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Presented by:

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*Topic*

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**Simulation of TBP distillation using Aspen HYSYS  
for the physicochemical properties of petroleum  
fractions.**

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Defended on June 14th, 2023.

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Oringo Simon, Bouhamza Ismail.

## *Dedication*

*This work is dedicated to all the curious minds, relentless explorers, and passionate seekers of knowledge. To those who embrace the pursuit of understanding and push the boundaries of human understanding, this work is an homage to your unwavering spirit.*

*To our mentors and advisors, thank you for guiding us on this intellectual journey and instilling in us the values of rigorous inquiry. Your wisdom and guidance have been invaluable in shaping this research. We extend our deepest gratitude to our families and loved ones for their unwavering support, patience, and belief in our abilities. Your encouragement and understanding have been the bedrock of our academic pursuit. May this dedication serve as a testament to the dedication and perseverance required in the pursuit of scientific excellence.*

*With utmost gratitude,*

*Oringo Simon, Bouhamza Ismail.*

# Acronym

	IBP .....21
<b>A</b>	<b>L</b>
acentric factor	Liquefied Natural Gas
$\omega$ 49	LNG .....31
American Petroleum Institute gravity	
API.....49	<b>T</b>
American Society for Testing and Materials	True boiling point
ASTM.....10	TBP.....6
Atmospheric distillation unit	
ADU .....15	<b>U</b>
	Universal Oil Products company
<b>C</b>	UOP .....43
Critical Pressure	
Pc .....49	<b>V</b>
Critical Temperature	Vacuum distillation unit
Tc .....49	VDU .....15
critical volume	Vapor pressure
Vc .....49	Ps61
	Pv .....61
<b>E</b>	
End Boiling Point	<b>W</b>
EBP.....21	Watson factor
	Kuop .....49
<b>I</b>	
Initial Boiling Point	

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# **General Introduction**

The distillation process plays a crucial role in the petroleum industry as it enables the separation of crude oil into various valuable components based on their boiling points. Understanding the behavior and properties of these petroleum fractions is essential for efficient refining processes and product development. Accurate knowledge of the physicochemical properties of these fractions is vital for optimizing their utilization and ensuring compliance with product specifications.

Traditionally, the determination of physicochemical properties of petroleum fractions involved time-consuming experimental methods that require meticulous accuracy and expensive equipment. However, advancements in computational techniques and simulation software have revolutionized the field, offering a more efficient and cost-effective approach.

This master's thesis focuses on the simulation of TBP (true boiling point) distillation using Aspen HYSYS, a widely recognized and powerful process simulation tool. The objective is to investigate the suitability and accuracy of Aspen HYSYS in predicting the physicochemical properties of petroleum fractions obtained through distillation.

By employing Aspen HYSYS, this study aims to simulate the distillation process and generate data on the physicochemical properties of various petroleum fractions. These properties may include boiling points, densities, viscosities, and composition profiles, among others. Comparisons will be made between the simulation results obtained from Aspen HYSYS and data derived from traditional experimental techniques and analytical methods.

The utilization of simulation software offers several advantages, including reduced time requirements, cost-effectiveness, and flexibility in assessing various scenarios. Additionally, simulation allows for the exploration of parameters that are difficult to manipulate in laboratory experiments, enabling a deeper understanding of the distillation process and the behavior of petroleum fractions.

The outcomes of this research have the potential to provide valuable insights into the accuracy and reliability of Aspen HYSYS as a simulation tool for predicting the physicochemical properties of petroleum fractions. Furthermore, it can contribute to the development of more efficient and sustainable refining processes, aiding in the optimization of product quality and resource utilization in the petroleum industry.

To achieve the objectives of this study, a comprehensive literature review will be conducted to gather existing knowledge on distillation processes, petroleum fractions, and simulation techniques. Subsequently, the simulation experiments using Aspen HYSYS will be performed, and the obtained results will be compared and evaluated against reference data. Any discrepancies or deviations will be analyzed and discussed, providing critical insights into the strengths and limitations of the simulation approach.

# **Chapter 1**

## **TBP Distillation**

## 1. Chapter 1 TBP Distillation

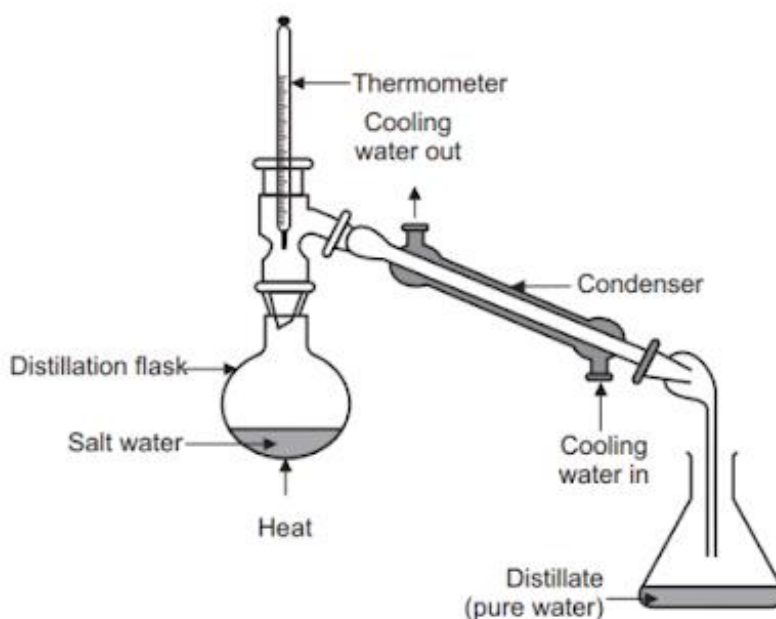
### 1.1 Introduction

Distillation is a separation technique that is widely used in the chemical, pharmaceutical, and petroleum industries for purifying and separating liquids. The process is based on the principle that different components of a mixture have different boiling points, and it involves heating the mixture to produce vapor, which is then condensed back into a liquid to separate the individual components. The general process is demonstrated in Figure 1.1.[1]

The earliest recorded use of distillation dates back to the 10th century, when Arab chemists used it to produce perfumes and distilled beverages. Over the years, the technique has been refined and has become a crucial tool for the separation of liquids in various industrial applications.[1]

In the chemical industry, distillation is used to purify chemicals, separate mixtures of liquids, and produce high-purity products. In the petroleum industry, distillation is used to refine crude oil into different fractions, such as gasoline, diesel, and jet fuel.[1]

There are various types of distillation processes, including simple distillation, fractional distillation, vacuum distillation, and steam distillation. The choice of the process depends on the composition of the mixture, the desired purity of the product, and the operating conditions.[1]



**Figure 1.1.** A simple figure illustrates the general structure of distillation

### 1.1.1 Definition of TBP distillation

TBP distillation, also known as True Boiling Point distillation, is a type of fractional distillation process that separates a mixture of liquids based on their boiling points. The term "true boiling point" refers to the temperature at which a liquid boils at a given pressure, taking into account the composition of the mixture. In TBP distillation, a distillation column is used to separate the components of a mixture, with each component condensing at a different height in the column based on its boiling point. The resulting product is a series of fractions with each fraction containing a different range of boiling points.[2]

TBP distillation is commonly used in the petroleum industry to refine crude oil into different fractions, such as gasoline, diesel, and jet fuel. It is also used in the chemical industry for the separation of volatile and semi-volatile components in mixtures.

The TBP distillation process can be accurately predicted using thermodynamic models and simulation software, making it a valuable tool for the separation and purification of liquids in various industrial applications.[3]

### 1.1.2 A simple description of TBP distillation

This method, as described in Figure 1.2, uses a batch distillation operation that incorporates more than 100 theoretical plates and a high reflux ratio of 100. This is an idealized method to achieve the best possible separation in distillation, made possible by a large number of theoretical plates (stages) for liquid-vapor contact in the column and an extremely high reflux ratio.[4]

As an example, consider distillation of a binary mixture of compounds A (70% by volume) and B (30% by volume), with boiling points  $T_a$  and  $T_b$ , respectively. Figure 1.3 illustrates the distillation curve that would be obtained if this mixture were distilled using the TBP method, with an ideal separation of A and B as pure compounds. Because of the TBP distillation conditions, first the lower boiling component A is distilled off without any contamination with B, and following the complete vaporization of A, B is distilled off as a pure compound.[4]

Note that because a large number of plates and a high reflux ratio in the column, temperature remains constant during evaporation of A until this entire compound is boiled off, as would be seen in the distillation of a pure compound.[4]

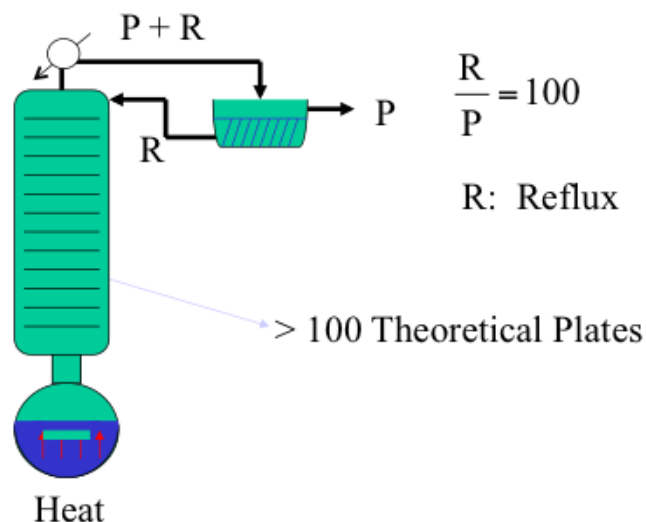


Figure 1.2. TBP distillation apparatus

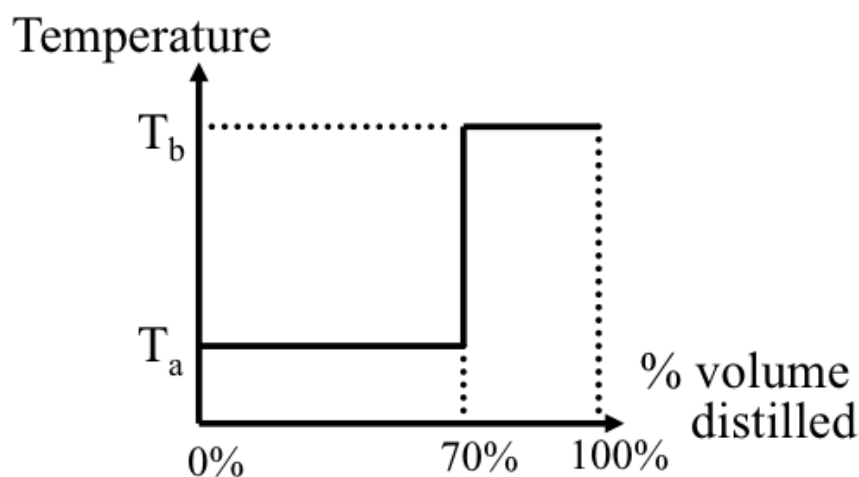


Figure 1.3. Distillation curve for an ideal separation of the components A and B in a binary mixture

### 1.1.3 Importance and applications of TBP distillation

TBP distillation is an important technique in the petroleum industry as it provides a detailed and accurate characterization of the composition of crude oil and its fractions. TBP distillation involves heating a sample of crude oil under carefully controlled conditions and collecting the distillate at different temperature intervals to determine the boiling points of the various components.[3]

The importance of TBP distillation in the petroleum industry can be seen in the following ways:



- **Product quality control:** TBP distillation is used to control the quality of various petroleum products such as gasoline, diesel, jet fuel, and lubricating oils. The boiling point range of each product is specified to meet the required performance characteristics, and TBP distillation is used to ensure that the product meets these specifications.[3]
- **Process optimization:** TBP distillation is used to optimize the refining process by determining the properties of different crude oil fractions. The information obtained from TBP distillation is used to design the appropriate refining processes and equipment for the specific crude oil, resulting in increased efficiency and reduced costs.[3]
- **Environmental regulation:** TBP distillation is used to determine the composition of crude oil and its fractions, which is important for environmental regulation. The information obtained from TBP distillation is used to determine the content of harmful impurities such as sulfur and metals, which can be harmful to the environment and public health.[3]
- **Research and development:** TBP distillation is an important tool for research and development in the petroleum industry. The information obtained from TBP distillation is used to develop new products and improve existing products, as well as to develop new refining processes and equipment.[3]

Moreover, distillation is a key process in oil refining, as it is used to separate crude oil into its various components based on their boiling points. The different fractions obtained from distillation are further processed to produce various products such as gasoline, diesel, jet fuel, and lubricating oils. Some of the applications of distillation in oil refining are:

- **Separation of crude oil:** The first step in oil refining is the separation of crude oil into its various components by distillation. The crude oil is heated in a distillation column, and the vapors that rise up the column are condensed and collected in different trays according to their boiling points.[3]
- **Production of gasoline:** The gasoline fraction obtained from crude oil distillation is further processed in a catalytic cracking unit to produce high-octane gasoline.[3]
- **Production of diesel:** The diesel fraction obtained from crude oil distillation is further processed in a hydrocracking unit to produce high-quality diesel fuel.[3]

- **Production of jet fuel:** The kerosene fraction obtained from crude oil distillation is further processed in a hydrotreating unit to produce jet fuel.[3]
- **Production of lubricating oils:** The heavy fractions obtained from crude oil distillation are further processed in a hydrocracking unit to produce lubricating oils.[3]
- **Removal of sulfur:** Distillation is used to remove sulfur from crude oil to produce low-sulfur fuels, which are less polluting.[3]
- **Recovery of solvents:** Distillation is used to recover solvents used in various refining processes, reducing waste and saving costs.[3]
- **Fractionation of intermediate products:** Distillation is used to separate intermediate products, such as naphtha and gas oil, into different fractions based on their boiling points, which are then further processed to produce various products[3]

## 1.2 Fundamentals of Distillation

### 1.2.1 Overview of the basic principles of distillation

The main principle of distillation is to separate individual components from a mixture of multiple components.

Distillation is a well-defined separation unit consisting of the partial evaporation of a liquid mixture and successive condensation, to obtain a product with a composition that differs from that of the original mixture. Distillation had a broader meaning in ancient and medieval times because nearly all purification and separation operations were subsumed under the term distillation, such as filtration, crystallization, extraction, sublimation, or mechanical pressing of oil.[5]

In industrial applications, distillation is a unit operation of practically universal importance, but is a physical separation process and not a chemical separation process. It is used for separating a liquid mixture.

The process of distillation works basing on the principle of volatility of the different components that are available in the mixture. This is caused by the difference in boiling points of the individual components where that with a lower boiling point us considered most volatile and vice versa.[5]

As the process begins the vapors of the least volatile liquid rise and are then condensed back into a liquid which is close to a pure substance. The addition of a thermometer is to closely monitor

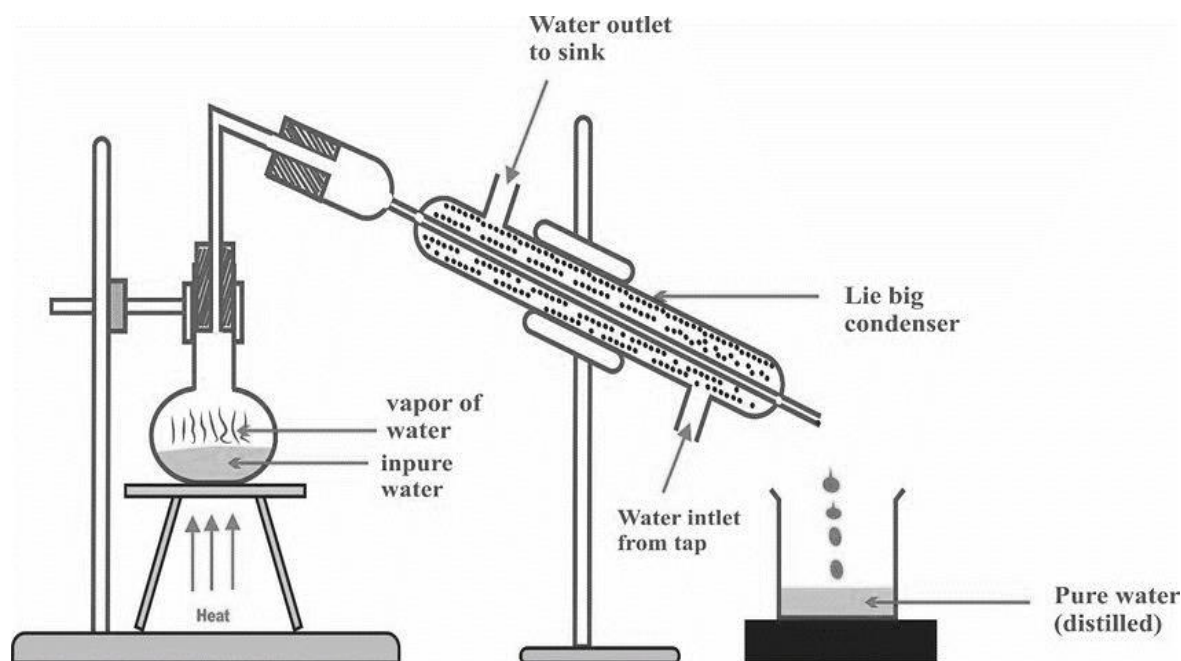
the current temperature of the vapors formed to ensure that the distillate obtained is as close to pure as possible.[5]

When it comes to the refining of petroleum, fractional distillation is used on a large scale in a process called ASTM distillation.

### 1.2.2 TBP Comparison with other distillation techniques

True boiling point (TBP) distillation is one of several distillation techniques used in the petroleum industry to separate crude oil into its various components. The following describes how TBP distillation compares to other distillation techniques:

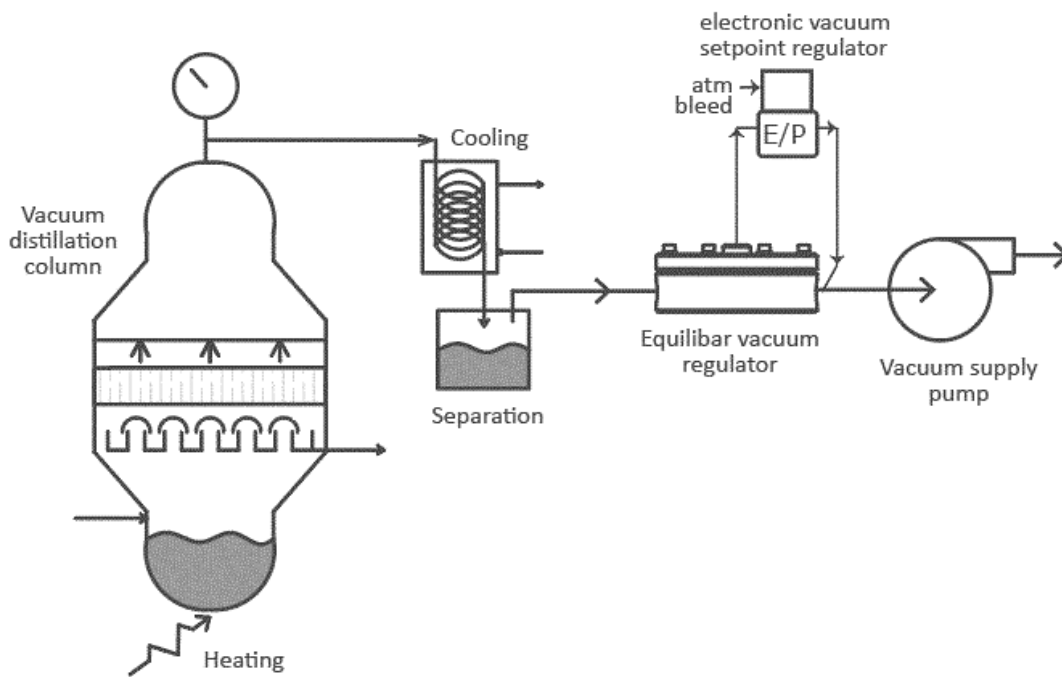
- A. Simple Distillation:** Simple distillation as illustrated in Figure 1.4 is a basic technique that uses a single distillation column to separate two or more components in a mixture based on their boiling points. It is typically used for the separation of low-boiling components in crude oil, such as natural gas liquids, but is not suitable for the separation of high-boiling components. TBP distillation, on the other hand, can separate a much wider range of components in crude oil based on their boiling points, making it a more versatile technique for the analysis of crude oil.[6]



**Figure 1.4.** A figure representing simple distillation

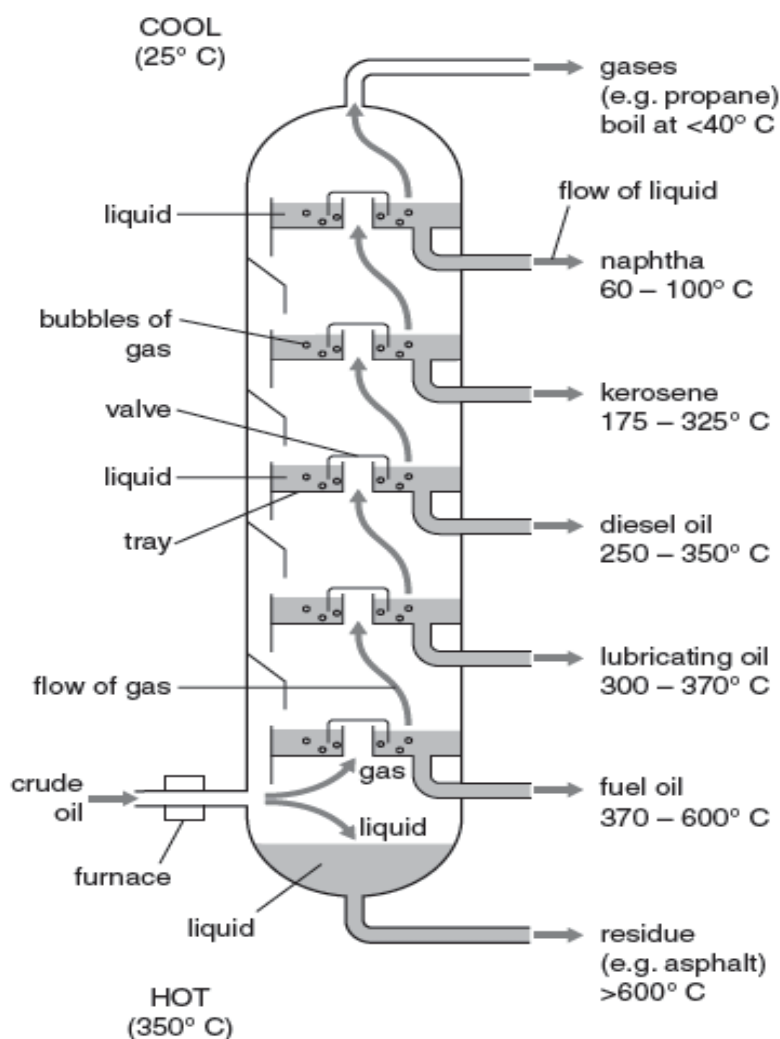
- B. Vacuum Distillation:** Vacuum distillation as illustrated in Figure 1.5 is a technique that reduces the boiling point of high-boiling components in crude oil by lowering the pressure

in the distillation column. This allows the separation of heavier components that would otherwise decompose or polymerize at atmospheric pressure. TBP distillation can also be performed under vacuum conditions, but it typically requires a larger and more complex distillation apparatus than vacuum distillation.[7]



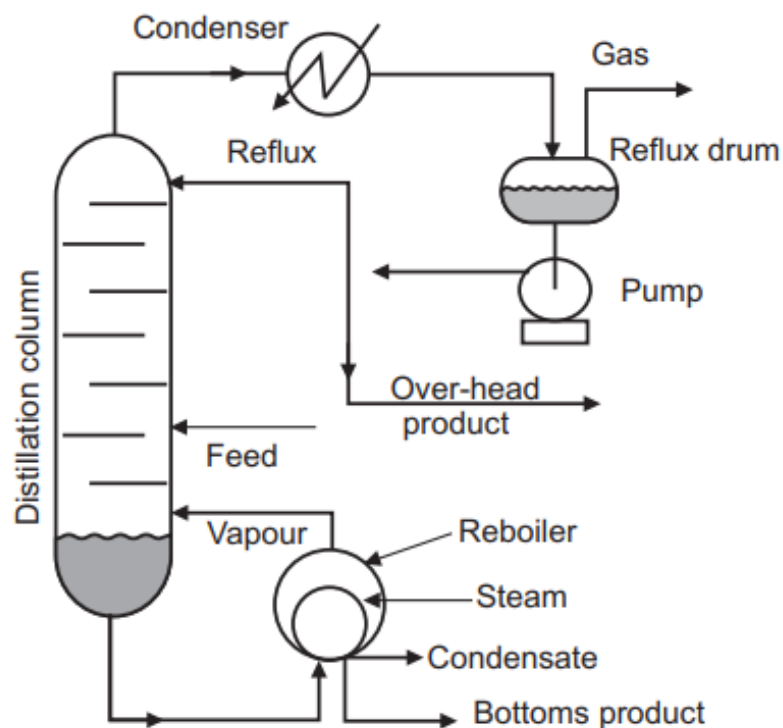
**Figure 1.5.** A figure illustrates the structure of vacuum distillation

**C. Fractional Distillation:** Fractional distillation as illustrated in Figure 1.6 is a technique that uses multiple distillation columns or trays to separate a mixture into multiple fractions based on their boiling points. It is typically used for the separation of intermediate-boiling components in crude oil, such as gasoline, kerosene, and diesel fuel. TBP distillation can also be used for the separation of these components, but it is more commonly used for the analysis of the entire boiling point range of crude oil.[8]



**Figure 1.6.** A figure illustrates the general structure of fractional distillation

**D. Molecular Distillation:** Molecular distillation as illustrated in Figure 1.7 is a technique that uses high vacuum and short residence times to separate components in a mixture based on their molecular size and shape. It is typically used for the separation of high-purity specialty chemicals and pharmaceuticals. TBP distillation is not typically used for the separation of individual molecules in a mixture, but it can provide a detailed analysis of the boiling point range and composition of crude oil.[9]



**Figure 1.7.** A figure illustrates the general structure of molecular distillation

In summary, TBP distillation is a versatile and widely used technique for the analysis of crude oil, as it can separate a wide range of components based on their boiling points. Although other distillation techniques may be more suitable for specific applications or components, TBP distillation is a key tool in the petroleum industry for characterizing and refining crude oil.

### 1.3 Equipment and Process of TBP Distillation

#### 1.3.1 Overview of the equipment used in TBP distillation

TBP distillation is an important technique used in refineries to separate and analyze the components of crude oil and petroleum products based on their boiling points. The equipment used in TBP distillation in refineries typically includes the following components

- Atmospheric distillation unit (ADU): The ADU is the primary distillation unit in a refinery and is used to separate the crude oil into different fractions based on their boiling points. The ADU consists of a distillation column with trays or packing material to provide a large surface area for vapor-liquid contact, a reboiler to vaporize the crude oil, and a condenser to condense the vaporized components. The ADU typically operates at atmospheric pressure.[6]
- Vacuum distillation unit (VDU): The VDU is used to distill the heavy fractions from the ADU that have higher boiling points and are not efficiently separated at atmospheric pressure. The VDU operates under reduced pressure, typically around 10-50 mmHg, to lower the boiling points of the components and increase the separation efficiency. The VDU consists of a distillation column with trays or packing material, a reboiler, a vacuum pump to reduce the pressure in the column, and a condenser to condense the vaporized components.[6]
- Fractionation column: A fractionation column is used to further separate the individual components obtained from the ADU or VDU into more specific fractions based on their boiling points. The fractionation column is typically smaller than the ADU or VDU and may be operated at atmospheric pressure or under reduced pressure, depending on the requirements of the separation.[10]
- Temperature probes: Temperature probes are used to measure the temperature of the distillation column, reboiler, and condenser to monitor and control the distillation process.[10]
- Heat exchangers: Heat exchangers are used to transfer heat between the incoming and outgoing streams of crude oil or petroleum products, as well as between the distillation column and the reboiler or condenser. [10]
- Product tanks: Product tanks are used to store the individual fractions obtained from the distillation process. The tanks are typically equipped with level sensors and pressure relief valves to maintain safe operating conditions.[10]

- Control systems: Control systems are used to regulate the temperature, pressure, and flow rates of the incoming and outgoing streams in the distillation units, as well as to monitor the performance of the distillation process.[10]

Overall, the equipment used in TBP distillation in refineries is designed to handle large volumes of crude oil and petroleum products and to provide high separation efficiency and accuracy. The specific equipment used may vary depending on the type of crude oil and petroleum products being processed and the requirements of the distillation process.[6]

### **1.3.2 Explanation of the TBP distillation process, including sample preparation, heating, vaporization, condensation, and collection**

Crude oil introduced into refinery processing contains many undesirable impurities, such as sand, inorganic salts, drilling mud by-products, polymers, corrosion by products, etc. The salt content in the crude oil varies depending on the source of the crude oil and how it is transported. When a mixture from many crude oil sources is processed in the refinery, the salt content can vary greatly. [11]

These undesirable impurities, especially salts and water, need to be removed prior to distillation. Two processes are used:

- Dewatering, removes water and constituents of brine that accompany the crude oil.
- Desalting, as illustrated in Figure 1.8 is a water-washing operation that removes water-soluble minerals and entrained solids.[11]

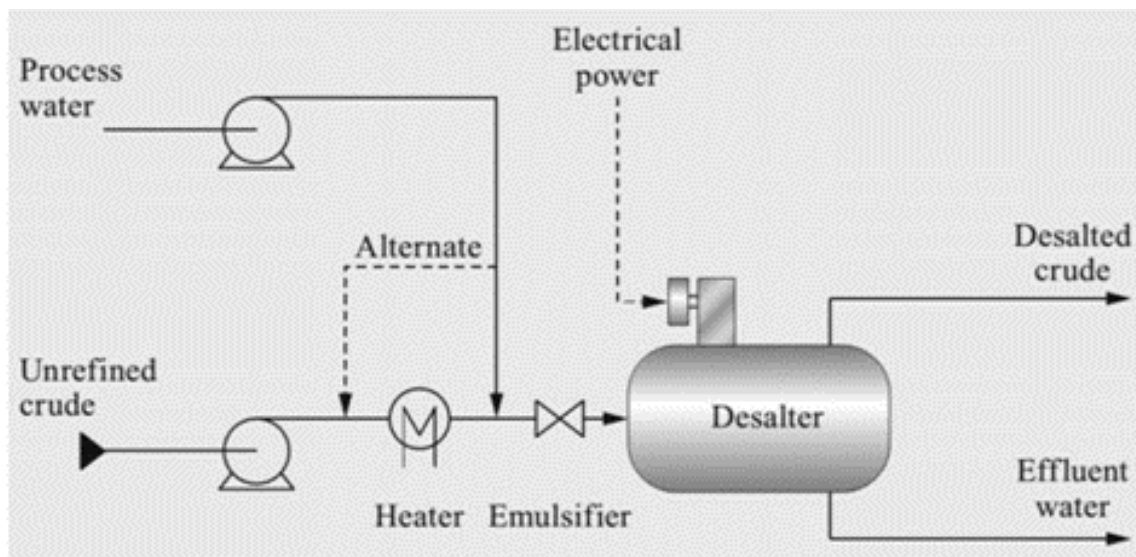
Both operations can be performed at the production field, at the refinery, or both places.

The impurities of most concern in crude oil include:

- The inorganic salts, which can be decomposed to form acids or alkali in the crude oil pre-heat exchangers and heaters. Salts that are most frequently present in crude oil are  $\text{CaCl}_2$ ,  $\text{NaCl}$  and  $\text{MgCl}_2$ , which can form hydrogen chloride when heated in the presence of water. Hydrogen chloride gas condenses to aqueous hydrochloric acid at the overhead systems of distillation columns, causing serious corrosion of equipment.[11]
- Naphthenic and carboxylic acids, as measured by the total acid number (TAN) test, also induce corrosion.[11]



- Sand, silt, or salt cause deposits and foul heat exchangers. They can also cause significant damage to pumps, pipelines, etc. due to abrasion or erosion.[11]
- Inorganic and organic compounds of sodium, calcium nickel, vanadium, iron, arsenic, and other metals in the crude can poison and deactivate catalysts.[11]



**Figure 1.8.** Flow diagram of the desalting process

Crude oil must first be desalted, by heating to a temperature of 100-150 °C and mixing with 4-10% fresh water to dilute the salt. Crude oil exits from the desalted at temperature of 250–260 °C[11]

Organo-silicon compounds are added to crudes to improve flow rates through pipelines and pumps. These Si compounds degrade catalysts by weakening alumina or aluminosilicate supports. They are only partly removed by desalting.

At the refinery, the crude is treated with hot water in one or more desalters. Desalters employing either chemical or electrostatic precipitators to remove dissolved salts and collect remaining solids. In chemical desalting, water and surfactants are added to the crude, heated to dissolve salts and other impurities, then sent to a settling tank, where the water and oil separate. [11]

The oil is then heated to a suitable temperature of 350–360 °C by a tube-still heater and sent to the distillation column where it is separated into individual components at their corresponding temperatures.[11]

**Table 1.1.** Boiling range and its corresponding distillation product

Boiling range		Distillation product
°F	°C	
<85	<29	Petroleum Gas (butane and lighter)
90–200	30–90	Light Naphtha (Gasoline, Petrochemicals)
200–400	90–200	Heavy Naphtha (Gasoline
300–525	150–275	Kerosene (Jet fuel, Heating oil)
350–650	180–345	Distillate (Diesel, Heating oil), Straight-run gas oil
650–1050	345–565	Vacuum gas oil (Lubricant oil)
>1050	>566	Vacuum residuum (Residual fuel oil, Asphalt, Coke)

### 1.3.3 Discussion of process parameters

TBP distillation is a complex process that involves several process parameters such as temperature, pressure, and flow rate. In the following, we will explore how these parameters affect the distillation process and the quality of the final products.

#### a) Temperature

Temperature is a critical parameter in TBP distillation. The boiling points of the components in the crude oil mixture vary widely, and heating the mixture to the right temperature is essential to achieve the desired separation. Typically, the TBP distillation process is conducted in a fractionating column with a temperature gradient along the length of the column. The temperature is highest at the bottom of the column and decreases gradually towards the top. As the crude oil mixture rises through the column, the components with lower boiling points vaporize and rise to the top, where they condense and are collected.[12]

The optimal temperature for TBP distillation depends on the composition of the crude oil mixture and the desired products. Typically, temperatures range from 200°C to 400°C. Higher temperatures can increase the separation efficiency but may also cause thermal cracking and degradation of the components. On the other hand, lower temperatures can result in incomplete separation and lower yields of the desired products.[12]

#### b) Pressure

Pressure is another important parameter in TBP distillation. The pressure inside the fractionating column affects the boiling points of the components, and thus, the separation efficiency. Typically, TBP distillation is conducted at atmospheric pressure or slightly above atmospheric pressure.[12]

The optimal pressure for TBP distillation depends on the composition of the crude oil mixture and the desired products. Higher pressures can increase the boiling points of the components and improve separation efficiency, but they also require more energy and may result in thermal cracking of the components. On the other hand, lower pressures can reduce energy consumption but may result in incomplete separation and lower yields of the desired products.[12]

### c) Flow rate

Flow rate is another important parameter in TBP distillation. The flow rate of the crude oil mixture and the flow rate of the cooling water affect the temperature and pressure inside the column and the rate of separation of the components.[13]

The optimal flow rate for TBP distillation depends on the size of the fractionating column, the composition of the crude oil mixture, and the desired products. Typically, the flow rate is adjusted to maintain the desired temperature and pressure inside the column and to ensure a steady flow of the components through the column.[13]

Overall, TBP distillation is a complex process that requires careful control of several process parameters to achieve the desired separation and quality of the final products. The optimal values of temperature, pressure, and flow rate depend on the composition of the crude oil mixture and the desired products. Advanced simulation tools such as Aspen HYSYS can optimize the TBP distillation process by predicting the optimal process parameters for given crude oil mixture and desired products.

### 1.3.4 Explanation of how to interpret TBP distillation results and determine the boiling point of a liquid

TBP distillation is a widely used method to characterize the boiling range distribution of petroleum products, such as crude oil, gasoline, diesel, and jet fuel. TBP stands for True Boiling Point, which refers to the temperature at which a petroleum product starts to boil and the temperature at which all of it has boiled off.[14]

The TBP distillation process involves heating a petroleum sample in a distillation apparatus under controlled conditions and collecting the condensed fractions at different temperature intervals. The collected fractions are then analysed to determine their composition and boiling points.[14]

Interpreting TBP distillation results involves analysing the distribution of the different fractions collected and their respective boiling points. The key parameters that are typically used to interpret TBP distillation results include:

1. Initial Boiling Point (IBP): This is the temperature at which the first drop of distillate is collected. It indicates the lowest boiling point of the sample.[15]
2. End Boiling Point (EBP): This is the temperature at which the last drop of distillate is collected. It indicates the highest boiling point of the sample. [15]
3. Volume % Recovered: This is the volume percentage of the sample that has been collected at a given temperature interval. It offers an indication of the yield of the different fractions.[15]
4. Distillation Curve: This is a graphical representation of the volume % recovered as a function of the boiling point temperature. It provides a visual representation of the distribution of the different fractions.(see Figure 1.9aand 1.9b) [15]
5. ASTM D86 or ASTM D2892: These are standards that provide guidelines for TBP distillation and provide a basis for comparing TBP distillation results across different laboratories, [15]

Overall, interpreting TBP distillation results involves understanding the boiling range distribution of the sample, identifying the key parameters such as IBP, EBP, volume % recovered, and using them to compare and evaluate the sample against standards and specifications.

#### **1.4 How to determine the boiling point of a liquid**

Consider a binary mixture of liquids (a) and (b), to determine the boiling point of any of the two components, one need to accurately measure these parameters.

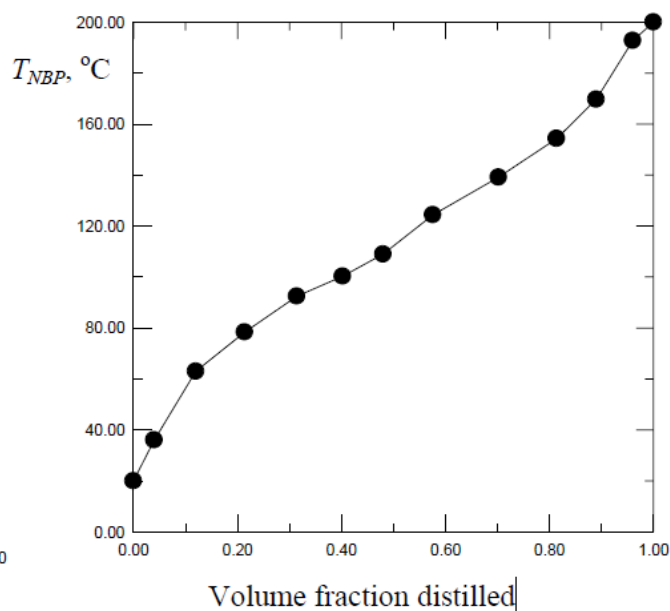
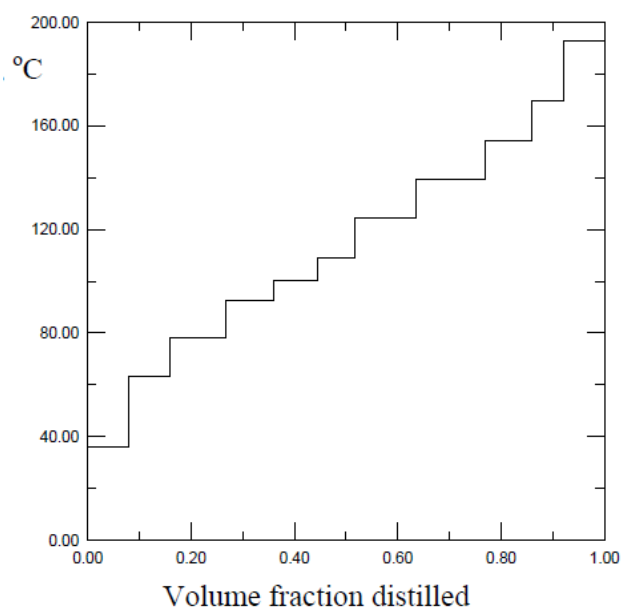
- a. Temperature
- b. Pressure
- c. Percentage of volume distilled.

The reason for measuring pressure is because pressure can affect the boiling point of any liquid.

When a graph of temperature against % of volume distilled is plotted it should present a graph similar to the graph illustrated in Figure 1.3.

When a liquid in a mixture reaches its boiling point, a horizontal line will be achieved indicating its boiling point temperature. Once all the liquid of the less volatile component is recovered, the temperature will rise again and then remain constant until the next liquid is fully recovered.

Crude oil on the other hand contains a mixture of many components that have boiling points close to one another hence multiple samples are taken and multiple distillations are carried out on a laboratory scale to receive a more accurate determination on the boiling points of the components present.



**Figure 1.9.** Theoretical TBP curve      **Figure 1.10.** True TBP curve

The figures above demonstrate the difference between theoretical and true TBP curves as obtained from distilling a sample of crude oil.

### 1.5 Discussion of the accuracy and precision of TBP distillation results

In the context of distillation, accuracy refers to how closely the measured value of a certain parameter (such as the temperature, pressure, or composition) corresponds to the true or actual value of that parameter. Precision, on the other hand, refers to how consistently the same value can be measured over multiple trials or measurements.[16]

In the case of TBP (true boiling point) distillation, accuracy and precision are both important factors to consider. The TBP distillation is a widely used method in the petroleum industry to determine the boiling range distribution of crude oil and its fractions. [16]

To achieve accurate and precise results, it is important to ensure that the distillation equipment is properly calibrated and maintained. The distillation apparatus must also be operated within a specific range of operating conditions (such as temperature and pressure) to ensure that the boiling range distribution is accurately captured. [16]

The accuracy of TBP distillation can be affected by several factors, including the type and quality of the crude oil or product being distilled, the composition of the distillation apparatus, and the operating conditions used during the distillation. Calibration of the equipment, including the temperature sensors and pressure gauges, is essential to ensure that accurate measurements are being obtained. [16]

Precision in TBP distillation can be evaluated by performing replicate measurements on the same sample under identical conditions. The repeatability of the results can be assessed using statistical techniques such as standard deviation, coefficient of variation, or relative standard deviation.[6]

Overall, accurate and precise TBP distillation results are important for ensuring the quality of petroleum products and for making critical decisions related to the refining and processing of crude oil

## **1.6 Advantages and Limitations of TBP Distillation**

### **1.6.1 Discussion of the advantages of TBP distillation**

TBP distillation is a widely used method for the separation and characterization of complex mixtures of hydrocarbons and other compounds in the petroleum industry. Some of the advantages of TBP distillation include:

- Determination of boiling point: TBP distillation allows for the determination of the boiling point of complex mixtures of hydrocarbons and other compounds with high accuracy and precision. This information can be used to identify and quantify individual components in the mixture and to optimize the distillation process.[17]
- High accuracy and precision: TBP distillation is a highly precise method for analyzing complex mixtures of hydrocarbons and other compounds. The results

obtained from TBP distillation are highly reproducible, making it a valuable tool for quality control and process optimization in the petroleum industry. [17]

- Suitable for a wide range of applications: TBP distillation is suitable for use in a wide range of applications in the petroleum industry, including crude oil characterization, product development, and process optimization. It can also be used to analyze other types of complex mixtures, such as polymers, food products, and pharmaceuticals.[17]

Simple and reliable method: TBP distillation is a simple and reliable method for analyzing complex mixtures of hydrocarbons and other compounds. It does not require specialized equipment or extensive training, making it accessible to a wide range of users.[17]

### 1.6.2 Explanation of the limitations of TBP distillation

TBP (True Boiling Point) distillation is a widely used technique for the separation and analysis of complex mixtures. However, there are several limitations associated with this technique, which need to be considered when using it. One of the significant limitations of TBP distillation is the need for specialized equipment, which includes a high-precision distillation column and other associated instruments. The instrument requires accurate temperature control and pressure control systems, which can be expensive to maintain and operate. Moreover, the selection of appropriate column packing material and distillation column design is also critical to achieve accurate and reliable results. The required specialized equipment can make TBP distillation an expensive technique, which may not be feasible for smaller laboratories with limited resources. [17]

Another limitation of TBP distillation is the time and resources required for sample preparation. Before distillation, the sample needs to be purified to remove impurities, which can affect the boiling point and compromise the accuracy and precision of the TBP results. Purification of the sample can be a time-consuming process and may involve several steps, such as filtration, solvent extraction, and concentration. The sample may also require pre-treatment with chemicals, such as sulfuric acid, to remove any unwanted species. These pre-treatment and purification steps can add to the overall cost and time of the analysis.[17]

TBP distillation can also be susceptible to interference from impurities in the sample. Impurities can cause a shift in the boiling point, which can result in errors in the TBP results. The presence of impurities can also lead to the overlapping of boiling points, which can make it difficult to

accurately separate the target compounds from the impurities. Hence, it is crucial to have a well-characterized and purified sample for TBP distillation to obtain accurate and reliable results.[17]

In conclusion, TBP distillation has several limitations that need to be considered before using it for the separation and analysis of complex mixtures. However, with proper preparation and appropriate instrument calibration, TBP distillation can be a highly accurate and precise technique for the analysis of petroleum and other complex mixtures.[17]

### **1.7 Discussion of the future direction of TBP distillation research and development**

TBP (True Boiling Point) distillation is a commonly used technique for separating complex mixtures of hydrocarbons into their individual components. This technique has been widely used in the petroleum and petrochemical industries to produce fuels, chemicals, and other products. In the future, TBP distillation is likely to continue to play an important role in these industries, but there are several potential directions in which it could evolve.[18]

One potential direction for TBP distillation is the development of more efficient and automated processes. This could involve the use of advanced process control systems that can optimize distillation conditions in real-time, as well as the integration of sensors and other monitoring devices that can provide detailed information about the composition and properties of the feed and product streams. This would improve the accuracy and efficiency of the distillation process, reducing waste and improving product quality.[18]

Another direction for TBP distillation is the development of new materials and techniques for column construction. This could include the use of advanced materials such as graphene, nanotubes, or other carbon-based materials that could provide improved thermal and chemical stability, or the development of new packing materials that could increase separation efficiency and reduce pressure drop.[18]

In addition, there may be opportunities to combine TBP distillation with other separation technologies, such as membrane separation, to improve overall process efficiency and product quality. For example, membrane distillation can be used to remove impurities from the feed stream before it enters the TBP distillation column, reducing the energy required to achieve the desired separation.[18]



Finally, TBP distillation may also find new applications in emerging industries such as biorefining, where it could be used to separate complex mixtures of biomass-derived compounds into their individual components. This could enable the production of a range of bio-based chemicals and fuels, providing a sustainable alternative to traditional fossil fuel-based products.[18]

Overall, the future direction of TBP distillation is likely to involve the continued optimization and refinement of existing processes, as well as the development of new technologies and applications that can improve efficiency, reduce waste, and enable the production of new and innovative products.

### **1.8 Conclusion**

This chapter mainly covers the following key points. First introduction, it talks about the background of distillation, the definition of TBP distillation and its importance and applications. It goes on further to include the usefulness of said method of distillation in the refinery industry and the products obtained. Secondly, the fundamentals of Distillation. In this section, the underlying principles of distillation are explained. As distillation mainly works along the principle of volatility between liquids, it explores how to measure the boiling point of a liquid as well as comparison between TBP and other forms of distillation. Thirdly, equipment and Process of TBP Distillation. Here the section covers major and essential equipment units needed to realize TBP distillation on an industrial scale as well as a brief explanation of how the process occurs starting from pre-treatment to separation and collection, fourth analysis of TBP Distillation Results. This section covers the methods of analyzing results, including gas chromatography and mass spectrometry, as well as simple graphs for the corresponding data. Finally, the advantages and limitations of TBP Distillation, this section covers the advantages and limitations of TBP as a method of separation of complex mixtures.

### **1.9 Summary of key points covered in the chapter**

This chapter mainly covers the following key points.

#### **a) Introduction**

In this section, it talks about the background of distillation, the definition of TBP distillation and its importance and applications. It goes on further to include the usefulness of said method of distillation in the refinery industry and the products obtained.

#### **b) Fundamentals of Distillation**

This section goes on to explain the underlying principles of distillation. As distillation mainly works along the principle of volatility between liquids, it explores how to measure the boiling point of a liquid as well as comparison between TBP and other forms of distillation.

#### **c) Equipment and Process of TBP Distillation**

Here the section covers major and essential equipment units needed to realize TBP distillation on an industrial scale as well as a brief explanation of how the process occurs starting from pre-treatment to separation and collection.

#### **d) Analysis of TBP Distillation Results**

This section covers the methods of analyzing including gas chromatography and mass spectrometry as well as simple graphs for the corresponding data.

#### **e) Advantages and Limitations of TBP Distillation**

Lastly this section covers the advantages and limitations of TBP as a method of separation of complex mixtures.

# **Chapter 2**

## **The Aspen HYSYS Software**

## 2. Chapter 2 The Aspen HYSYS Software

### 2.1 Introduction about simulation

Refining and chemical simulation is an essential process in the field of chemical engineering. In refining processes, simulation software can be used to model various processes such as distillation, cracking, and hydro processing. This software allows engineers to simulate and optimize the entire refining process, from crude oil feedstock to final product distribution.[19]

The simulation software can predict the behavior of different chemical compounds under various conditions such as temperature, pressure, and catalysts. This is important because it helps engineers to predict how the different components of the feedstock will behave during the refining process. It also enables them to optimize the conditions under which the reactions take place to ensure that the products obtained are of high quality and meet the required specifications. For instance, simulation software can be used to optimize the design of distillation columns. In a distillation column, crude oil is separated into different components based on their boiling points. The software can model the behavior of the different components and optimize the design of the distillation column to ensure maximum efficiency and product yield. This saves time and resources, as engineers can test different design options and evaluate their effectiveness before committing to a particular design.[19]

Simulation software can also be used to predict the behavior of chemical reactions. In chemical engineering, chemical reactions play a critical role in the design and optimization of chemical processes. By modeling chemical reactions, engineers can predict the products that will be formed under different conditions, and optimize the process to ensure that the desired products are obtained in high yield and purity. In addition to predicting the behavior of chemical reactions and refining processes, simulation software can also be used to simulate the behavior of materials in different environments. For example, it can be used to model the behavior of catalysts used in refining processes, or the behavior of materials used in the construction of chemical reactors. This can help engineers to identify potential problems, such as corrosion or erosion, and design solutions to mitigate them.[19]

### 2.2 Simulation software used in the refining industry

Refining simulation software refers to computer programs that simulate the refining process in oil and gas production. These programs are designed to model the various physical and chemical

reactions that occur during the refining process, including separation, cracking, and hydro processing. The goal of refining simulation software is to optimize the refining process by predicting the behavior of the various components and identifying potential issues before they arise.[20]

There are many different types of refining simulation software available, each with its own set of features and capabilities. Some of the more popular types of refining simulation software include:

1. **Aspen HYSYS:** is a widely used process simulation tool that is designed to simulate the behavior of chemical processes. It includes a wide range of modules that can be used to simulate everything from distillation to catalytic reforming. Aspen HYSYS is known for its user-friendly interface and powerful simulation capabilities[20]
2. **PRO/II:** is a process simulation software tool that is used to model chemical processes and refine refining operations. It is designed to be highly customizable and can be used to simulate everything from simple distillation to complex reaction systems. PRO/II is often used in the petrochemical industry.[19]
3. **ChemCAD:** is a process simulation software tool that is designed to simulate chemical processes. It includes a wide range of modules that can be used to model everything from simple distillation to complex reaction systems. ChemCAD is known for its user-friendly interface and powerful simulation capabilities. [20]
4. **UniSim Design:** is a process simulation software tool that is used to model refining operations. It includes a wide range of modules that can be used to simulate everything from distillation to hydro processing. UniSim Design is known for its advanced modeling capabilities and is often used in the oil and gas industry.[19]
5. **SimSci:** is a process simulation software tool that is used to simulate refining operations. It includes a wide range of modules that can be used to model everything from simple distillation to complex reaction systems. SimSci is known for its powerful simulation capabilities and user-friendly interface.[19]

In addition to these specific software tools, there are many other refining simulation software tools available on the market. Some of these tools are designed for specific industries or applications, whereas others are more general-purpose.[19]

When it comes to refining simulation software, it is important to choose the right tool for the job. Some software tools may be better suited for specific applications or industries, may be more

general-purpose. Additionally, it is important to consider factors such as ease of use, simulation capabilities, and compatibility with other software tools when selecting a refining simulation software tool. [20]

In order to improve the simulation software, there are a few key steps that need to be taken. These include:

- Identifying the key features and capabilities of the software - Before one can begin refining simulation software, one needs to understand its capabilities and features. This can be done by reading through the software documentation or consulting with the software vendor.[19]
- Analyzing the performance of the software: Once you understand the capabilities and features of the software, one can begin to analyze its performance. This can be done by running simulations and comparing the results to real-world data.[19]
- Identifying areas for improvement: Based on analysis, one can identify areas where the software can be improved. This may include improving simulation accuracy, adding new features, or optimizing the software for specific applications.[19]
- Implementing changes and testing: Once you have identified areas for improvement, one can begin to implement changes to the software. This may involve modifying the code, adding new modules, or tweaking existing algorithms. After making changes, it is important to test the software to ensure[19]

### **2.3 Introduction about ASPEN HYSYS**

Aspen HYSYS is a computer software tool developed by Aspen Technology that is widely used for process simulation, design, and optimization in the oil and gas industry. It stands for "Hydrocarbon Yield Simulation System." The software enables engineers to simulate complex processes, including separation, distillation, and reaction processes, in hydrocarbon processing plants. By optimizing these processes, Aspen HYSYS can improve plant efficiency and minimize operating costs. Aspen HYSYS has become a valuable tool in the oil and gas industry, as it enables companies to improve their production processes and maximize profits.[13]

Aspen HYSYS was first introduced in 1983 and has since undergone numerous updates and improvements. The software is known for its user-friendly interface, robust simulation capabilities, and ability to integrate with other process simulation tools. In this section, we provide

an overview of Aspen HYSYS, its features and capabilities, and its role in the oil and gas industry. We also discuss some of the resources used in our research.[13]

### **2.3.1 Features and Capabilities of Aspen HYSYS**

Aspen HYSYS is a process simulation tool that enables engineers to model and optimize complex hydrocarbon processing plants. It provides a range of features and capabilities that make it an essential tool for the oil and gas industry. Some of these features and capabilities include:

1. **Process simulation:** Aspen HYSYS enables engineers to simulate complex chemical processes using advanced thermodynamic models. It provides a range of unit operation models, such as distillation, absorption, and extraction, as well as reaction kinetics models for chemical reactions.[21]
2. **Optimization:** Aspen HYSYS enables engineers to optimize their processes to improve plant efficiency and minimize operating costs. The software provides a range of optimization tools, such as sensitivity analysis, design space exploration, and parameter estimation. [21]
3. **Equipment sizing and rating:** Aspen HYSYS enables engineers to size and rate process equipment, such as distillation columns, heat exchangers, and compressors. The software provides a range of sizing and rating tools, such as tray sizing, heat exchanger rating, and compressor performance. [21]
4. **Data management:** Aspen HYSYS enables engineers to manage their process data efficiently. The software provides a range of data management tools, such as data reconciliation, data validation, and data reporting. [21]
5. **Integration with other software:** Aspen HYSYS integrates seamlessly with other process simulation tools, such as Aspen Plus and Aspen Exchanger Design and Rating, to provide a comprehensive solution for process simulation and design. [21]

### **2.3.2 Role of Aspen HYSYS in the Oil and Gas Industry**

Aspen HYSYS has played a significant role in advancing process simulation and design in the oil and gas industry. The software enables engineers to optimize their production processes, improve plant efficiency, and minimize operating costs. By doing so, companies can maximize their profits and remain competitive in the market.[22]

Aspen HYSYS is used in a range of applications in the oil and gas industry. Some of these applications include:

1. Refinery modeling and optimization: Aspen HYSYS is used to model and optimize refinery processes, such as crude oil distillation, catalytic cracking, and hydro processing. The software enables engineers to optimize these processes to improve product yields, reduce energy consumption, and minimize emissions.[22]
2. Gas processing: Aspen HYSYS is used to model and optimize gas processing plants, such as natural gas processing plants and LNG facilities. The software enables engineers to optimize these processes to improve product yields, reduce energy consumption, and minimize emissions.[22]
3. Petrochemicals: Aspen HYSYS is used to model and optimize petrochemical processes, such as ethylene production, propylene production, and aromatics production. The software enables engineers to optimize these processes to improve product yields, reduce energy[22]

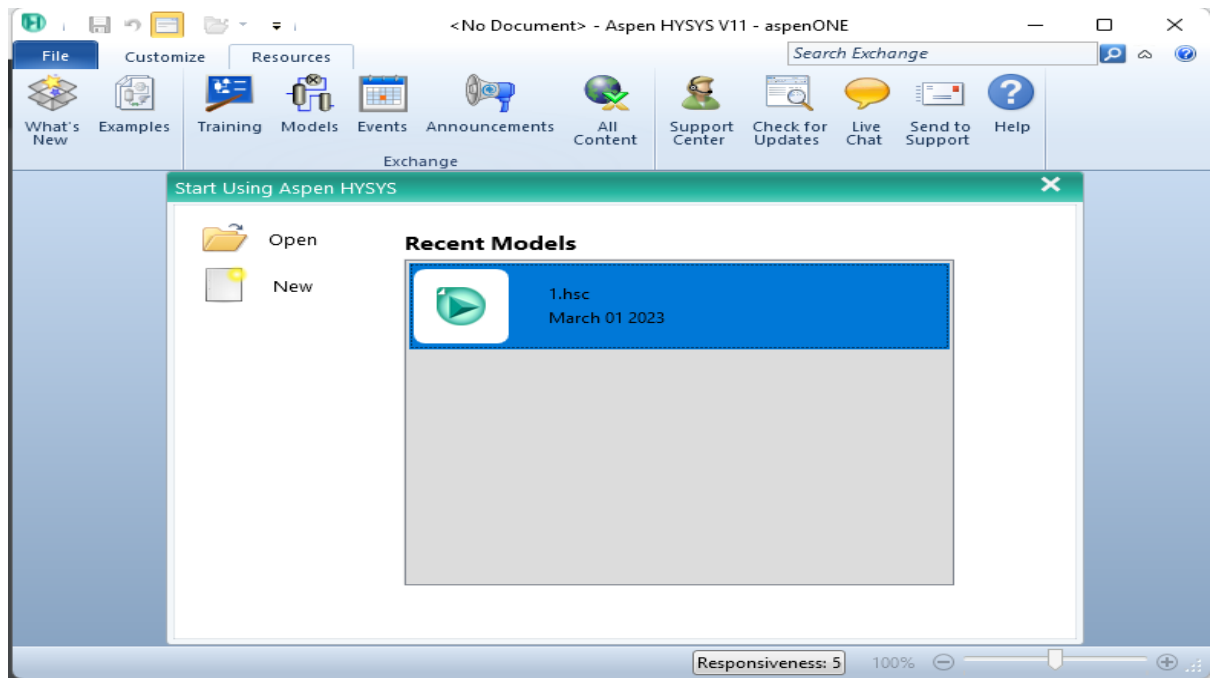
#### **2.4 Starting Aspen HYSYS**

The installation process creates the following shortcut to Aspen HYSYS:

1. Click on the Start menu.
2. Select All apps | Aspen Tech | Aspen HYSYS | Aspen HYSYS V11.

The Aspen HYSYS startup interface appears as illustrated in Figure 2.1.

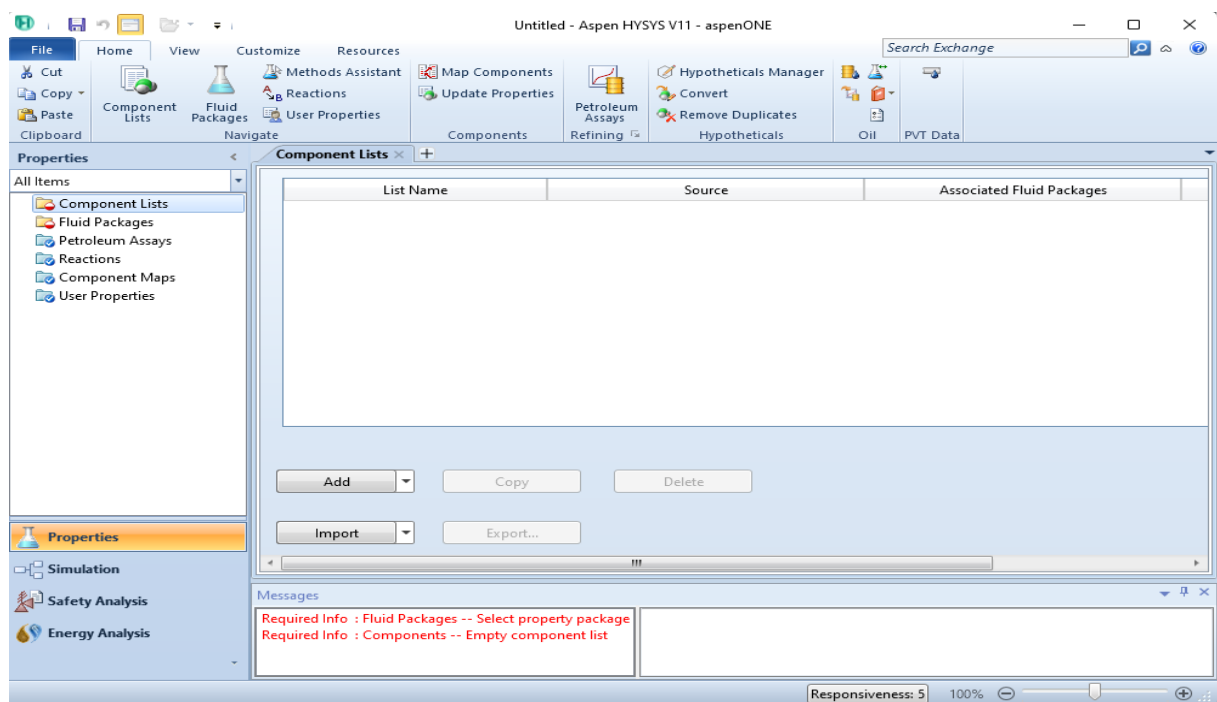




**Figure 2.1.** A figure illustrates the HYSYS startup interface

## 2.5 Creating A New Simulation

Select File/New/Case or press Ctrl+N or click on the New Case to start a new case. In HYSYS, simulation is referred to as a “case”. This will open up Navigation Pane which is where all of the components list, fluid packages and their properties can be specified as illustrated in Figure 2.2



**Figure 2.2.** A figure illustrates the navigation pane in ASPEN HYSYS

Aspen HYSYS utilizes the concept of the fluid package, which encompasses all essential information for conducting flash and physical property computations. This approach enables users to specify all pertinent details - including property package, components, hypothetical components, interaction parameters, reactions, tabular data, and other related data - within a single entity.

There are four key advantages to this approach:

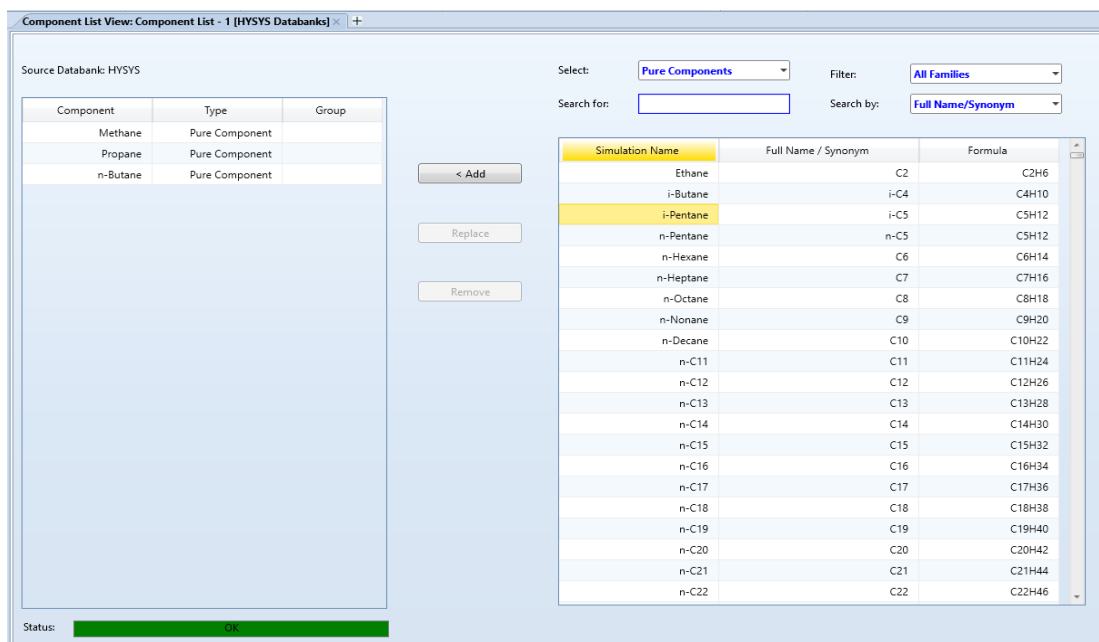
- 1 All associated information is defined in a single location, allowing for easy creation and modification of the information.
- 2 Fluid packages can be stored as completely defined entities for use in any simulation.
- 3 Component lists can be stored out separately from the Fluid Packages as completely defined entities for use in any simulation.
- 4 Multiple Fluid Packages can be used in the same simulation. However, they are defined inside the common Basis Manager.

**NOTE:** Before proceeding any further, save file in an appropriate location. Select File/Save As and select where to save the file. Do not save the file to the default location.

### **2.6 Adding components**

The initial phase in establishing the simulation foundation involves defining the chemical constituents that will be included in the simulation.

1. To add components, click on the Add button.
2. Clicking on Add will bring up the Component List View which is a list of all the components available in HYSYS as illustrated in Figure 2.3



**Figure 2.3.** A figure illustrates the Components List View

3. Select the desired components for simulation. One can search through the list of components in one of three ways:

- a. Simulation Name
- b. Full Name
- c. Formula

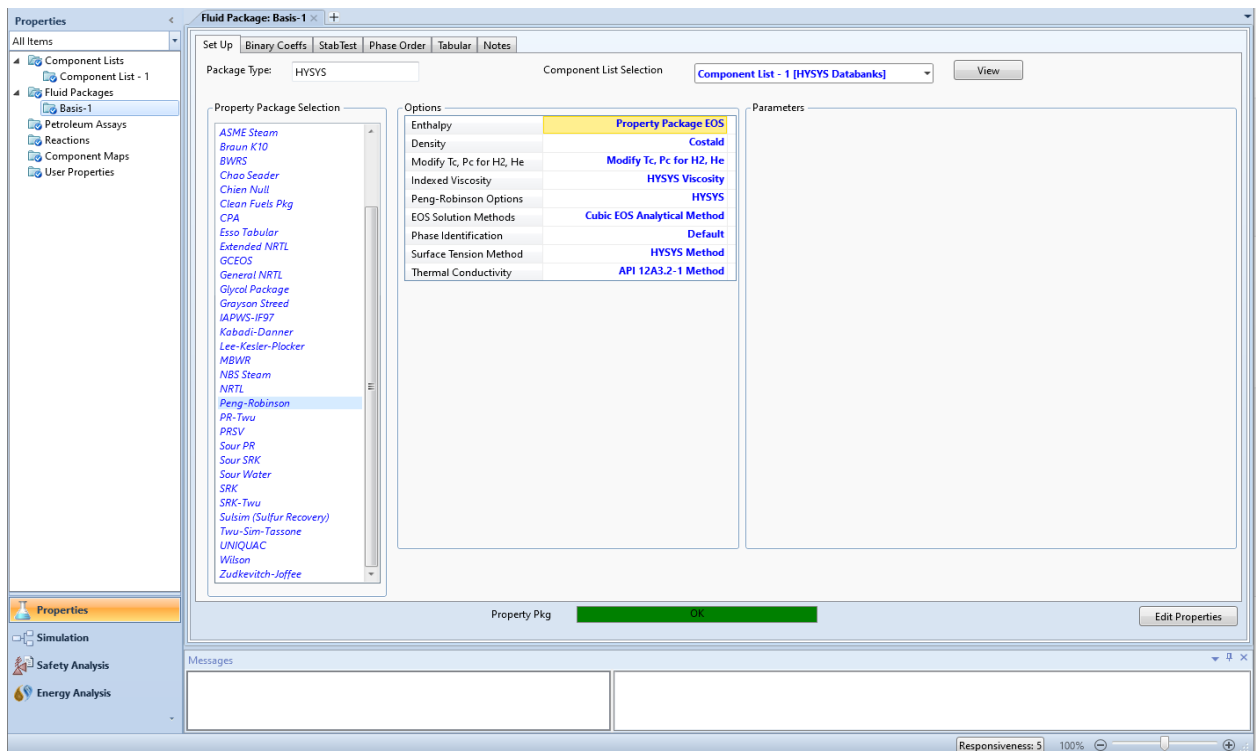
Which match term one want of the three above types by selecting the corresponding button above the list of components, once the component name has been entered, click the search button.

4. Once have located the desired component, either double click on the component or click Add to add it to the list of components for the simulation.
5. Once this is complete, one can switch to another window from the windows in the left panel.

## 2.7 Selecting the Fluids Package

After specifying the chemical components for simulation, the next step is to establish the fluid package. This package serves as a means of computing the thermodynamic properties of the components and mixtures in simulation, such as enthalpy, entropy, density, and vapor-liquid equilibrium. As such, selecting the appropriate fluid package is crucial, as it forms the foundation for the simulation's outcomes.

1. From the Navigation Pane (Figure 2.4), select the Fluid Pkgs tab.
2. Click the Add button to create a new fluid package as demonstrated below



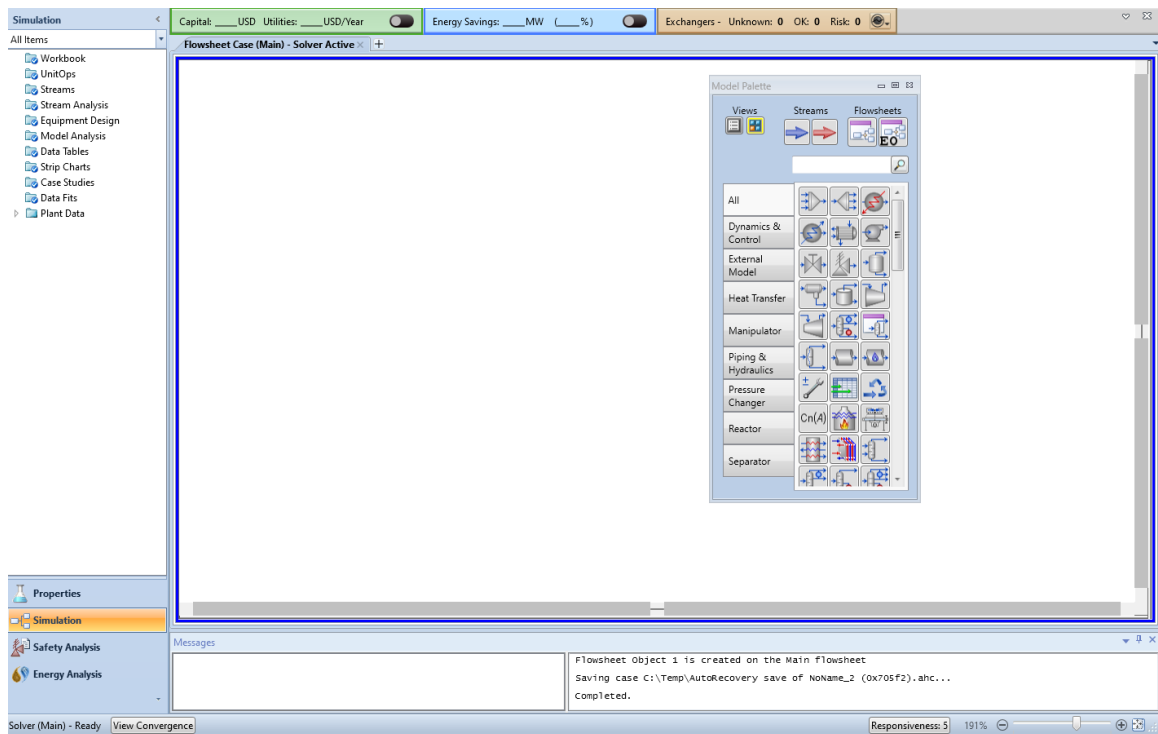
**Figure 2.4.** A figure illustrates the Fluid Package Menu

From the list of fluid packages, select the desired thermodynamic package.

3. Once the desired model has been located, select it by clicking on it once (no need to double click). For example, select Peng-Robinson property package for simulation.
1. 5. One can present fluid package a name at the side of the screen (right click on Basis-1 then click rename).

## 2.8 Entering the Simulation Environment

One has now completed all necessary input to begin simulation. Click on the Simulation button in the left panel as illustrated in Figure 2.5



**Figure 2.5.** A figure illustrates the basic simulation worksheet

On the right-hand side, one will notice a vertical toolbar. This is known as the Model Palette. If for any reason this palette is not visible, got to view and then click on model palette and it will appear on the worksheet. It is from this toolbar that one will add streams and unit operations to simulation.

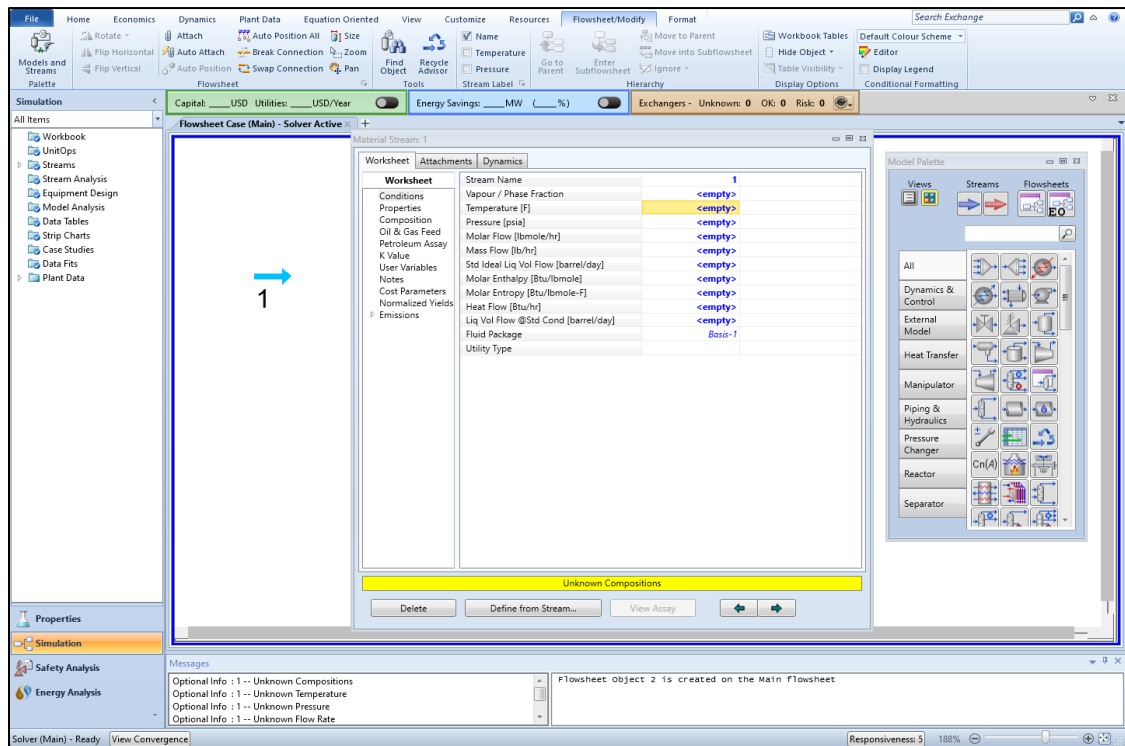
### 2.8.1 Adding Material Streams

Material Streams are used to transport the material components from process units in the simulation. A material stream can be added to the flow sheet in one of two ways:

1. Click on the blue arrow button on the Object Palette
2. Pressing F11

Using any of the above methods will create a new material stream (a blue arrow) on the flow sheet. The HYSYS default names the stream in increasing numerical order (i.e., the first stream created will have the name “1”). This name can be modified at any time. Specifying Material Streams to enter information about the material stream, double click on the stream to reveal the window illustrated in Figure 2.6. It is within this window that the user specifies the details regarding the material stream. For a material stream that will be used as an input, we need to specify four variables. Within the HYSYS environment, input material streams have four degrees

of freedom at all times. Meaning, we need to supply four information in order to fulfill the requirement for HYSYS to start its calculations.



**Figure 2.6.** A figure illustrates the material steam conditions

From Figure 2.6, one will see the warning yellow message bar at the bottom of the window indicating what information is needed (unknown compositions). Just follow what the message wants. For example, the first detail that one needs to supply is compositions. In order to specify the composition of the stream, select the “Composition” option from this list to display the window in Figure 2.7. It is within this window that the user specifies the composition of the stream.

Note that only the components that are specified in the simulation will appear in this list. The HYSYS default is mole fractions. However, the user can also specify mass fractions, liquid volume fractions, or flows of each component. If the user is specifying fractions, all fractions must add up to 1.

The yellow warning message bar signals that the input temperature for this stream needs to be specified. To do so, access the "Conditions" option from the list, which will bring up the window demonstrated in Figure 2.8. Within this window, the user can input the temperature of the stream.

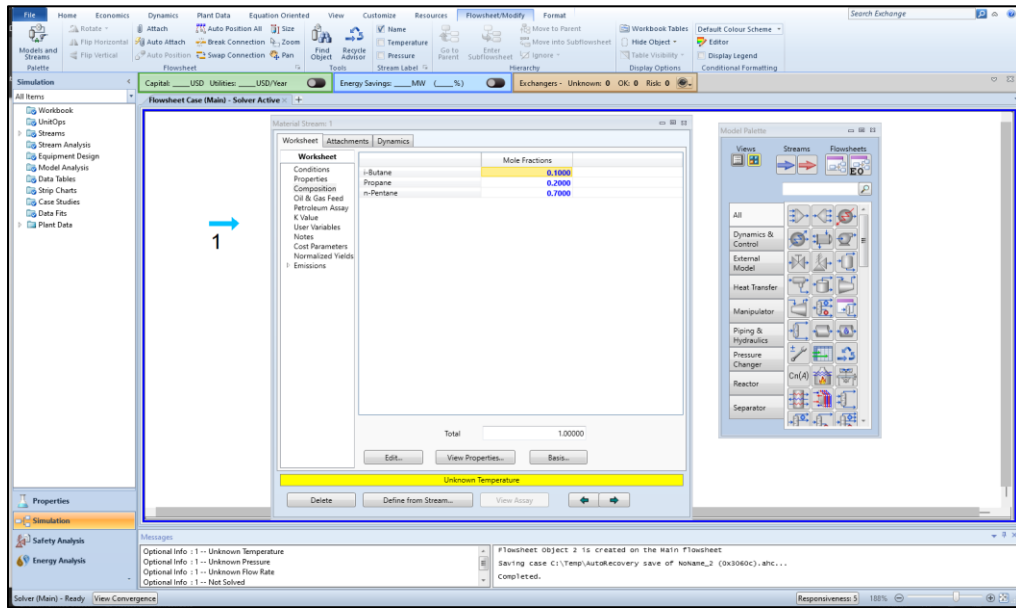


Figure 2.7. A figure illustrates the input steam compositions

It's not mandatory to input values in the default units provided when entering the conditions for a stream. As the user enters a value in a cell, a drop-down arrow appears in the adjacent unit's box. By selecting this drop-down arrow, the user can input the value into any unit desired for the corresponding parameter, and HYSYS will automatically convert the value to the default unit set. To indicate a temperature of 77 °F, input the value of 77 in the temperature section. Subsequently, the yellow warning message bar will prompt the user to specify the input pressure for this stream. Within the same window, input the pressure of 14.5 psia in the pressure section to indicate the pressure of 1 bar, as illustrated in Figure 2.8.

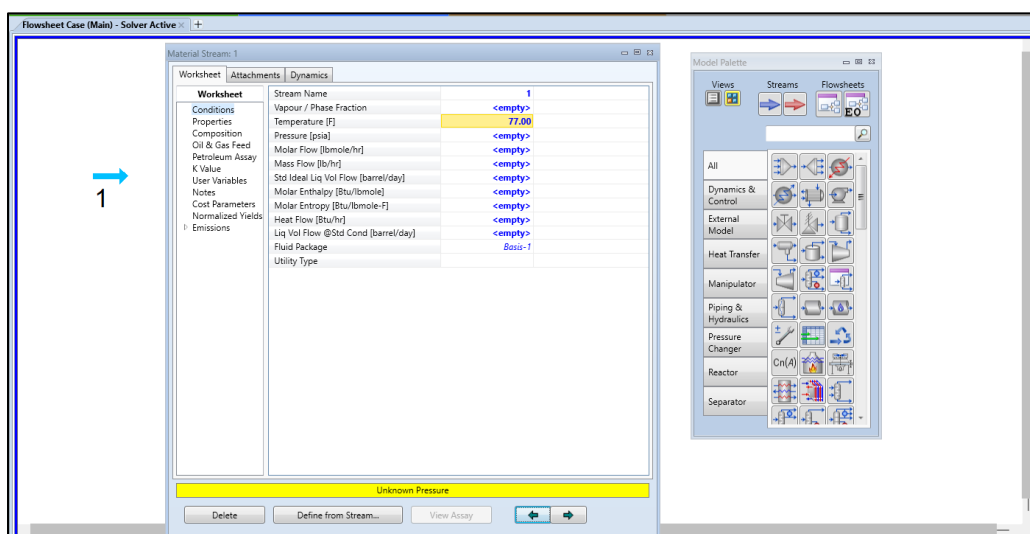
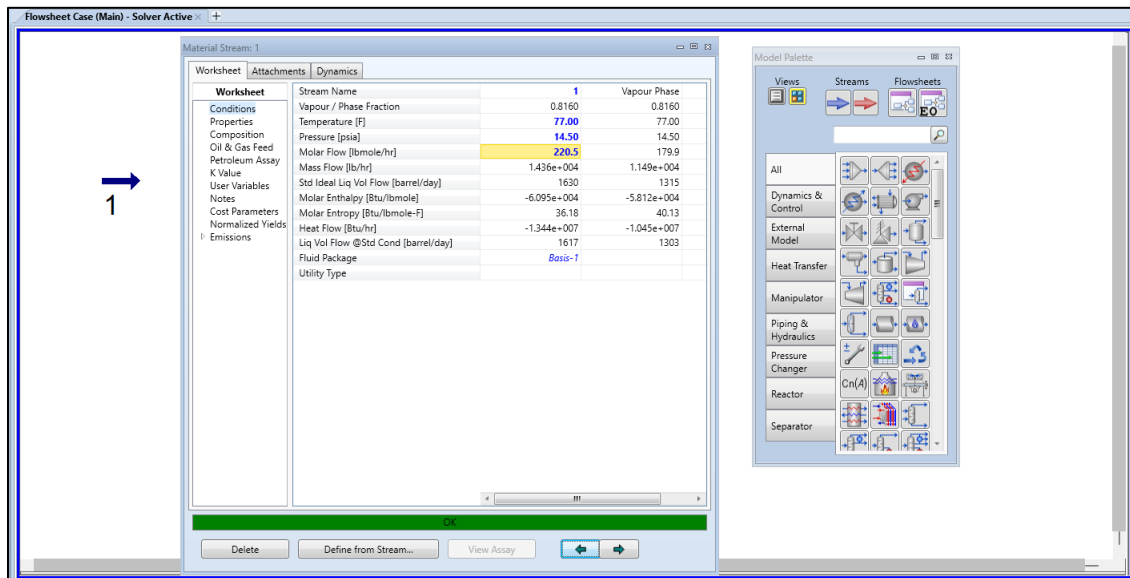


Figure 2.8. A figure illustrating input stream temperature

Next, the last variable that one needs to specify is flow rate. For this, one has two options either to specify molar flow rate or mass flow rate. In the same window, enter the molar flow rate of 220 in the molar flow rate section to indicate the flow rate of 220lbmole/h as illustrate in Figure 2.9.

**Note:** these values are only an example to approximate the image.



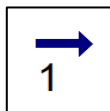
**Figure 2.9.** A figure illustrates Input stream pressure and molar flow rate

After all the necessary stream information is entered, HYSYS will calculate the remaining properties and data, provided there is enough information available from the rest of the flow sheet. When a stream is completely characterized, a green message bar appears at the bottom of the window in the stream input view, indicating that everything is "OK" (refer to Figure 2.9). However, if any information is missing, the input window will display a yellow message bar at the bottom of the window indicating which information needs to be added.

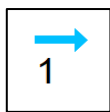
Values that are demonstrated in **blue** have been specified by the user and can be modified, whereas values demonstrated in **black** have been calculated by HYSYS and cannot be modified. For example, in Figure 2.9 the temperature, pressure and molar flow rate have been specified whereas all other values shown have been calculated.

The following color code for material streams on the flow sheet indicates whether HYSYS has enough information to completely characterize the stream:





Royal Blue = properly specified and completely solved



Light blue = incompletely specified, properties not solved

### 2.9 Conclusion

In conclusion, Aspen HYSYS stands out as the premier simulation software among various refining and chemical engineering software options. Its exceptional features, robust capabilities, and extensive industry adoption make it the preferred choice for professionals in the field.

First and foremost, Aspen HYSYS offers a comprehensive suite of tools that empower engineers to simulate, analyze, and optimize complex processes in the refining and chemical engineering industries. Its user-friendly interface, coupled with powerful modeling capabilities, enables engineers to efficiently design, troubleshoot, and improve processes.

One of the key strengths of Aspen HYSYS is its wide range of thermodynamic models and property packages. These models accurately represent real-world behaviors of various chemical compounds, enabling engineers to achieve precise simulations and predictions. The software also supports a diverse range of unit operations and equipment models, allowing for detailed process representation and accurate results.

Furthermore, Aspen HYSYS boasts a vast library of pre-built components and process templates, which significantly speeds up simulation setup and reduces the need for manual input. This feature enhances productivity and allows engineers to focus on analyzing and optimizing their processes rather than spending excessive time on model creation.

Another significant advantage of Aspen HYSYS is its integration capabilities. It seamlessly integrates with other Aspen Tech software products, such as Aspen Plus, Aspen EDR, and Aspen Economic Evaluation, forming a comprehensive suite that covers the entire process lifecycle. This integration streamlines data exchange, facilitates interdisciplinary collaboration, and enables engineers to leverage a broader range of tools and functionalities. Moreover, Aspen HYSYS has gained widespread adoption and recognition in the industry. It is extensively used by major refining and chemical engineering companies worldwide, making it a standard choice for process

simulation and optimization. The large user community fosters knowledge sharing, facilitates support, and ensures continuous software improvement through updates and enhancements.

In conclusion, Aspen HYSYS stands out as the best simulation software among its peers in the refining and chemical engineering field. Its advanced features, versatile modeling capabilities, ease of use, integration capabilities, and widespread industry adoption make it an indispensable tool for engineers seeking to design, analyze, and optimize complex processes. With Aspen HYSYS, professionals can confidently tackle the challenges of process simulation and unlock valuable insights for the development and improvement of refining and chemical engineering operations

# **Chapter 3**

## **The Experimental Part**

### 3. Chapter 3 The Experimental Part

#### 3.1 Introduction

The physicochemical characteristics of crude oil play a crucial role in various industries, from petroleum refining to environmental impact assessment. Traditionally, these characteristics have been determined through laboratory analysis following standardized procedures, such as those established by ASTM. However, with advancements in technology, software tools like Aspen HYSYS offer the capability to calculate physicochemical properties of crude oil based on thermodynamic models.

This chapter aims to compare the physicochemical characteristics of crude oil obtained through laboratory analysis at the Boumerdes Research and Development Center (CRD), using ASTM standards, with the characteristics calculated by Aspen HYSYS. Specifically, the focus will be on evaluating the reliability and accuracy of the properties calculated by the software compared to the results obtained from the rigorous laboratory analysis.

The analyzed crude oil in this study is the Algerian reference crude oil known as Sahara blend. The main objective is to determine its physicochemical properties, which are essential for understanding its behavior during processing and utilization. Furthermore, this chapter will also present the main characteristics of the processed crude oil sampled from the storage center, along with the yields of different cuts obtained from the true boiling point (TBP) distillation.

By comparing the laboratory-derived characteristics with the ones calculated using Aspen HYSYS, we can assess the software's capability to accurately predict the physicochemical properties of crude oil. This analysis will provide valuable insights into the reliability and suitability of Aspen HYSYS as a predictive tool in the oil and gas industry.

Overall, this chapter seeks to bridge the gap between laboratory analysis and software predictions, offering valuable information for decision-making processes and ensuring the accuracy and reliability of physicochemical data used in various petroleum-related applications.

#### 3.2 Determination of the main characteristics of crude oil

The various properties of crude oil, including its density, Reid vapor pressure, viscosity, acidity index, as well as flash, pour, and freeze points, were measured in the laboratory. The contents of paraffins, carbon residue, and asphaltenes were also determined. The presence of elements other

than hydrocarbons, such as water, sediments, sulfur, mercury, and metallic elements, was also identified.

The characterization factor and molecular weight were obtained by reading from the UOP 375-59 chart. The calorific value was determined using the "Hougen & Watson" chart. The different characteristics obtained are presented in the tables below.

**Table 3.1.** The different experimental characteristics obtained.

Characteristics	Results
<ul style="list-style-type: none"> <li>• Density at 20°C,</li> <li>• Density at 15°C,</li> <li>• Specific gravity at 60/60°F,</li> <li>• °API</li> </ul>	0,7978 0,8015 0.8022 44.87
<ul style="list-style-type: none"> <li>• Reid vapor pressure at 37.8°C (100°F)kg/cm<sup>2</sup></li> <li>• Kinematic viscosity at:                20.0°C (68°F) cSt                37.8°C (100°F) cSt</li> </ul>	0.594  2.324 1.996
<ul style="list-style-type: none"> <li>• Flash point, °C</li> <li>• Freezing point, °C</li> <li>• Pour point °C</li> <li>• Acidity index, mg KOH/g</li> <li>• Water amount by extraction, % vol</li> <li>• Water and sediment amount (BSW), % vol</li> <li>• Sulfur amount by X-ray, % wt</li> <li>• Asphaltene content, % wt</li> <li>• Carbon residue amount, % wt</li> <li>• Mercury amount, mg/L</li> <li>• Paraffin amount, % wt</li> <li>• Characterization factor "KUOP"</li> <li>• Molecular weight, g/mol</li> <li>• Higher Heating Value, kcal/kg</li> </ul>	<-3.9 -39 -36 0.5 None To be determined 0.1 <0.05 1.8 7.52 1.10 11.89 225 11045

**Table 3.2.** Metal Elements amount in Crude Oil

<b>Metallic elements.</b>	<b>Amount in parts per million (ppm).</b>
<b>Fe</b>	0.2
<b>Cr</b>	0.2
<b>Pb</b>	2.5
<b>Cu</b>	0.1
<b>Al</b>	0.3
<b>Ni</b>	0.9
<b>Ag</b>	0.3
<b>Mo</b>	1.6
<b>V</b>	1.3
<b>B</b>	0.1
<b>Zn</b>	0.3
<b>Si</b>	0.4
<b>Na</b>	0.5

### 3.3 Petroleum Distillation

#### 3.3.1 ASTM D86 Distillation

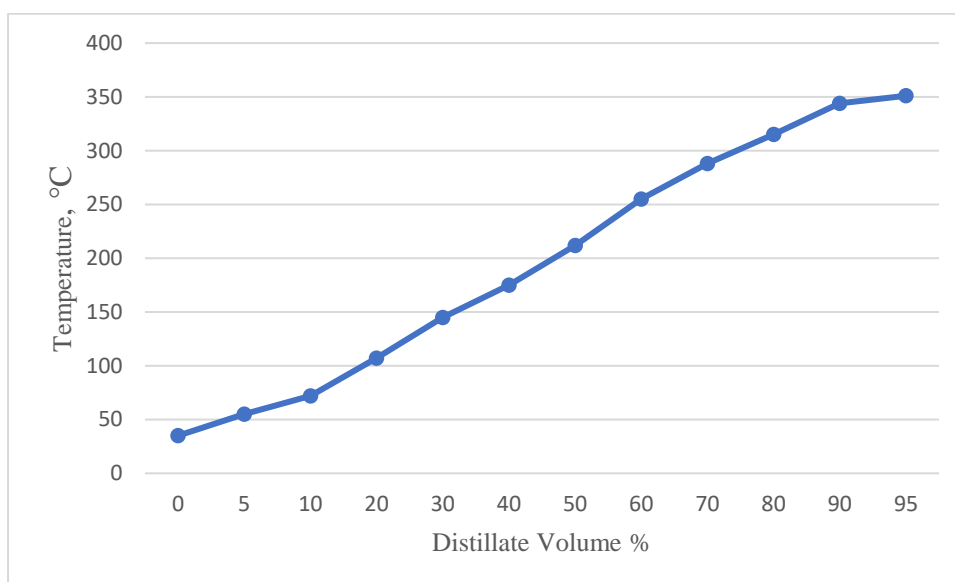
An analytical distillation was conducted on a 100 ml sample of this petroleum following ASTM D86 standard. The different temperatures determined based on the volume percentages distilled are summarized in the following table.

**Table 3.3.** ASTM D86 Distillation Data of Crude Oil

<b>Distillate Volume %</b>	<b>Temperature, °C</b>
<b>Initial Point</b>	35
<b>05 % Vol</b>	55
<b>10</b>	72
<b>20</b>	107
<b>30</b>	145
<b>40</b>	175
<b>50</b>	212

<b>60</b>	255
<b>70</b>	288
<b>80</b>	315
<b>90</b>	344
<b>95</b>	351
<b>Final Point</b>	353
<b>Distillate, % Vol</b>	96
<b>Residue</b>	Coke

**Note:** The residue percentage could not be measured due to the formation of coke, and therefore the percentage is unavailable.



**Figure 3.1.** ASTM D86 Distillation Curve

### 3.3.2 True Boiling Point (T.B.P.) Distillation

A charge of 1.4 liters was distilled in an Oldershaw column with 30 actual trays. The dissolved gases present in the crude oil were recovered in a cooled trap to prevent their volatilization.

Fifty narrow petroleum fractions and an atmospheric residue were collected. The different distillates were weighed, and their densities and refractive indices were measured at 20°C. The densities at 15°C were calculated using conversion tables according to ASTM D1250-80 standard. Thus, the volume of each distillate was calculated based on the density at 15°C and the measured

weight. The yields, expressed as mass percentages and volume percentages, of the different narrow cuts and atmospheric residue were calculated.

The various results obtained are presented in the table provided below.

**Table 3.4.** TBP Distillation Data of Crude Oil

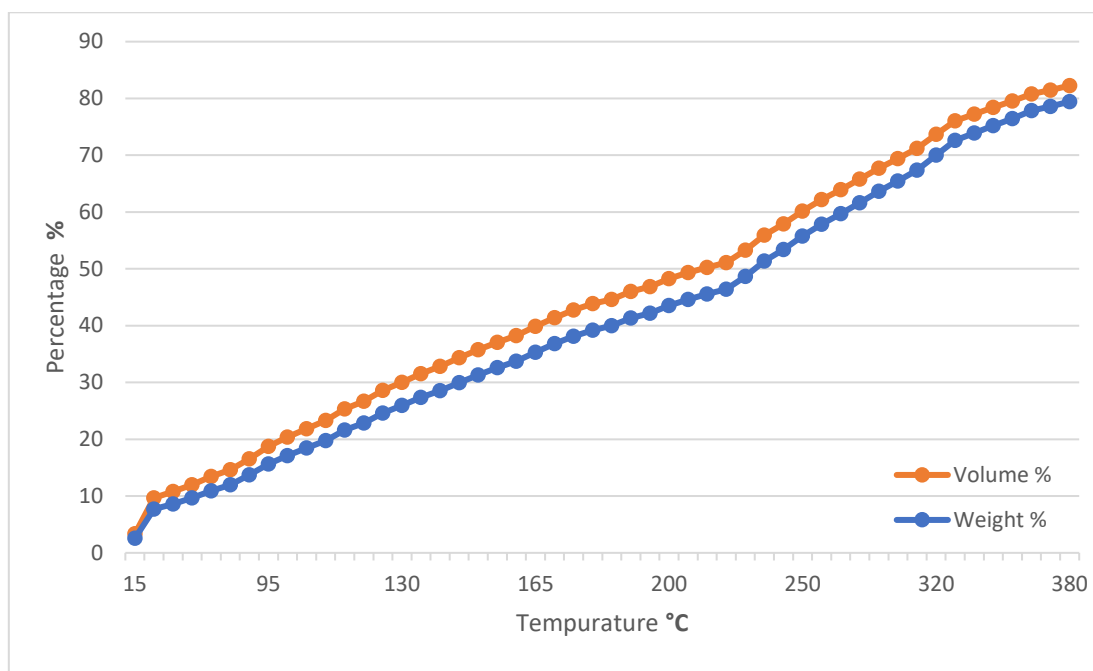
N° Cuts	Temp °C	Weight %	Cumulative Weight %	Density at 20°C	Density at 15°C	%Vol	Cumulative Vol%	Refractive Index	KUOP
Light	<15.0°C	2.56	2.56	*	*	3.34	3.34	-	-
1	15-65	5.12	7.68	0.6424	0.6473	6.34	9.68	1.3741	12.75
2	65-70	0.94	8.62	0.6887	0.6933	1.09	10.77	1.381	12.24
3	70-75	1.04	9.66	0.6897	0.6943	1.2	11.97	1.3896	12.28
4	75-80	1.27	10.93	0.6937	0.6983	1.46	13.43	1.3923	12.27
5	80-85	1.03	11.96	0.6988	0.7034	1.17	14.6	1.3945	12.24
6	85-90	1.75	13.71	0.7074	0.712	1.97	16.57	1.399	12.15
7	90-95	1.94	15.65	0.7083	0.7128	2.18	18.76	1.3994	12.19
8	95-100	1.44	17.09	0.7176	0.7223	1.6	20.36	1.4045	12.09
9	100-105	1.35	18.44	0.7277	0.7224	1.5	21.85	1.409	12.14
10	105-110	1.31	19.75	0.7279	0.7226	1.45	23.31	1.4092	12.19
11	110-115	1.85	21.6	0.728	0.7227	2.05	25.36	1.4098	12.24
12	115-120	1.24	22.84	0.73	0.7345	1.35	26.71	1.4106	12.1
13	120-125	1.75	24.59	0.7369	0.7413	1.89	28.61	1.4142	12.04
14	125-130	1.34	25.93	0.7488	0.7532	1.43	30.03	1.4236	11.89
15	130-135	1.41	27.34	0.7555	0.7599	1.49	31.52	1.4247	11.84
16	135-140	1.22	28.56	0.756	0.7604	1.29	32.81	1.4234	11.88
17	140-145	1.41	29.97	0.7623	0.7367	1.53	34.34	1.4271	12.31
18	145-150	1.35	31.32	0.7669	0.7712	1.4	35.75	1.4315	11.81
19	150-155	1.28	32.6	0.7684	0.7726	1.33	37.08	1.4322	11.83
20	155-160	1.14	33.74	0.7705	0.7747	1.18	38.26	1.4337	11.85
21	160-165	1.55	35.29	0.7773	0.7812	1.59	39.85	1.4359	11.79
22	165-170	1.53	36.82	0.7778	0.7817	1.57	41.42	1.4365	11.83
23	170-175	1.28	38.1	0.778	0.7819	1.31	42.73	1.4374	11.87
24	175-180	1.12	39.22	0.7822	0.7859	1.14	43.87	1.4384	11.86
25	180-185	0.74	39.96	0.7871	0.7908	0.75	44.62	1.441	11.83
26	185-190	1.38	41.34	0.7876	0.7913	1.4	46.02	1.4412	11.86
27	190-195	0.82	42.16	0.788	0.7917	0.83	46.85	1.4419	11.9



28	195-200	1.39	43.55	0.7941	0.7977	1.4	48.25	1.4448	11.85
29	200-205	1.08	44.63	0.7952	0.7988	1.08	49.33	1.4462	11.88
30	205-210	0.94	45.57	0.8029	0.8065	0.93	50.27	1.4504	11.8
31	210-215	0.83	46.4	0.803	0.8066	0.83	51.09	1.4505	11.84
32	215-220	2.25	48.65	0.8116	0.8152	2.21	53.31	1.4536	11.76
33	220-230	2.72	51.37	0.8184	0.8219	2.65	55.96	1.4581	11.72
34	230-240	2.04	53.41	0.8261	0.8296	1.97	57.93	1.4634	11.69
35	240-250	2.34	55.75	0.8309	0.8338	2.25	60.18	1.467	11.71
36	250-260	2.12	57.87	0.8335	0.837	2.03	62.21	1.4686	11.74
37	260-270	1.84	59.71	0.8401	0.8435	1.75	63.96	1.471	11.72
38	270-280	1.94	61.65	0.8422	0.8456	1.84	65.8	1.4716	11.76
39	280-290	2.02	63.67	0.8427	0.8461	1.91	67.72	1.4733	11.83
40	290-300	1.76	65.43	0.8472	0.8506	1.66	69.38	1.4738	11.83
41	300-310	1.96	67.39	0.8502	0.8536	1.84	71.22	1.4753	11.86
42	310-320	2.63	70.02	0.8658	0.8592	2.45	73.67	1.4845	11.85
43	320-330	2.58	72.6	0.8704	0.8738	2.37	76.04	1.4883	11.72
44	330-340	1.32	73.92	0.8764	0.8798	1.2	77.24	1.492	11.7
45	340-350	1.3	75.22	0.8776	0.881	1.18	78.43	1.4923	11.75
46	350-360	1.25	76.47	0.8778	0.8812	1.14	79.56	1.4925	11.81
47	360-370	1.37	77.84	0.8783	0.8817	1.25	80.81	1.4928	11.87
48	370-375	0.72	78.56	0.8791	0.8825	0.65	81.46	1.4933	11.9
49	375-380	0.89	79.45	0.8808	0.8842	0.81	82.27	1.4938	11.91
50	380+	20.55	100	0.9266	0.9297	17.73	100	1.494	11.34

**N.B.:**

- The conversion of densities from 20 to 15°C is carried out using the ASTM D1250-80 tables.
- (\*) Chromatographic analysis of the light fractions (C5) could not be determined due to technical reasons, and therefore the density of the light fractions cannot be calculated.



**Figure 3.2.** TBP Distillation Curve of Crude Oil

### Fractionation of crude oil

A second distillation was carried out on this sample of oil under the same conditions as indicated in the following table, in order to recover different broad cuts for their characterization. The fractionation scheme used in this table is presented below.

**Table 3.5.** Different Broad Cuts of Crude Oil

Cuts	Boiling Temperature in °C
Light Naphtha	15-80°C
Heavy Naphtha	80-165°C
Kerosene	165-250°C
Light Gasoil	250-320°C
Heavy Gasoil	320-380°C
Atmospheric Residue	R380°C +

### 3.4 Calculating and Comparing the Characteristics Results

#### 3.4.1 Introduction

We used the experimental results obtained: boiling temperature, density at 20 °C ( $d^{20}$ ), Watson factor (Kuop), refractive index at 20 °C ( $n^{20}$ ), for the 50 fractions to calculate the values of critical temperature ( $T_c$ ), critical pressure ( $P_c$ ), critical volume ( $V_c$ ), and acentric factor ( $\omega$ ) using the Riazi-Daubert correlation.

We conducted calculations of critical properties in a TBP distillation using Aspen Hysys. The simulation was based on the API value of 44.84 and the molecular weight of 225 g/mol, whereas referencing the ASTM D86 distillation data of crude oil. By inputting these parameters into the HYSYS simulation, we calculated the critical temperature ( $T_c$ ), critical pressure ( $P_c$ ), critical volume ( $V_c$ ), and acentric factor ( $\omega$ ) for the fractions obtained from the distillation process.

Subsequently, we compared these simulated values with the calculated results obtained from Riazi-Daubert analysis. The purpose of this comparison was to evaluate the accuracy and reliability of the HYSYS simulation in predicting the critical properties of fractions, specifically in relation to the calculated findings provided by the Riazi-Daubert correlation.

#### 3.4.2 Peng-Robinson correlation

The Peng-Robinson correlation is a widely used thermodynamic model for calculating the properties of fluids, especially in the context of phase equilibrium calculations. It is particularly suitable for hydrocarbon systems, including gases, liquids, and their mixtures.[23]

The Peng-Robinson equation of state incorporates parameters such as temperature, pressure, and composition to estimate various thermodynamic properties. It provides a mathematical representation of the intermolecular forces and interactions within the fluid, allowing for the prediction of critical properties, vapor-liquid equilibrium, and other phase behavior characteristics. [23]

The Peng-Robinson equation of state can be written as follows:

$$P = \frac{RT}{V - b} - \frac{a}{V(V + b) + b(V - b)}$$

$$Z^3 + (1 - b)Z^2 + (a - 2b - 3b^2)Z - (ab - b^2 - b^3) = 0$$

**P** represents the pressure

**T** is the temperature

**R** is the gas constant

**V** is the molar volume

**a** is the attractive parameter

**b** is the co-volume parameter[23]

The equation is based on a cubic equation of state and includes correction factors to account for the effects of molecular size and shape. It accounts for the attractive forces between molecules (using the term "a") and the repulsive forces due to molecular volume (using the term "b").[23]

By using the Peng-Robinson correlation, one can estimate critical temperature ( $T_c$ ), critical pressure ( $P_c$ ), critical volume ( $V_c$ ), and other properties of interest for various substances and mixtures. The accuracy of the correlation depends on the specific system and the accuracy of the input parameters. [23]

It is important to note that the Peng-Robinson correlation is a widely used and reliable model, it may have limitations for certain systems, such as polar substances or mixtures involving highly asymmetric molecules. In such cases, alternative correlations or modifications may be employed to improve the accuracy of the predictions. [23]

### 3.4.3 Error Calculation

The error ( $\epsilon$ ) can be calculated using the following formula:[24]

$$\epsilon = \left( \frac{\theta_{cal} - \theta_{exp}}{\theta_{exp}} \right) \times 100$$

$\epsilon$ : Errors relative

$\theta_{Exp}$ : Experimental Value.

$\theta_{Cal}$ : Calculated Value [24]

### 3.4.4 Critical Temperature

In thermodynamics, the critical temperature refers to the highest temperature at which a substance can exist in a distinct liquid and gas phase. Above this temperature, known as the critical temperature, the substance exhibits properties that are intermediate between those of a liquid and a gas, forming a supercritical fluid.[25]

We utilized Aspen Hysys, to calculate the critical temperature using the Peng-Robinson correlation. The results of these calculations are presented in the following table.

**Table 3.6.** Obtained Values of Critical Temperature

Fraction	Tc1	Tc2	E
1	476.7740	457.0334	4.13965094
2	502.7247	485.4633	3.43265667
3	509.3575	506.503	0.5589495
4	516.2108	524.3825	1.58317493
5	523.1744	536.4174	2.53213265
6	525.3968	542.3801	3.2338124
7	547.2455	547.9669	0.13283366
8	552.5552	553.4417	0.16137008
9	557.6444	558.8807	0.22248696
10	562.0720	564.3174	0.39984038
11	566.4997	569.7233	0.5707544
12	571.4234	575.1291	0.64910037
13	576.8985	580.5281	0.63064661
14	581.9877	585.903	0.67408075
15	585.5333	591.247	0.97638196
16	594.0405	596.6072	0.43216598
17	598.6335	601.9846	0.56038273
18	603.5573	607.3505	0.62969512
19	609.6939	612.6626	0.48755887
20	614.8383	617.8905	0.49778035
21	619.7620	623.1207	0.54225289
22	624.6307	628.8405	0.67407171
23	629.1686	635.0706	0.93943618
24	636.0219	641.2752	0.82626451

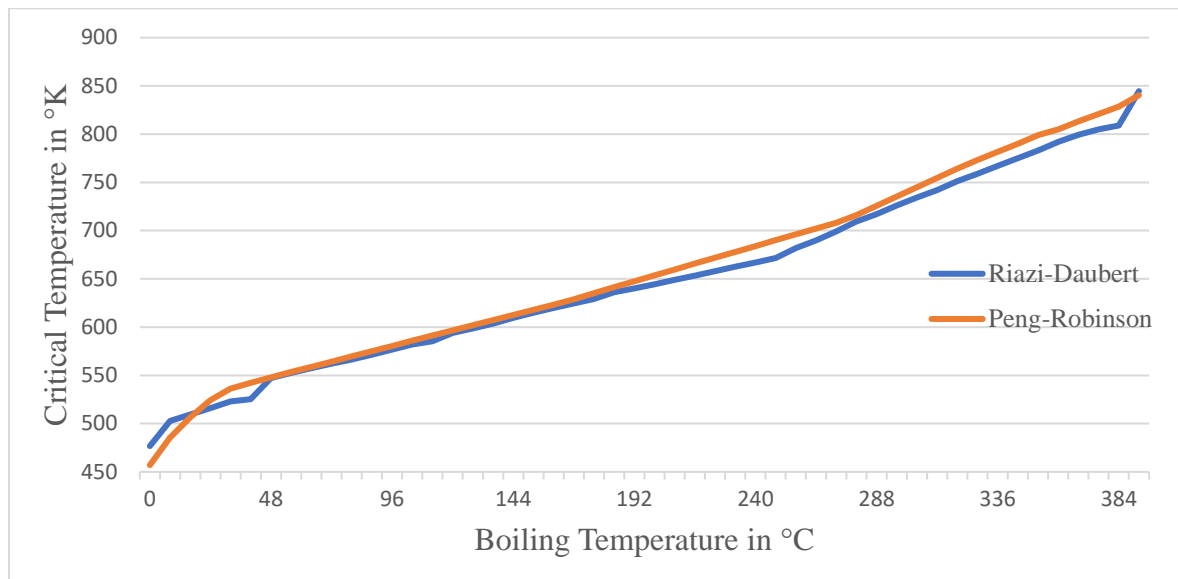
25	640.1188	647.4894	1.15282996
26	644.4913	653.6633	1.42333768
27	648.9189	659.8142	1.6803885
28	653.4568	665.9126	1.90719989
29	658.0498	671.9863	2.11936464
30	662.6428	678.0254	2.32183246
31	666.9601	684.0613	2.56407286
32	671.6634	690.0898	2.74391548
33	681.7780	696.0859	2.09981922
34	689.7512	702.054	1.78382821
35	699.2129	708.0317	1.26167221
36	709.2810	716.0327	0.95204345
37	716.9233	725.7892	1.23712333
38	725.8888	735.4297	1.31560982
39	734.3582	745.0555	1.45782556
40	742.0557	754.5632	1.68629761
41	751.2417	764.0049	1.69917507
42	758.9943	773.0643	1.85434196
43	767.0226	781.8536	1.93392306
44	775.2714	790.1122	1.91446124
45	782.9689	798.8343	2.02747133
46	791.8793	804.8561	1.63992563
47	799.1909	813.2065	1.753836
48	804.9503	820.8099	1.97030083
49	808.8266	828.4046	2.42137955
50	844.5594	840.375	0.4943461
Mean	1.41807604		
Error			

$T_{c1}$ : Critical temperature using Riazi-Daubert correlation

$T_{c2}$ : Critical temperature using Peng-Robinson correlation

$E$ : Errors relative to the Riazi-Daubert correlation

Based on the previous values, we calculated the error for each correlation. We also plotted the variation curve for each correlation, representing the values of  $T_c$ .



**Figure 3.3.** A graph of Critical Temperature versus Boiling Temperature of the petroleum fractions

We utilized Aspen Hysys, to calculate the critical temperature using the Peng-Robinson correlation. The results of these calculations are presented in the previous table. A comparison was made between the critical temperature obtained from the simulation and the critical temperature measured through laboratory analysis. The results were analyzed and interpreted to evaluate the reliability of the simulation and its ability to predict the critical temperature of crude oil.

To facilitate the presentation of the findings, a comprehensive table was constructed, incorporating the critical temperatures obtained from both the simulation and the laboratory analysis. This error analysis provided valuable insights into the level of agreement between the simulated and calculated critical temperatures.

The analysis revealed a maximum error of 4.1% and an average error of 0.49% in the calculated critical temperatures. These values serve as indicators of the degree of deviation between the simulation results and the calculated data. The average error being lower than the maximum error suggests that, on average, the simulation results were in close agreement with the calculated values. However, it is important to note that there still exists some variation between the simulated and calculated critical temperatures.

To visually represent the comparison between the simulated and calculated data, a graph was created. The graph demonstrated a close alignment between the two sets of temperatures, indicating a substantial similarity between them. This visual representation further reinforces the

notion that, despite the presence of discrepancies, the simulation was able to effectively capture the essential characteristics of crude oil and provide reasonably accurate predictions of its critical temperature.

In conclusion, the interpretation of the results underscores the performance of the simulation conducted in this study. The errors calculated reveal the accuracy of the simulation in estimating the critical temperature of crude oil. Although some room for improvement remains, the simulation yielded valuable insights into the behavior of crude oil and validated the efficacy of the simulation approach employed.

### 3.4.5 Critical pressure

Critical pressure refers to the specific pressure at which a substance undergoes a phase transition from its gas phase to a liquid phase or from its liquid phase to a solid phase, at its critical temperature. It is the highest pressure at which a substance can exist as a gas or a liquid. Above the critical pressure, the substance cannot exist in a distinct liquid or gas phase, and instead exhibits properties that are intermediate between the two phases, often referred to as a supercritical fluid. The critical pressure is a characteristic property of a substance and varies depending on the nature of the substance itself.[25]

The obtained results and the values calculated from the correlations are represented in the following table.

**Table 3.7.** Obtained Values of Critical Pressure

<b>Fraction</b>	<b>P<sub>c1</sub></b>	<b>P<sub>c2</sub></b>	<b>E</b>
<b>1</b>	34.1978	36.89499	7.310457
<b>2</b>	29.7712	35.82984	16.90948
<b>3</b>	29.4232	34.84739	15.56556
<b>4</b>	29.1373	33.48928	12.99515
<b>5</b>	28.8709	32.36996	10.80959
<b>6</b>	27.9917	31.82885	12.05559
<b>7</b>	30.1316	31.29275	3.710608
<b>8</b>	29.5802	30.75549	3.821409
<b>9</b>	29.0118	30.23162	4.034918
<b>10</b>	28.3462	29.71568	4.608607



11	27.7152	29.21736	5.141322
12	27.1857	28.73068	5.377445
13	26.7595	28.26199	5.316308
14	26.2816	27.81007	5.496105
15	25.6027	27.36816	6.450778
16	25.6595	26.93526	4.736407
17	25.1527	26.52172	5.161887
18	24.7165	26.1226	5.382705
19	24.4586	25.73702	4.967229
20	24.0692	25.35187	5.05946
21	23.6706	24.96395	5.180862
22	23.2777	24.54963	5.18107
23	22.8492	24.0943	5.1676
24	22.7241	23.64708	3.903166
25	22.2704	23.20952	4.046267
26	21.8639	22.79197	4.071897
27	21.4702	22.38473	4.085514
28	21.1074	21.98883	4.008548
29	20.7617	21.59685	3.86698
30	20.4264	21.21542	3.719098
31	20.0717	20.84215	3.6966
32	19.7678	20.48265	3.490022
33	19.6335	20.13734	2.502037
34	18.924	19.7994	4.421337
35	18.391	19.46938	5.538839
36	17.9469	19.05083	5.794638
37	17.311	18.56032	6.731158
38	16.8227	18.07822	6.944926
39	16.3188	17.61189	7.342153
40	15.8276	17.16682	7.801206
41	15.3954	16.73123	7.984034
42	14.8944	16.31106	8.685277
43	14.4546	15.90186	9.101201
44	14.0821	15.59371	9.693722
45	13.6308	15.27931	10.78917
46	13.309	15.05722	11.61048

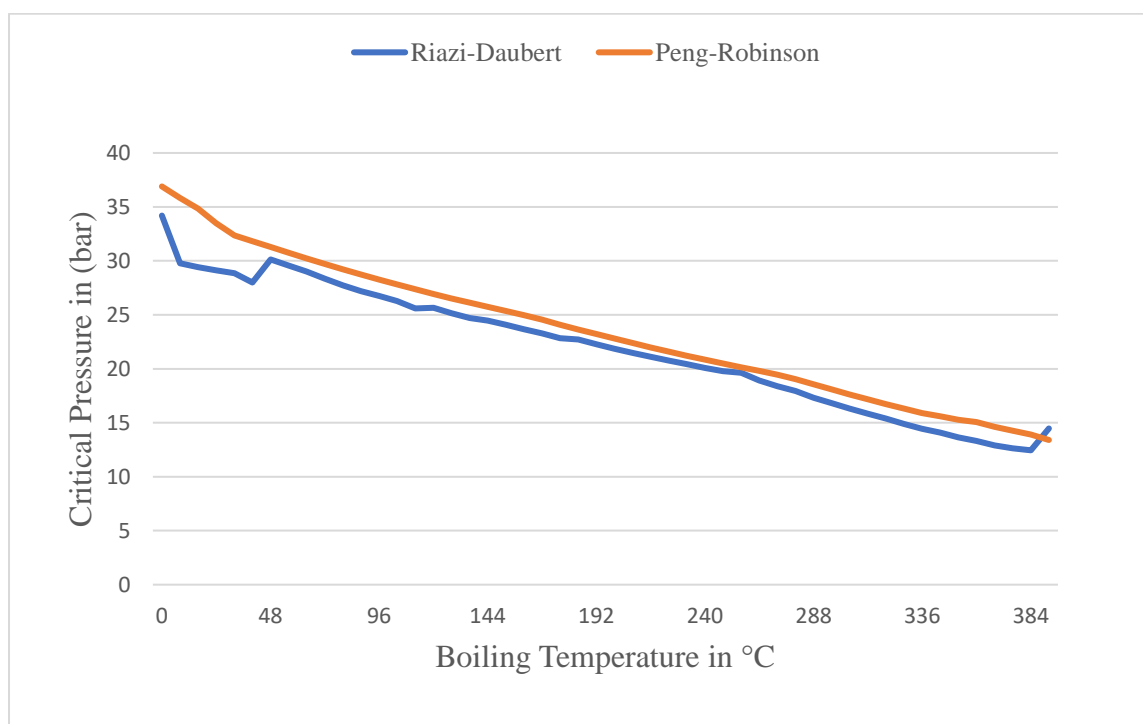
<b>47</b>	12.9008	14.62854	11.81074
<b>48</b>	12.6244	14.25957	11.46716
<b>49</b>	12.4477	13.90213	10.46191
<b>50</b>	14.4726	13.40569	7.958658
<b>Mean</b>	6.839346		
<b>Error</b>			

**P<sub>c1</sub>**: Critical Pressure using Riazi-Daubert correlation

**P<sub>c2</sub>**: Critical Pressure using Peng-Robinson correlation

**E**: Errors relative

Based on the previous values, we determined the error. We also plotted the variation curve for each correlation and demonstrate the P<sub>c</sub> (critical pressure) values.



**Figure 3.4.** A graph of Critical Pressure versus Boiling Temperature of the petroleum fractions

The objective was to examine the accuracy of a simulation performed to determine the critical pressure of a substance. By comparing the critical pressure obtained from the simulation with the critical pressure obtained through Riazi-Daubert correlation, the reliability of the simulation in predicting the substance's critical pressure was evaluated. The results were thoroughly analyzed

and interpreted to gain insights into the performance of the simulation and its ability to estimate the critical pressure accurately.

In order to present the findings effectively, a comprehensive table was constructed, incorporating the critical pressures obtained from both the simulation and the Riazi-Daubert correlation. Additionally, the errors between the two sets of pressures were calculated, employing appropriate methodologies. The analysis revealed a maximal error of 16.9% and an average error of 6.83% in the calculated critical pressures.

Notably, the maximal error observed in this study is comparatively higher than the maximal error encountered in the determination of critical temperature, indicating a greater discrepancy between the simulated and critical pressures. Moreover, the average error for critical pressure is also higher than the average error observed for critical temperature.

These results highlight the challenges and complexities associated with accurately estimating the critical pressure of the substance using the simulation approach. The higher maximal and average errors suggest that the simulation might not fully capture the intricate factors influencing the substance's behavior near its critical pressure point.

It is crucial to acknowledge the limitations and sources of error in the simulation process. Factors such as assumptions made during the simulation, uncertainties in input parameters, and the inherent complexity of the substance's behavior near critical conditions could contribute to the observed discrepancies.

The interpretation of these results underscores the need for further investigation and refinement of the simulation methodology used in estimating critical pressures. Future studies may explore alternative simulation approaches or consider additional factors that could influence the accuracy of the results.

In conclusion, the interpretation of the results emphasizes the challenges encountered in accurately determining the critical pressure of the substance through simulation. The higher maximal and average errors in critical pressure, compared to critical temperature, indicate the need for continued research and improvement in simulation techniques for estimating critical pressures. These findings contribute to the understanding of the limitations and complexities involved in predicting critical pressures, providing valuable insights for further advancements in this field.

### 3.4.6 Density at 15°C

Density at 15 degrees Celsius (°C) refers to the amount of mass per unit volume of a substance at a temperature of 15°C. It is typically expressed in units of kilograms per cubic meter (kg/m<sup>3</sup>) or grams per milliliter (g/mL).[26]

The density of a substance at a specific temperature is determined by the substance's molecular weight, the spacing between its molecules, and the temperature and pressure of the environment in which it is measured and its composition. [26]

It is an important property that to identify and differentiate various materials. In this report, we compare the density of the crude oil at a temperature of 15 degrees Celsius using two different correlations - the Riazi-Daubert and Peng-Robinson correlations.

**Table 3.8.** Obtained Values of Density

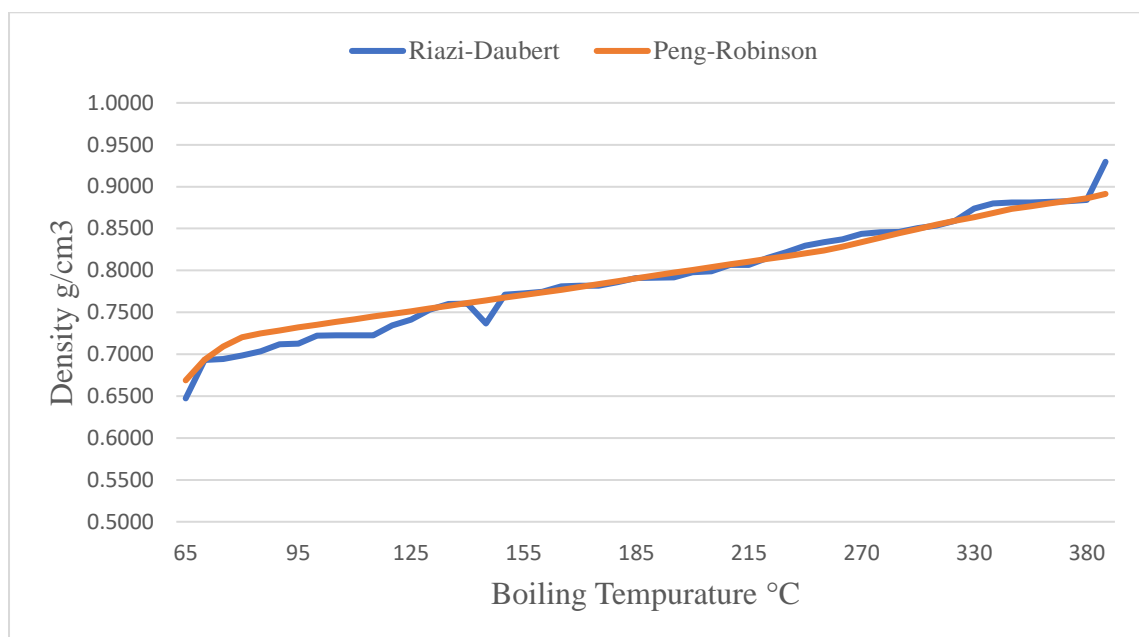
<b>Fraction</b>	<b>D<sub>1</sub></b>	<b>D<sub>2</sub></b>	<b>E</b>
<b>1</b>	0.6473	0.6688	3.2178
<b>2</b>	0.6933	0.6936	0.0434
<b>3</b>	0.6943	0.7094	2.1236
<b>4</b>	0.6983	0.7204	3.0615
<b>5</b>	0.7034	0.7250	2.9770
<b>6</b>	0.7120	0.7284	2.2562
<b>7</b>	0.7128	0.7320	2.6222
<b>8</b>	0.7223	0.7353	1.7721
<b>9</b>	0.7224	0.7386	2.1932
<b>10</b>	0.7226	0.7418	2.5893
<b>11</b>	0.7227	0.7450	2.9935
<b>12</b>	0.7345	0.7482	1.8285
<b>13</b>	0.7413	0.7514	1.3434
<b>14</b>	0.7532	0.7546	0.1877
<b>15</b>	0.7599	0.7578	0.2787
<b>16</b>	0.7604	0.7610	0.0744
<b>17</b>	0.7367	0.7642	3.6040
<b>18</b>	0.7712	0.7675	0.4761
<b>19</b>	0.7726	0.7708	0.2312
<b>20</b>	0.7747	0.7739	0.1016

21	0.7812	0.7769	0.5515
22	0.7817	0.7802	0.1921
23	0.7819	0.7836	0.2232
24	0.7859	0.7870	0.1447
25	0.7908	0.7904	0.0467
26	0.7913	0.7939	0.3230
27	0.7917	0.7973	0.6992
28	0.7977	0.8006	0.3674
29	0.7988	0.8039	0.6384
30	0.8065	0.8072	0.0868
31	0.8066	0.8105	0.4763
32	0.8152	0.8138	0.1766
33	0.8219	0.8171	0.5891
34	0.8296	0.8204	1.1245
35	0.8338	0.8237	1.2292
36	0.8370	0.8282	1.0624
37	0.8435	0.8337	1.1706
38	0.8456	0.8391	0.7799
39	0.8461	0.8443	0.2093
40	0.8506	0.8495	0.1268
41	0.8536	0.8546	0.1139
42	0.8592	0.8592	0.0048
43	0.8738	0.8636	1.1802
44	0.8798	0.8683	1.3188
45	0.8810	0.8733	0.8772
46	0.8812	0.8767	0.5181
47	0.8817	0.8799	0.2022
48	0.8825	0.8830	0.0555
49	0.8842	0.8861	0.2095
50	0.9297	0.8914	4.2999
<b>Mean error</b>			1.0595

**D<sub>1</sub>** – Density obtained from Riazi-Daubert correlation

**D<sub>2</sub>** – Density obtained from Peng Robinson correlation

**E** – error relative



**Figure 3.5.** A graph of density versus boiling temperature of the petroleum fractions

The graph illustrates the density values of the crude oil at 15°C as predicted by two different correlations: the Riazi-Daubert and the Peng-Robinson equations. The Riazi-Daubert equation is known to be a simple and fast method for estimating the density of hydrocarbons, whereas the Peng-Robinson equation is a more complex equation of state that takes into account molecular interactions.

As we can see from the plot, the two correlations generally agree with each other, with a few exceptions. The mean error between the two correlations is about 1.06%, which is relatively small.

Based on the general trend of the slope indicated on the graph, the graph demonstrates a more stable progression showed by the Peng Robinson correlation as opposed to the Riazi-Daubert correlation. This is more pronounced at the 14<sup>th</sup> fraction which may suggest an overestimation of the density at this point by the Riazi-Daubert correlation probably due to calculation errors whereas the other correlation indicated a more stable value with reference to the rest of the trend.

Another feature of the plot is the general trend of increasing density as the fraction increases. This is to be expected, as the fractions are becoming more concentrated in the number of total molecules as we move towards the right side of the plot. However, there are a few points where the density decreases even as the fraction increases, such as around fractions 1 and 17. This

suggests that there may be some non-linearities or complexities in the behavior of crude oil at these points.

Overall, the results suggest that both the Riazi-Daubert and Peng-Robinson correlations are reasonable approximations for the density of this liquid at 15°C. The small mean error between the two correlations indicates that they are generally in useful agreement with each other. Thus, it's accurate to use Aspen Hysys to estimate the density of a crude oil sample.

### 3.4.7 Acentric Factor

The acentric factor  $\omega$  is a conceptual number introduced by Kenneth Pitzer in 1955, proven to be useful in the description of fluids. The acentric factor is said to be a measure of the non-sphericity (centricity) of molecules. As it increases, the vapor curve is "pulled" down, resulting in higher boiling points[26]

Fluids containing non spherical molecules, or those with polar groups, demonstrate systematic deviations in their thermodynamic properties from their spherical counterparts. It is these deviations which are correlated with the acentric factor.[26]

Mathematically, it is expressed as:

$$\omega = \frac{\ln\left(\frac{P_c}{P_v}\right)}{\ln\left(\frac{P_c}{P_s}\right)}$$

Where  $P_c$  is the critical pressure,  $P_v$  is the vapor pressure at the boiling point, and  $P_s$  is the vapor pressure of a hypothetical spherical fluid with the same critical temperature and pressure.[26]

Or it can be expressed as

$$\omega = -\log_{10} P_T^{sat} - 1 \text{ at } T_r = 0.7.$$

Where  $P_T^{sat} = \frac{P^{sat}}{P_c}$  is the reduced saturation vapor pressure and  $T_r = \frac{T}{T_c}$  is the reduced temperature.[26]

With  $T_c$  and  $P_c$  are the critical temperature and critical pressure respectively.

The closer the value is to 0, the more spherical the molecules of the liquid or gas and vice versa.[26]

The following table reveals the comparison between the calculated values using the correlation of Riazi-Daubert and values simulated by Aspen Hysys using the Peng Robinson correlation.

**Table 3.9.** Obtained Values of Acentric factor

<b>fractions</b>	<b><math>\omega_1</math></b>	<b><math>\omega_2</math></b>	<b>E</b>
<b>1</b>	0.1238	0.2360	90.5993
<b>2</b>	0.2034	0.2735	34.4377
<b>3</b>	0.2337	0.2811	20.2773
<b>4</b>	0.2505	0.2888	15.2894
<b>5</b>	0.2641	0.2966	12.2974
<b>6</b>	0.2679	0.3031	13.1561
<b>7</b>	0.2750	0.3162	14.9860
<b>8</b>	0.2827	0.3241	14.6323
<b>9</b>	0.2905	0.3320	14.2818
<b>10</b>	0.2984	0.3397	13.8329
<b>11</b>	0.3063	0.3474	13.4182
<b>12</b>	0.3142	0.3554	13.0983
<b>13</b>	0.3222	0.3638	12.9288
<b>14</b>	0.3300	0.3720	12.7204
<b>15</b>	0.3379	0.3796	12.3276
<b>16</b>	0.3459	0.3896	12.6239
<b>17</b>	0.3538	0.3978	12.4269
<b>18</b>	0.3617	0.4063	12.3276
<b>19</b>	0.3695	0.4155	12.4371
<b>20</b>	0.3775	0.4242	12.3619
<b>21</b>	0.3858	0.4329	12.2171
<b>22</b>	0.3948	0.4416	11.8456
<b>23</b>	0.4051	0.4502	11.1440
<b>24</b>	0.4154	0.4603	10.8009
<b>25</b>	0.4259	0.4687	10.0390
<b>26</b>	0.4364	0.4773	9.3797
<b>27</b>	0.4469	0.4861	8.7715



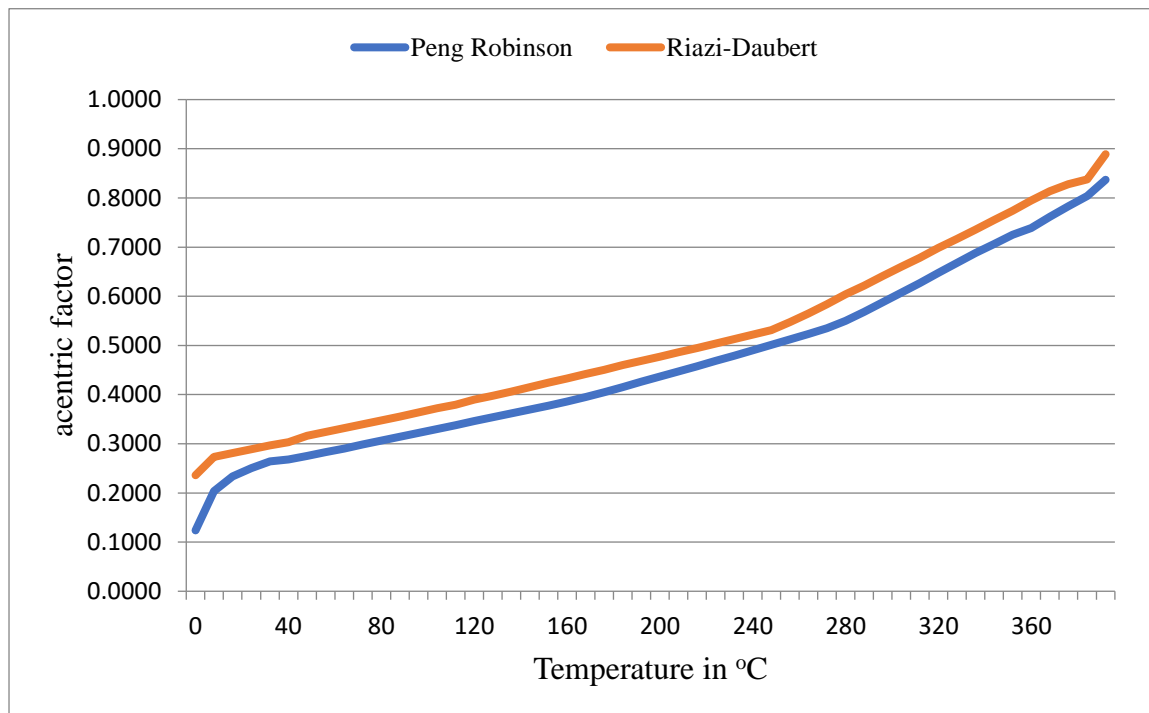
28	0.4575	0.4949	8.1796
29	0.4683	0.5039	7.6066
30	0.4792	0.5129	7.0415
31	0.4902	0.5217	6.4303
32	0.5012	0.5309	5.9237
33	0.5122	0.5473	6.8444
34	0.5234	0.5649	7.9310
35	0.5347	0.5840	9.2242
36	0.5498	0.6039	9.8479
37	0.5684	0.6217	9.3695
38	0.5876	0.6409	9.0652
39	0.6072	0.6599	8.6720
40	0.6270	0.6781	8.1447
41	0.6473	0.6981	7.8447
42	0.6676	0.7167	7.3547
43	0.6881	0.7358	6.9399
44	0.7059	0.7552	6.9885
45	0.7250	0.7741	6.7739
46	0.7387	0.7947	7.5823
47	0.7617	0.8133	6.7701
48	0.7828	0.8277	5.7385
49	0.8041	0.8374	4.1387
50	0.8369	0.8889	6.2121
<b>Mean error</b>	12.3057		

**ω1-** Acentric factor obtained by Peng Robinson correlation form Aspen HYSYS

**ω2-** Acentric factor calculated based on the Riazi-Daubert correlation.

**E-** Error relative.

Using the results above a graph of acentric factor versus boiling temperature to compare the two values is plotted.



**Figure 3.6.** A graph of acentric factor versus boiling temperature of the petroleum fractions

Using Aspen HYSYS, data showing the acentric factor using the correlation of Peng Robinson is generated and a graph of acentric factor versus temperature was plotted.

In general, the lower the value of acentric factor, the higher the degree of sphericity and the more the fluid acts as an ideal fluid. By comparing the acentric factor obtained from the simulation with the acentric factor measured through the calculated, the reliability of the simulation evaluated.

In order to present the findings effectively, a comprehensive table was constructed, incorporating the data obtained from both the simulation and the calculated. Additionally, the errors between the two sets were calculated, employing appropriate methodologies. Based on the results obtained the data shows a minimum error of 4.14% and a maximum error of 90.60% and an average error of 12.30%

Notably, the maximal error observed in this study is comparatively high, indicating a greater discrepancy between the simulated and calculated acentric factors. However, as shown in the graph, the general slope of both correlations seems consistent and similar without any intersecting points. This may suggest that the performance of the two methods is consistent across different amounts of data, but since the correlation of Riazi-Daubert has a higher degree of variability than

the other, it may indicate that the performance of that method is either less consistent or more affected by certain types of data.

The higher maximal and average errors suggest that the simulation might not fully capture the intricate factors influencing the substance's behavior concerning the acentric factor. Thus, it is crucial to acknowledge the limitations and sources of error in the simulation process. Factors such as assumptions made during the simulation, uncertainties in input parameters, and the inherent complexity of the substance's behavior as well as impurities could contribute to the observed discrepancies. Therefore, it may be better to use a different correlation to simulate the acentric factor or change the underlying equation of the correlation to receive more accurate values.

### 3.4.8 Watson k

The Watson characterization factor (Watson K) is an important parameter used in the petroleum industry to estimate the behavior and properties of crude oil fractions. [27]

The K factor or characterization factor is defined from Rankine boiling temperature  $^{\circ}\text{R}=1.8T_b[\text{k}]$  and relative to water density  $\rho$  at  $60^{\circ}\text{F}$ . [27]

The K factor is a systematic way of classifying a crude oil according to its paraffinic, naphthenic, intermediate or aromatic nature. The K(UOP) is also referred to as the UOP K factor or just UOPK. [27]

**Table 3.10.** Obtained Values of Watson K factor

Fractions	$W_{c1}$	$W_{c2}$	E
1	11.99	12.75	6.3386
2	11.907	12.24	2.7967
3	11.856	12.28	3.5762
4	11.846	12.27	3.5793
5	11.889	12.24	2.9523
6	11.887	12.15	2.2125
7	11.883	12.19	2.5835
8	11.883	12.09	1.7420
9	11.883	12.14	2.1628
10	11.884	12.19	2.5749

11	11.885	12.24	2.9870
12	11.885	12.1	1.8090
13	11.885	12.04	1.3042
14	11.884	11.89	0.0505
15	11.883	11.84	-0.3619
16	11.882	11.88	-0.0168
17	11.879	12.31	3.6283
18	11.875	11.81	-0.5474
19	11.871	11.83	-0.3454
20	11.87	11.85	-0.1685
21	11.869	11.79	-0.6656
22	11.869	11.83	-0.3286
23	11.871	11.87	-0.0084
24	11.873	11.86	-0.1095
25	11.875	11.83	-0.3789
26	11.875	11.86	-0.1263
27	11.876	11.9	0.2021
28	11.876	11.85	-0.2189
29	11.877	11.88	0.0253
30	11.878	11.8	-0.6567
31	11.88	11.84	-0.3367
32	11.88	11.76	-1.0101
33	11.879	11.72	-1.3385
34	11.878	11.69	-1.5828
35	11.877	11.71	-1.4061
36	11.873	11.74	-1.1202
37	11.868	11.72	-1.2471
38	11.866	11.76	-0.8933
39	11.863	11.83	-0.2782
40	11.86	11.83	-0.2530
41	11.859	11.86	0.0084
42	11.86	11.85	-0.0843

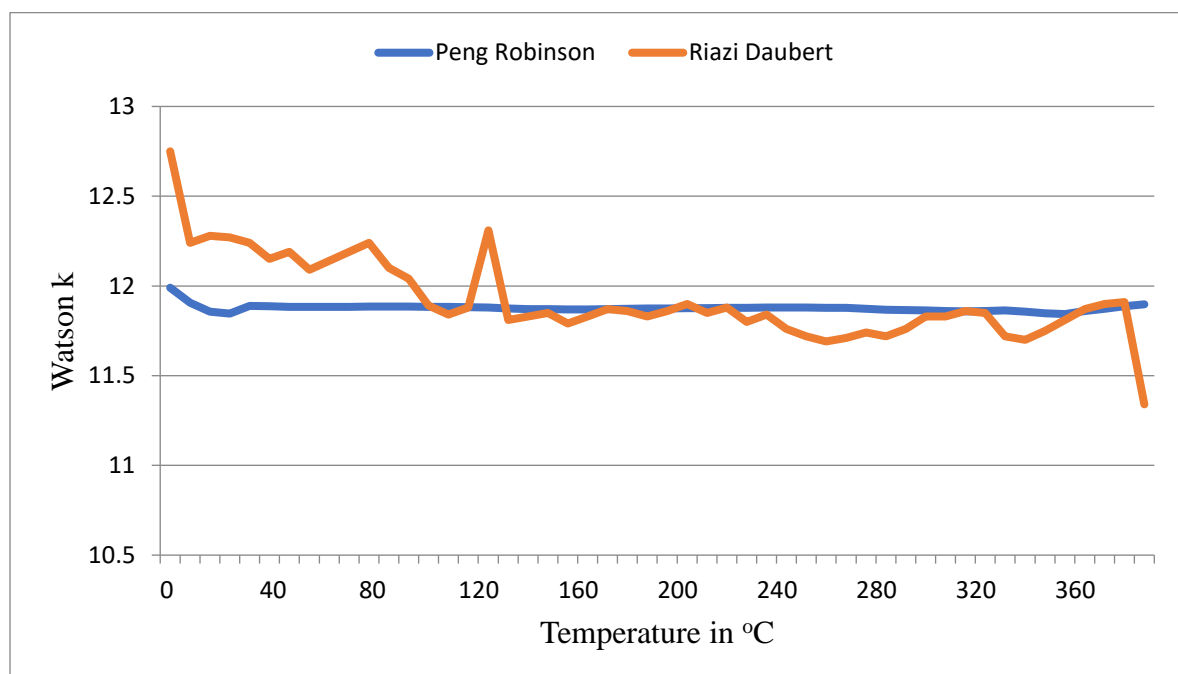
43	11.864	11.72	-1.2138
44	11.856	11.7	-1.3158
45	11.847	11.75	-0.8188
46	11.843	11.81	-0.2786
47	11.86	11.87	0.0843
48	11.873	11.9	0.2274
49	11.886	11.91	0.2019
50	11.898	11.34	-4.6899
average error	0.3849		

$W_{c1}$ -Watson K factor obtained from Peng Robinson correlation.

$W_{c2}$ -Watson K factor obtained from Riazi Daubert correlation.

E-Error relative.

Using the data presented above, a graph of Watson k versus boiling temperature is plotted for comparison.



**Figure 3.7.** A graph of Watson K factor versus boiling temperature of the petroleum fractions

The table provided compares the Watson K values obtained from the Peng-Robinson and Riazi-Daubert correlations for a set of crude oil fractions. To assess the accuracy of the Peng-Robinson method relative to the Riazi-Daubert method, we can analyze the average error.

The average error between the two methods is calculated as 0.3849. This value represents the average difference between the Watson K values obtained from the Peng-Robinson and Riazi-Daubert correlations across the dataset.

A positive average error indicates that the Peng-Robinson method tends to underestimate the Watson K values compared to the Riazi-Daubert method. Conversely, a negative average error would indicate an overestimation by the Peng-Robinson method.

Based on the average error of 0.3849, it can be inferred that the Peng-Robinson method generally provides slightly lower Watson K values compared to the Riazi-Daubert method for these crude oil fractions.

The Watson characterization factor is calculated based on the specific gravity (API gravity) and the boiling point of a crude oil sample. This is a constant value for a particular blend of hydrocarbons and does not change during the distillation process. Although the composition and properties of the fractions obtained during distillation will vary, the Watson characterization factor remains constant for a specific crude oil sample. It is a characteristic property of crude oil and is used as a fundamental parameter for various correlations and calculations in the petroleum industry.[24]

Based on these results, it may be safe to assume that the correlation of Peng Robinson may be better suited to calculating the Watson factor for this specific crude oil sample as opposed to using that of Riazi Daubert.

### **3.5 Conclusion**

After comparing each property with its average error, we can draw the following general conclusion:

- Temperature: The average error for temperature is 1.418, indicating a relatively low error compared to the range of temperature values. This suggests that the predictions for temperature are fairly accurate.

- Pressure: The average error for pressure is 6.839, which is relatively high compared to the range of pressure values. This indicates that the predictions for pressure have a higher level of uncertainty and may not be as accurate as desired.
- Density: The average error for density is 1.0595, which is low compared to the range of density values. This suggests that the predictions for density are relatively accurate.
- Acentric Factor: The average error for the acentric factor is 12.809, which is relatively high compared to the range of acentric factor values. This indicates that the predictions for the acentric factor have a higher level of uncertainty and may not be as accurate.
- Watson K: Based on the average error of 0.3849, it can be inferred that the simulated values give a result that is within the expected range. However, as demonstrated in the graph by the instability in the values generated by Riazi Daubert, it might require a change of the models used to simulate these values for a more accurate and detailed comparison.

Based on these comparisons, it can be concluded that the predictions for temperature and density are relatively accurate, whereas the predictions for pressure and the acentric factor have higher levels of uncertainty and may not be as accurate.

# **General Conclusion**



### **General conclusion**

In this master's thesis, we investigated the simulation of TBP distillation using Aspen HYSYS for predicting the physicochemical properties of petroleum fractions. The objective was to assess the accuracy and reliability of Aspen HYSYS as a simulation tool in comparison to traditional experimental methods and analytical techniques.

Through a comprehensive literature review, we gained a deep understanding of distillation processes, petroleum fractions, and simulation techniques. This foundation allowed us to design and execute simulation experiments using Aspen HYSYS, generating data on the physicochemical properties of various petroleum fractions.

Our findings revealed that Aspen HYSYS offers a valuable and efficient approach for simulating TBP distillation and predicting the properties of petroleum fractions. The simulation results closely aligned with the reference data obtained from traditional experimental methods and analytical techniques, demonstrating the accuracy and reliability of the software.

The advantages of utilizing Aspen HYSYS became evident throughout the research process. The software significantly reduced time requirements compared to traditional experimental approaches, allowing for rapid exploration of various scenarios and conditions. Additionally, simulation provided a cost-effective alternative, eliminating the need for expensive equipment and consumables.

Furthermore, simulation enabled us to analyze and understand the behavior of petroleum fractions in greater detail. We could observe the effects of different parameters and variables on the distillation process, providing valuable insights for refining optimization and product development.

However, it is essential to acknowledge the limitations of simulation. While Aspen HYSYS proved to be a powerful tool, it relies on accurate input data and models that represent the real-world conditions adequately. Deviations between simulation and experimental results could arise due to uncertainties in the input data or assumptions made during modeling. Therefore, it is crucial to validate simulation results with experimental data whenever possible.

In conclusion, this master's thesis contributes to the field of petroleum refining by showcasing the capabilities and benefits of using Aspen HYSYS for the simulation of TBP distillation and

prediction of physicochemical properties of petroleum fractions. The results emphasize the accuracy and reliability of the software, which can lead to improved efficiency, cost savings, and informed decision-making in the petroleum industry.

Future research can explore further refinements of the simulation models, incorporating additional complexities and considering different types of crude oils. Additionally, the integration of optimization algorithms can enhance the potential of Aspen HYSYS for refining process optimization and product quality improvement.

Overall, this study highlights the significance of simulation techniques in understanding and analyzing complex processes within the petroleum industry. By bridging the gap between theory and practice, simulation contributes to the advancement and sustainability of the industry, ultimately leading to more efficient utilization of petroleum resources and improved product quality.

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## Abstract

This study investigates the simulation of TBP distillation using Aspen HYSYS to predict the physicochemical properties of petroleum fractions. The objective is to assess the accuracy and reliability of Aspen HYSYS in comparison to traditional experimental methods. Through a comprehensive literature review and simulation experiments, the research demonstrates that Aspen HYSYS accurately predicts the properties of petroleum fractions, aligning closely with reference data. The software offers advantages such as reduced time requirements and cost-effectiveness. The findings provide valuable insights into the behavior of petroleum fractions and contribute to refining optimization. While simulation has limitations, validation with experimental data ensures reliability. Overall, this study highlights the capabilities and benefits of Aspen HYSYS in simulating TBP distillation and emphasizes its potential for efficient utilization of petroleum resources and improved product quality.

**Keywords:** Distillation, petroleum fractions, TBP, Aspen Hysys, physical and chemical properties, PR correlation.

## ملخص

هدفت هذه الدراسة إلى هذه محاكاة التقطير النقطي لنقاط الغليان الحقيقية باستخدام برنامج أسبن هايسيس لتوقع الخواص الفيزيوكيميائية لكسور النفط الخام. الهدف هو تقييم دقة وموثوقية أسبن هايسيس مقارنةً بالطرق التجريبية التقليدية. من خلال استعراض شامل للمصادر وتنفيذ تجارب المحاكاة، تبين البحث أن أسبن هايسيس يتنبأ بدقة بخواص كسور النفط، ويتفق تقريبًا مع البيانات المرجعية. يوفر البرنامج مزايا مثل تقليل الوقت المطلوب وتوفير التكاليف. تقدم النتائج رؤى قيمة حول سلوك كسور النفط وتساهم في تحسين تكيف العمليات. على الرغم من وجود قيود في المحاكاة، فإن التحقق من النتائج باستخدام البيانات التجريبية يضمن الموثوقية. بشكل عام، تسلط هذه الدراسة الضوء على إمكانيات وفوائد أسبن هايسيس في محاكاة التقطير النقطي لنقاط الغليان الحقيقية وتؤكد إمكانية استخدامه في استخدام فعال لموارد النفط وتحسين جودة المنتج.

**الكلمات المفتاحية:** تقطير، كسور البترول، نقطة التقطير الحقيقية (TBP)، أسبن هايسيس، الخصائص الفيزيوكيميائية، ارتباط بين روبنسون.

## Résumé

Cette étude examine la simulation de la distillation TBP en utilisant Aspen HYSYS pour prédire les propriétés physico-chimiques des fractions de pétrole. L'objectif est d'évaluer l'exactitude et la

fiabilité d'Aspen HYSYS par rapport aux méthodes expérimentales traditionnelles. À travers une revue de littérature complète et des expériences de simulation, la recherche démontre qu'Aspen HYSYS prédit avec précision les propriétés des fractions de pétrole, en étroite corrélation avec les données de référence. Le logiciel présente des avantages tels que des exigences temporelles réduites et une rentabilité accrue. Les résultats fournissent des informations précieuses sur le comportement des fractions de pétrole et contribuent à l'optimisation du raffinage. Bien que la simulation présente des limitations, la validation avec des données expérimentales garantit la fiabilité. Dans l'ensemble, cette étude met en évidence les capacités et les avantages d'Aspen HYSYS dans la simulation de la distillation du TBP et souligne son potentiel d'utilisation efficace des ressources pétrolières et d'amélioration de la qualité des produits.

**Mots clés :** Distillation, fractions de pétrole, TBP, Aspen Hysys, propriétés physico-chimiques, corrélation PR.