condensates design, and simulated design specification.

II.2.3. HYSYS validation

After simulating the design parameters, comparing the simulated results to the designed ones, and after calculating the relative deviation, which was under 4%, we can conclude that our program is reliable and its results are correct. That leads us to use it to simulate the current case and to optimize with it.

III.3. Simulation of current case

Now we will simulate the current case in order to find the exact malfunction.

II.3.1. Display of current case

The following table are the current case's data:

a) Current composition

The table II.8 represents the current feed composition.

Feed component	Molar fractions
N₂	0,0000
CO₂	0,0000

CH₄	0,00
C₂H₆	0.0054
C₃H₈	0.2573
iC₄H₁₀	0.0935
nC₄H₁₀	0,1455
iC₅H₁₂	0.0869
nC₅H₁₂	0.0981
C₆H₁₄	0.0588
C₇H₁₆	0.0616
C₈H₁₈	0.0604
C₉H₂₀	0.0348
C₁₀H₂₂	0.0955
C₁₁H₂₄	0.0000
C₁₂H₂₆	0.0000
Total	1.0000

Table II.8 Current feed composition.

b) Current feed condition

The table II.9 shows the current feed condition.

Specification	Values
Mass flow (t/h)	49,4
Temperature (°C)	117,7
Pressure (Kg/cm²)	14,60

Table II.9 Current feed condition.

c) Current operating condition of the debutanizer

The table II.10 illustrates the current operating condition of the debutanizer.

Parameters	Current case
-------------------	---------------------

Top temperature (°C)	71,2
Bottom temperature (°C)	192,9
Reboiler temperature (°C)	206,4
Reflux flow rate (t/h)	26,2
Reboiler duty (t/h)	179,7

Table II.10 Current operating condition of the debutanizer.

II.3.1. Simulation of current case

a) Current case simulation

First, entering the feed parameters (composition and conditions) shown in the tables above. Then, converging the rectification column, by entering the parameters mentioned before.

b) Results display

After simulating the current case operating parameters, and current feed conditions we have results by HYSYS, the results will be shown in the following table:

The table II.11 shows the tower's conditions.

	Values
Top temperature (°C)	66.88
Bottom temperature (°C)	181.6
LPG (t/h)	14.93
CONDESATES (t/h)	34.47

Table II.11 shows the tower's conditions.

The table II.12 represents the condensates and the LPG's composition.

Component	Current case	
	Condensates	LPG
N ₂	0	0
CO ₂	0	0
CH ₄	0	0
C ₂ H ₆	0	0,011880
C ₃ H ₈	0,00002	0,565988
iC ₄ H ₁₀	0,0129765	0,190240
nC ₄ H ₁₀	0,007393	0,231780
iC ₅ H ₁₂	0,159838	0,0001
nC ₅ H ₁₂	0,180533	0
C ₆ H ₁₄	0,108212	0
C ₇ H ₁₆	0,113365	0
C ₈ H ₁₈	0,111156	0
C ₉ H ₂₀	0,064044	0
C ₁₀ H ₂₂	0,1757520	0
C ₁₁ H ₂₄	0	0
C ₁₂ H ₂₆	0	0
Total	1	1

The table **II.13** illustrates the LPG and condensate's specification.

Parameters	Current case
C ₂ ⁻ LPG %	1,2
C ₅ ⁺ LPG %	0,01
RVP Condensate (Kg/cm ²)	0.7839
LPG mass flow	14.62

Table **II.13** LPG and condensate's specification.

II.3.2. Result interpretation

Based on the values obtained, the operating conditions satisfy the required product specifications. The LPG composition remains within acceptable limits, with a low C5+ content of 0.01% and a controlled C2– content of 1.2%, indicating an efficient separation performance in the debutanizer column. For the condensate product, the Reid Vapor Pressure (RVP) is equal to 0.7839 kg/cm², which is still acceptable but relatively close to the upper desired range. This suggests that the condensate still contains a certain amount of light hydrocarbons, which may increase its volatility. Therefore, further optimization of the operating parameters could help reduce the RVP value and improve condensate stability and storage safety while maintaining the LPG specifications within the required limits

II.3.3. Adjustment with HYSYS

Figure II.6 represents the effect of the reflux rate on the condensate RVP. After studying the influence of the reflux rate on the condensate RVP, we notice that the RVP value increases when the reflux rate increases. This means that increasing the reflux rate makes the condensate more volatile because more light hydrocarbons are present in the product. Therefore, in order to reduce the RVP and obtain a more stable condensate, it is necessary to decrease and properly control the reflux rate while keeping suitable operating conditions for the separation process.

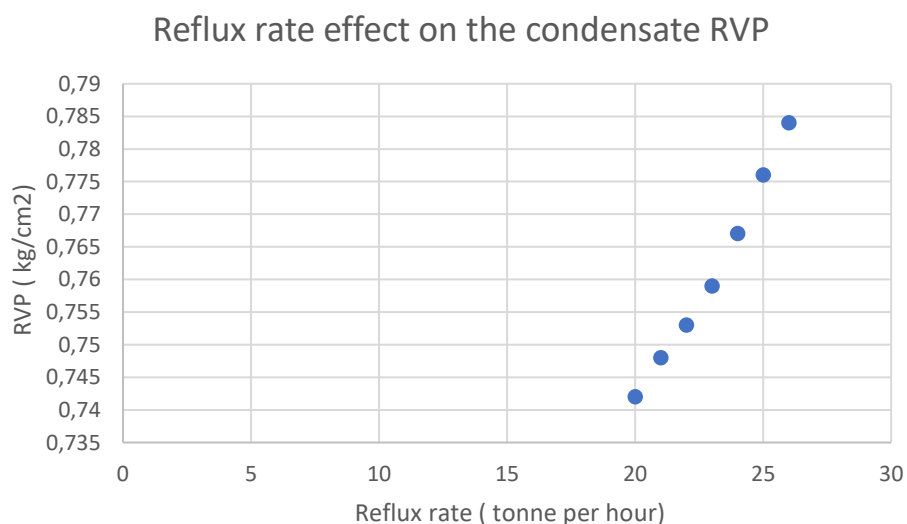


Figure II.6 reflux rate effect on the RVP

The results obtained indicate that the reflux rate has a significant effect on the condensate quality. Therefore, an Adjust operation was implemented in the simulation to automatically regulate this parameter and ensure that the desired product specifications are achieved.

The Adjust operation is a calculation tool in HYSYS that automatically modifies a selected process variable in order to satisfy a defined specification or operating target. It functions by varying an independent variable, known as the manipulated variable, until the required value of another parameter, referred to as the target variable, is achieved. In order to make this operation we follow these steps:

- From the tools pallets choose the adjuster;
- Choose the adjusted variables and the target variables and write down the target value;
- Specify the allowed tolerance, step size, maximum bound and the minimum one, and the maximum number of iterations;
- The last step click start.

The final results we get is a flow rate with 23 tonnes per hour, after we insert this value In our column we find the results shown in the table **II.14**:

Parameters	Current case
C2 ⁻ LPG %	1,17
C5 ⁺ LPG %	0,16
RVP Condensate (Kg/cm ²)	0.7589

Table **II.14** results after adjustment.

Conclusion

This chapter presented the development and validation of the Aspen HYSYS model of the C102 debutanizer. The comparison between the simulated and design cases confirmed the reliability of the simulation model, with acceptable deviations for the main operating parameters. The validated model was then used to evaluate the current operating conditions and identify the reflux flow rate as the operating parameter with the greatest influence on condensate RVP. Finally, the Adjust operation demonstrated that reducing the reflux flow rate from 26.2 t/h to 23 t/h improves condensate quality

while maintaining the required LPG specifications. These results establish the basis for the optimization study presented in the next chapter.

Chapter III

Optimization with PSO algorithm

Introduction

This chapter presents the application of the Particle Swarm Optimization (PSO) algorithm to optimize the operating conditions of the C102 debutanizer. Unlike the Adjust operation in Aspen HYSYS, which modifies a single variable to satisfy a predefined target, PSO is a global optimization algorithm capable of exploring the search space to determine the optimal operating conditions. In this study, PSO is applied to identify the reflux flow rate that minimizes the condensate Reid Vapor Pressure (RVP) while maintaining the required LPG quality specifications.

III.1. The PSO algorithm

III.1.1. Definition of PSO

Particle Swarm Optimization (PSO) is an optimization technique based on a group of candidate solutions called particles, inspired by the collective behavior of birds and fish, where particles explore the search space and improve their positions by learning from their own best experience and the best experience found by the whole swarm to reach an optimal solution [26].

III.1.2. Principle of Particle Swarm Optimization (PSO)

PSO is a swarm-based optimization method inspired by the behavior of birds searching for food. In this method, each particle updates its position and velocity based on its own best solution (pbest) and the global best solution (gbest). This update reduces the distance (gap) between the current position and the best solutions, allowing particles to gradually move toward the optimal solution [27].

Figure III.3 illustrates the fundamental mechanics of Particle Swarm Optimization

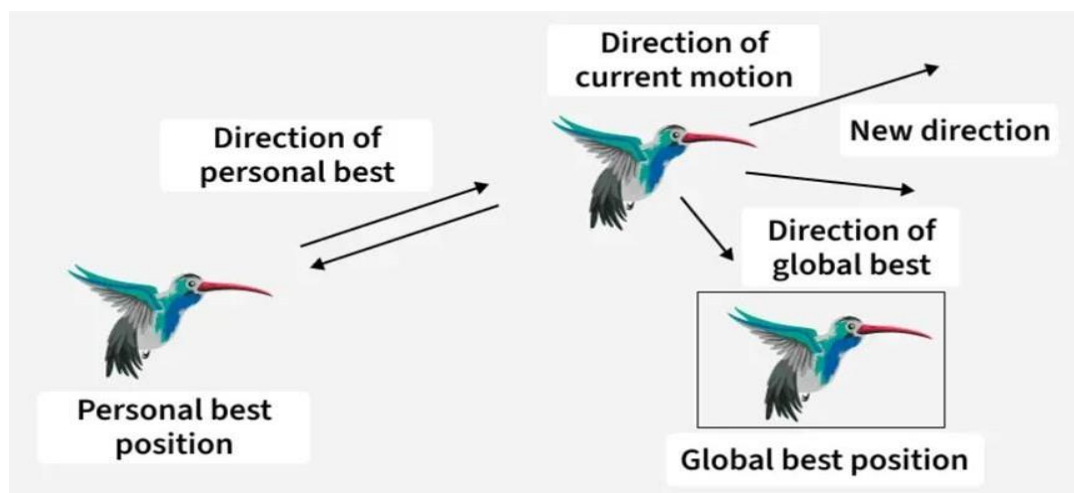


Figure III.3 the fundamental mechanics of the PSO [11].

III.1.3. Used equations

The PSO algorithm using MATLAB uses a set of equation in order to find the good velocity and position, these equations are the following [28]:

a) velocity equation

$$v_i(t+1) = w \cdot v_i(t) + C_1 \text{rand}_1(P_{\text{best } i}(t) - x_i(t)) + C_2 \text{rand}_2(G_{\text{best } i}(t) - x_i(t)) \quad (19)$$

b) Position equation

$$x_i(t+1) = x_i(t) + v_i(t+1) \quad (20)$$

Where :

i : Particle number.

t : Iteration number.

v : Particle velocity.

x: Particle position.

rand: Random function.

P_{best} : Best position visited by the particle.

G_{best} : Best position found by the entire swarm.

w: Inertia weight.

C_1, C_2 : Acceleration coefficients.

III.1.1. PSO algorithm using MATLAB Workflow

The Particle Swarm Optimization (PSO) algorithm works by following a specific set of steps, as shown in the flowchart below.

a) Each particle in PSO has

Position (x): current solution

Velocity (v): direction and speed of movement

Fitness value: quality of the solution

b) Each particle stores

P_{best} : The best position found by itself

G_{best} : The best position found by the entire swarm

The following figure **III.4** illustrates the flowchart of the PSO algorithm

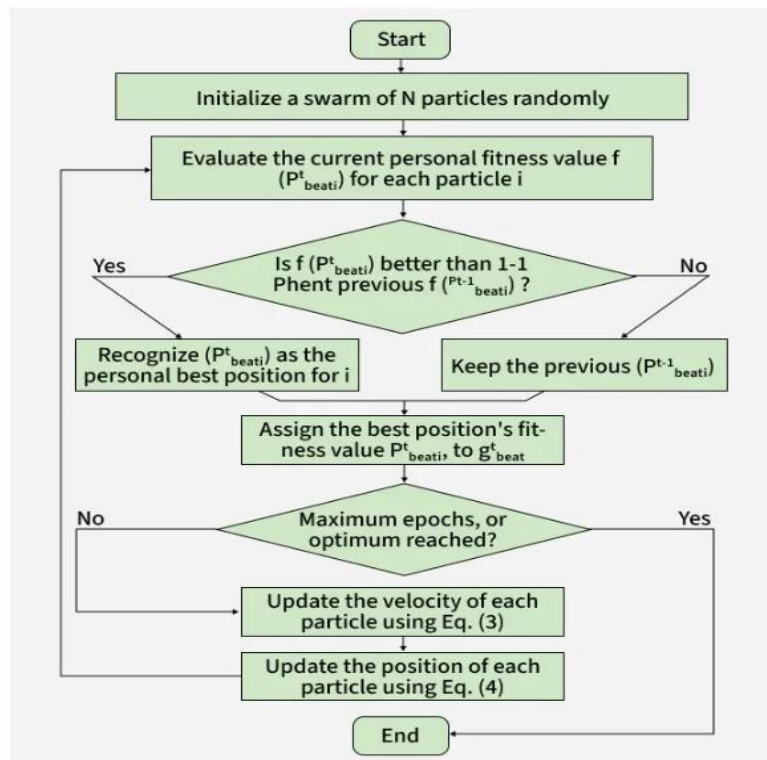


Figure III.4 the PSO workflow [12]

III.1. MATLAB definition

MATLAB (Matrix Laboratory) is a high-level programming and numerical computing environment developed by MathWorks. It is widely used for numerical analysis, algorithm development, and optimization. In this study, MATLAB was used to implement the Particle Swarm Optimization (PSO) algorithm and optimize the operating conditions of the C102 debutanizer in conjunction with Aspen HYSYS [29].

III.2. Optimization with PSO algorithm using MATLAB

The objective of the optimization is to minimize the condensate Reid Vapor Pressure (RVP), which is the main indicator of condensate stability. During the optimization, the LPG quality specifications were maintained within their acceptable limits. Therefore, the optimization problem can be expressed as:

Minimize: Condensate RVP

Subject to:

- C_2^- in LPG $\leq 1.2\%$

- C_5^+ in LPG $\leq 0.4\%$

Figure III.6 illustrates the Convergence of PSO optimization applied to column C102

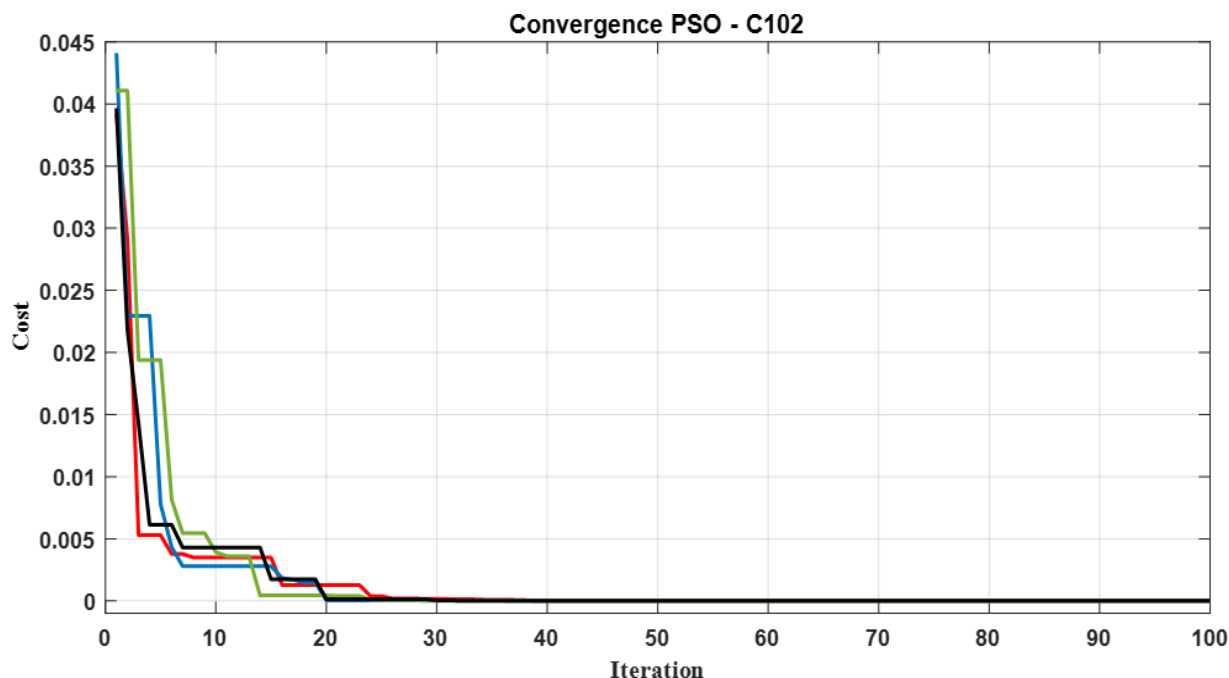


Figure III.6 Convergence of PSO optimization applied to column C102.

The results obtained from the PSO algorithm using MATLAB are resumed in the

table III.1.

Parameters	Reflux rate (t/h)	T bottom (°C)	T reboiler (°C)	RVP of condensate (kg/cm ²)	C2- LPG (%)	C5+ LPG (%)	LPG Flow (t/h)
The results	23.000	142.000	190.000	0.7589	1.1700	0.1600	14.6200

Table III.1 PSO algorithm using MATLAB results.

➤ Interpretation of Results

The figure shows the convergence curves obtained from several runs of the PSO algorithm using MATLAB for optimizing the operating parameters of column C102. A rapid decrease in the cost function is observed from the very first iterations, reflecting the algorithm's ability to quickly identify optimal regions within the search space. Despite the differences observed at the start of the simulations due to the random initialization of the particles, all curves converge to a very low final value, close to zero.

This convergence toward a single solution demonstrates the robustness and stability of the PSO, as well as its low sensitivity to initial conditions. The results obtained confirm that the algorithm is capable of effectively determining the optimal operating parameters for the C102

column while meeting the quality specifications for LPG and condensate. Thus, PSO is a powerful tool for optimizing separation processes at the Hassi R'Mel gas complex.

The results obtained after implementing the Adjust function show that the process has achieved a more stable operating state, with a notable improvement in condensate quality, reflected in a decrease in VAP from 0.7839 to 0.7589 kg/cm². However, this optimization is accompanied by a slight increase in the C5+ fraction in the LPG, indicating a trade-off between the quality of the two products. Overall, setting the reflux rate to 23 t/h allows for compliance with operational constraints while maintaining acceptable product specifications, confirming the validity of the control strategy adopted.

Conclusion

The PSO algorithm using MATLAB successfully optimized the operating conditions of the C102 debutanizer by minimizing the condensate Reid Vapor Pressure (RVP) while maintaining the required LPG quality specifications. The results demonstrate the robustness and effectiveness of PSO, making it a reliable optimization tool for improving the performance of the separation process.

General conclusion

Conclusion

The purpose of this study was to analyze and optimize the debutanizer column (C102) at the Hassi R'Mel natural gas complex. The thesis begins with an overview of the complex, its history, and the theoretical foundations of natural gas processing. It also presents the composition and treatment of natural gas, as well as the principles of rectification and the main operating parameters affecting separation performance and product quality.

A detailed Aspen HYSYS simulation was developed and validated using the design operating conditions. The validated model was then used to analyze the current operating conditions and identify the influence of key parameters on product specifications, particularly the effect of the reflux rate on condensate Reid Vapor Pressure (RVP).

To improve process performance, a Particle Swarm Optimization (PSO) approach was applied to determine the optimal operating conditions. The obtained results demonstrated that the selected operating parameters ensure compliance with product quality requirements while improving condensate stability and maintaining acceptable LPG specifications.

Overall, the results highlight the effectiveness of simulation and optimization tools in enhancing process performance and product quality. This study demonstrates the value of combining artificial intelligence techniques with process simulation to support decision-making and improve the operation of natural gas processing facilities.

In the end we suggest to apply process intensification in the natural gas process facilities, such as using one rectification column instead of two (combine the C101 and C102 in one column); Furthermore linking MATLAB and ASPEN HYSYS grant the chemical engineers a simple method to optimize.

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Annex

I. Presentation of the industrial site of Hassi R'Mel

A.1.1. Geographic location

Hassi R'Mel has a very strategic geographic location and a big surface, it extends for 2100 km² between the wilayas of Ghardaïa and Laghouat, in the middle of the Algerian desert, the coordination of its gas field are (2°55'–3°00'E; 33°15'–33°45'N) [4], nearly 50 km south Laghouat, it's altitude is about 760 stretches over 80 km in a NS direction and 60 km WE [5].

The figure A.1 represents the geographic location of HASSI R'MEL [1].

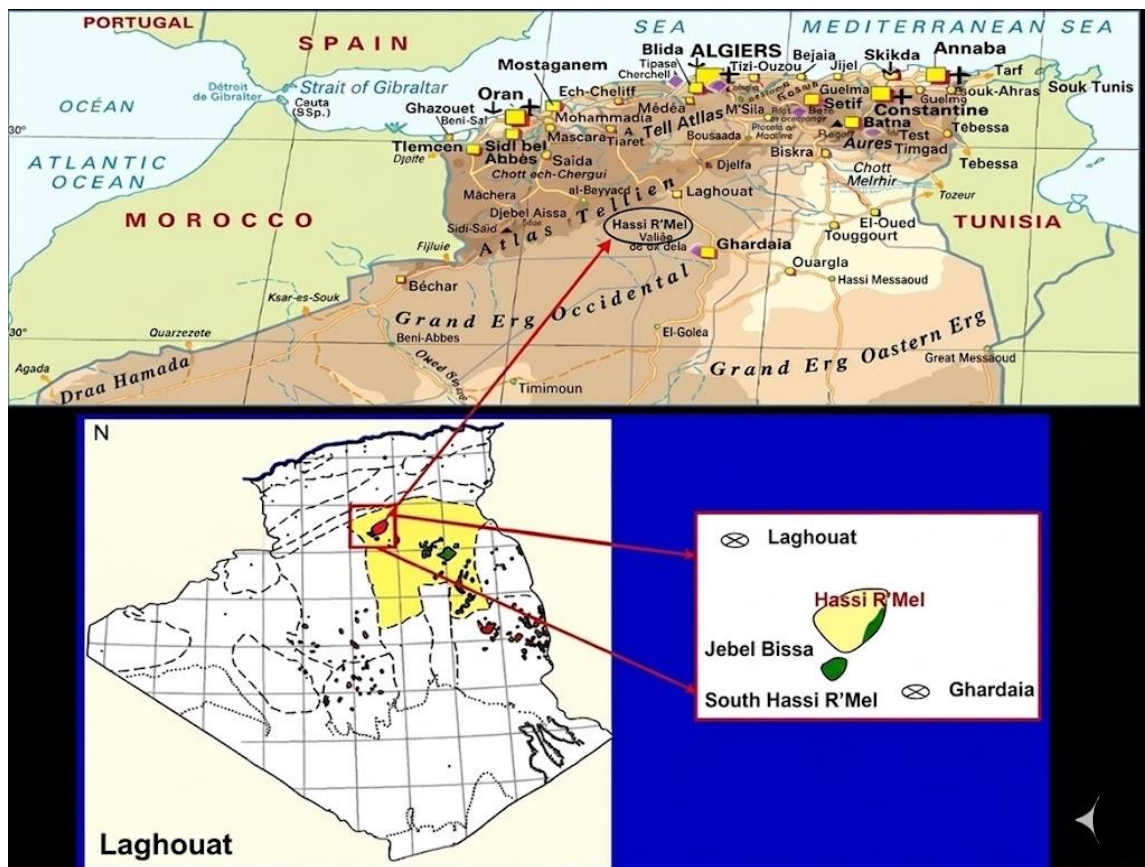


Figure A.1 Geographic location of Hassi R'Mel [1].

A.1.2. Installations and zones

Hassi R'mel's gas field consists of three main areas [6]:

a) North area

This area consists of:

- Module 3;
- The depropanizer unit;
- A northern compression station;

- The Oil Treatment Centre (CTH).

b) Center area

This area has:

- Modules 0, 1 and 4;
- The Storage and Transfer Centre (CSTF);
- The Gas Dispatching Centre (CNDG);
- The Oil Treatment Centre (CTH);
- The Phase B unit.

c) South area

This area consists of:

- Module 2;
- A southern compressor station;
- Djebel Bissa;
- Southern HR;
- The Oil Treatment Centre (CTH).