# MAXIMIZING LIGHT PETROLEUM GASES (LPG) YIELD FROM ATMOSPHERIC DISTILLER OF CRUDE OIL DISTILLATION USING RESPONSE SURFACE METHODOLOGY

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**by**

**VINODINI KANDASAMY**

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## LIST OF SYMBOLS

| | Symbol | Unit |
|---|---|---|
| API | American Petroleum Institute gravity | ° |
| | Duty / Power | W |
| Error | Error Percentage | % |
| | Flowrate | kg/s |
| T | Furnace Temperature | K |
| P | Pressure | Pa |
| | Steam to Feed Flowrate Ratio | % |
| TBP | True Boling Point | °F |
| | Yield | % |

## LIST OF ABBREVIATIONS

| | |
|---|---|
| ADU | Atmospheric Distillation Unit |
| AGO | Atmospheric Gas Oil |
| ANOVA | Analysis of Variance |
| API | American Petroleum Institute |
| bbl/d | Barrels per Day |
| bscfd | Billion Standard Cubic Feet per Day |
| CCD | Central Composite Design |
| CDU | Crude Distillation Unit |
| LPG | Light Petroleum Gas |
| PFD | Process Flow Diagram |
| OFAT | One Factor at a Time |
| RSM | Response Surface Methodology |
| V | Version |

**MEMAKSIMUMKAN PEROLEHAN BUTANA DAN HASIL HIDROKARBON RINGAN DARIPADA PENYULINGAN ATMOSFERA MINYAK MENTAH PETROLEUM DALAM RADAS SULING ATMOSFERA MENGGUNAKAN METODOLOGI PERMUKAAN RESPON**

## ABSTRAK

Gas petroleum ringan (LPG) merupakan produk ringan penyulingan atmosfera minyak galian yang digunakan untuk pelbagai aplikasi di seluruh dunia. Selaras dengan pembangunan perisian simulasi Aspen Plus dan Design Expert, kajian mensimulasikan dan mengoptimumkan proses tertentu untuk menghasilkan produk akhir seperti yang diinginkan mampu dilaksanakan. Dalam kajian ini, Aspen Plus digunakan untuk tujuan simulasi dan Design Expert untuk tujuan mengoptimumkan proses penyulingan atmosfera, menghasil LPG pada kadar maksimum oleh kerana pasaran pesat LPG di mata dunia. Simulasi penyulingan atmosfera dilakukan menggunakan radas PETROFRAC, dengan ciri minyak mentah dokumen 53016. Analisis simulasi menunjukkan bahawa tiga pembolehubah manupulasi terpilih: suhu relau, bilangan peringkat dan nisbah wap dan suapan minyak pada aliran masuk radas mempunyai pengaruh yang tinggi terhadap penghasilan LPG. Perolehan LPG didapati berkurang dengan suhu relau yang semakin meningkat dan bilangan peringkat turus penyulingan serta nisbah pula, meningkat hasil LPG sehingga kuantiti maksimum sebelum menurun secara mendadak. Kajian menunjukkan hasil LPG maksimum 5.177%, lebih tinggi daripada industri, 2.9% secara purata dan kadar aliran tertinggi, 26.2 kg/s LPG dihasilkan pada suapan 507 kg/s minyak galian. Hasil LPG maksimum diperoleh pada faktor optima : suhu relau 603.15 K, bilangan peringkat turus 33 tingkat dan nisbah wap ke suapan 1.90%.

**MAXIMIZING BUTANE AND LIGHTER HYDROCARBON YIELD FROM ATMOSPHERIC DISTILLER OF CRUDE OIL DISTILLATION USING RESPONSE SURFACE METHODOLOGY**

## ABSTRACT

Light petroleum gas (LPG) is a product of extruded oil ADU. LPG stands from refinery hydrocarbon gases such as methane, ethane, propane, butane and their existing isomers, used for various application worldwide. With the development of simulating software such as Aspen Plus and Design Expert, it is possible to simulate and optimize a specified process with desired end-product characteristics prior to plant running. As the LPG demand market grows tremendously worldwide, it is of utmost importance for LPG demand to be met. In this work, Aspen Plus is used to simulate and Design Expert is used to optimize an atmospheric distiller processing extruded crude into LPG and many more products. Simulation of the atmospheric distillation was done using a PETROFRAC distiller, crude assay 53016 beside operating parameters and inlet streams' properties. Sensitivity analysis on the same PETROFRAC distiller model shows that three chosen operating parameters : furnace temperature, number of stages and ADU steam to feed ratio had significant effects on LPG yield. The LPG yield is found to be decreasing with increasing furnace temperature, number of stages and steam to feed ratio after a maximum value. The optimization study conducted in Design Expert software resulted in maximum LPG yield of 5.177% and throughput of 26.2 kg/s LPG for simulation model fed with 507 kg/s of crude at optimum process conditions : 603.15K furnace temperature, 33 number of stages and 1.90% of steam to feed ratio. The optimized yield, 5.177% achieved was higher than common LPG yield in industry which is 2.9%.

## CHAPTER ONE

## INTRODUCTION

### 1.1 Crude Processing

#### 1.1.1 Atmospheric Distillation

Crude oil distillation is the first paramount operation of the petroleum refinery process in crude based product processing. Atmospheric distillation is a type of steam distillation since vaporization of crude occurs by introduction of steam in column (Heinemann et al., 2016). The extruded oil undergoes an atmospheric distillation producing light products such as light petroleum gases (LPG), gasoline, naphtha, kerosene and light fuel oils while the atmospheric distiller's residue undergoes vacuum distillation producing heavier distillate at higher pressure.

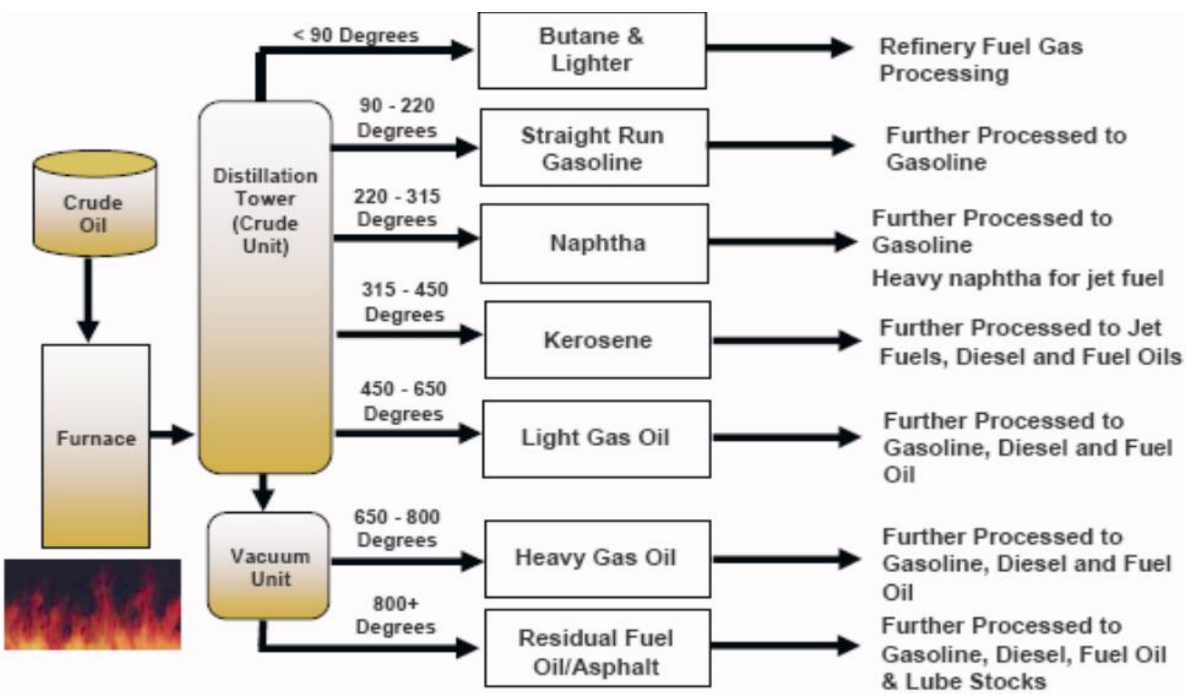


Figure 1.1: Crude Distillation Unit Diagram (Big West of California,2008)

In atmospheric distiller, the heated crude oil, mixture of hydrocarbons boils off producing different products, recovered at different temperatures of atmospheric pressure at different cuts of distillation column. The product fluid of lowest boiling point will be distilled at topmost tray of distillation column, which is also the lightest of all products (Fahim et al., 2010). As we go down the column, product pours out at higher boiling point and would be heavier.

In simple words, atmospheric distillation of crude oil involves fractional distillation of hot, pre-heated crude oil. The crude present in vapour form, is converted into product stream at varying boiling point being cooled by condenser to the pour temperature and refluxed by pumparounds and side-strippers to increase fractioned product flowrate and to reduce the heat captivated by column (Bagajewicz et al., 2001). The whole distillation occurs at atmospheric pressure of 101325 Pa. However, there would be small pressure drop in the fractionated distillation column.

### 1.1.2 Importance of LPG

LPG, a product from the distillation column, mixture of refinery gases compromising methane, ethane, propane, butane and their existing isomers (Fahim et al., 2010). Besides, petroleum, LPG could also be derived from another feedstock made of fossil fuel: natural gas (Heinemann, et al., 2016). The outlet of LPG at first is in vapor form from atmospheric distiller, which is then liquefied in the subsequent processes for eased transport and industrial use. This liquefaction is most vital to lower the pressure buildup in the pipeline caused by dual phase existence. Upon liquefaction, the LPG stream is also known commonly as liquefied petroleum gas stream. This pressure increase in pipeline could risk an explosion in plant (Benali et al., 2012b). The common LPG such as propane and butane evaporate under atmospheric pressure. LPGs have various applications and are used by the entire world population. In 2015, Malaysia's domestic gas consumption was at 2.6 BSCFD where 82% of the consumption was by Peninsular population, 8% consumed by Sarawak and another 10% by Labuan and Sabah population. LPG are used mostly by power stations which is 55% of all uses to produce electricity in Malaysia (Malaysia Gas Association, 2016). Light gases such as propane, ethane and the butane hydrocarbons are widely used in plastic manufacture industry, as cooking fuel and as heating element of other domestic uses (Fahim et al, 2010).

LPG has an average octane number of 104, higher than octane number of gasoline, a common petroleum-based fuel, 90.5. Octane number resembles numerical measure of fuel's ability to resist knocking or pinging during combustion of fuel during ignition. The higher the value is, the smoother the rides and better the engine performance is to be achieved by vehicles. Therefore, LPG stream is also a convenient automotive fuel (Demirbas, 2002). Moreover, LPG is the primary choice of cooking fuel surpassing kerosene and biomass fuel in demand. Thus, production of butane and lighter hydrocarbons by atmospheric distillation should be able to meet demand in market. LPG is considered to be a popular choice of fuel due to its clean and minimized impureness trait. LPG also causes less hazard and health harm at use. Setting operating conditions and parameters in such a way that these gas products of crude oil distillation are maximized, helps to achieve this market demand. As per statistics, heavy products of crude oil are more expensive to process and are not of domestic use compared to lighter hydrocarbon products (D'Sa et al., 2004).

### 1.1.3 Response Surface Methodology (RSM)

Khuri Andre I and Mukhopadhyay Siuli (2010) reported that RSM is the technique of generating model correlating experimental factors to responses. This is a statistical approach which functions to predict response values for desired set of variable manipulated, to determine significance of the factors and to determine factors' values that result in maximum response. The series of functions met is to be considered as optimization method.

The mathematical model necessary for RSM is either presented in first or second order. Both models have differing design method to generate regression model, determine significance and optimized factors. First order model uses either 2*k* factorial, Plackett–Burman, or simplex design. On the other hand, 3*k* factorial, central composite (CCD), and Box–Behnken designs are used by second order. CCD is the most popular choice for second order modelling as it is capable of generating graphical- contoured and tabulated data on regression model of 3D plot including axial point unlike other design technique (Bezerra et al., 2008). The CCD graph generated is also known as orthogonal graph design. This project simulation had CCD at use for Design Expert optimization. RSM has contour and surface plot as result representing illustration. Figure below shows an example of plot generated for RSM under CCD:

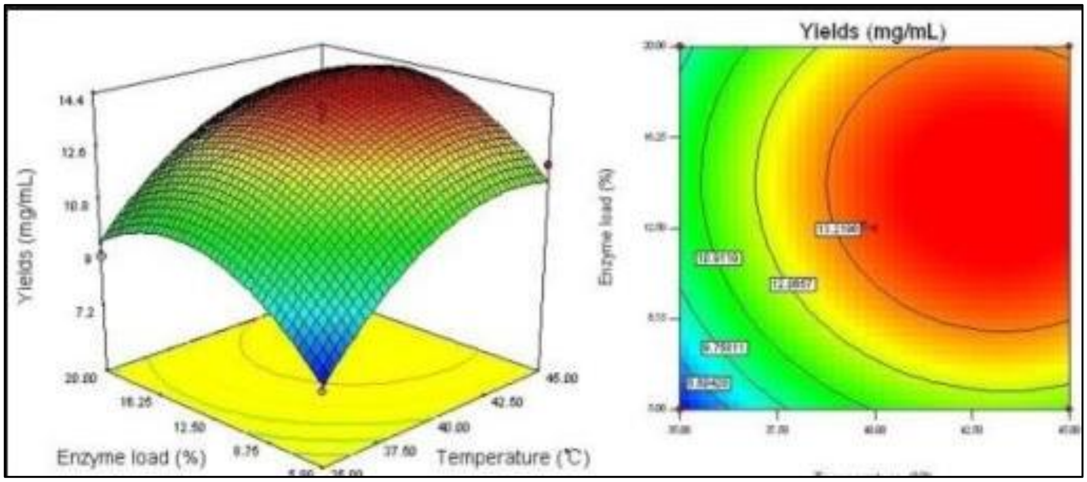


Figure 1.2: Surface Plot and Contour Plot of an Experimental (Box et al., 2005)

## 1.2 Problem Statement

Considering the importance of the LPG market, research has to be stepped up to improve the industrial atmospheric distillation process supplying the ever increasing needs of the market and at the same time, assuring high quality petroleum products. With the aid of softwares such as Aspen Plus and Design Expert, it is possible to simulate and optimize a particular process with desired end-product characteristics. In this case, simulation should be able to vary variables related to end product yield and most importantly, maximizing the LPG production throughput. A proper design of operating conditions and parameters of crude distillation unit can significantly improve the quality and yield of the butane and lighter hydrocarbon products. Such conditions can be said as manipulation of variables (Liu, 2012). Therefore, this research will focus on maximizing butane and lighter hydrocarbon or simply, the LPG yield from atmospheric distiller of crude oil distillation using RSM. It is common to produce LPG of yield 2.9% from atmospheric distillation of crude oil in industry (Colwell and Ronald, 2009). However, yielding a higher amount of LPG would be much pleasant for industrialists.

These manipulating variables or parameters include furnace temperature, number of stages or trays of column and steam to feed flowrate ratio of crude distillation unit (CDU). Previously, researches focus have been on ‘One Factor at a Time’ Technique (OFAT) instead of the cumulative effect of all relevant factors combined. This is due to the complicated correlation between the multiple factors and response. As a result, an optimum set of reaction conditions obtained from OFAT technique became less desirable and this was further proven by the inconsistency of results that existed from a previous work to another (Malaysia Gas Association, 2016). Considering multiple factors in experimental approach, without a proper design of experiment, the approach would be time-consuming, costly and tedious. Moreoever, bench-scale experimental results are nonpareil to be compared to industrial, real plant scale production. If researchers were to execute a set of experimental run at real, industrial scale crude processing plant, it is to be irrational as well. Manipulating a plant’s operating condition would need immense amount of crude and steam for runs. Besides, each shutdown and constructional change to plant is expensive. With software tools to help in designing the experiment in order to optimize the process parameters for the highest yield, the effort would be more effective and efficient. The results would be obtained faster and more accurately.

Therefore, in this project, the simulation software Aspen Plus V8.8 is used to study the individual and combined effects of the various manipulating variables on the yield of butane and lighter hydrocarbons. Then, Design Expert software was utilized for sensitivity analysis, conducted on the respective manipulating variables in a combined effect, followed by optimization of the distillation process to maximize the yield of LPG.

## 1.3 Research Objectives

The objectives of this research are as follow:

1. To simulate the atmospheric distillation of crude oil using the PETROFRAC distiller model and compare with literature data.

2. To investigate the effect of furnace temperature, number of trays in column and ratio of steam to crude feed flowrate on the yield of LPG by using sensitivity analysis in Aspen Plus software.

3. To study and optimize the production of petroleum products by maximizing the yield of butane and lighter hydrocarbons (LPG) using the optimization tool of Design Expert software.

## 1.4 Scope of Project

In this study, simulation-based work was done to simulate the atmospheric distillation of crude oil using Aspen Plus Version 8.8 producing LPG and other distillation products. This paper focuses solely on simulation-based approach rather than experimental approach in order to study the individual and combined effects of the various manipulating variables on the yield of LPG (overhead product). The equipments of the process were furnace followed by atmospheric distiller equipped with condenser, pump-around and side-stripper steams. The simulation was done comparatively to a literature article for validity of results

(Gu et al., 2014). The effect of various operating conditions such as column inlet temperature, number of trays in column and steam to feed flowrate ratio on yield of LPG are studied in order to obtain the optimum set of operating conditions for the process. The optimum reaction conditions are vital in order to produce high LPG yield in the production plant. LPG yield is also recovery percentage of LPG by plant.

### 1.5 Organization of Thesis

This thesis consists of five main chapters and each chapter contributes to the sequence of this study. The following are the contents for each chapter in this study:

**Chapter 1** introduces the overview of this research and the significance of LPG in real life, problem statement, research objectives, scope of this project and the organization of thesis.

**Chapter 2** discusses the literature review of this study. A short description on evolution of the petroleum refinery industry and its history were mentioned. Besides, the current atmospheric distillation process and its features were also discussed. Finally, previous research works on maximizing LPG yield were also included.

**Chapter 3** covers the experiment materials required for this study and the details of methodology from the start of this research project. It discusses on the description of equipment and materials used and steps of simulation run until optimization of factors.

**Chapter 4** refers to the results data and discussions of the data obtained. Further elaboration on the factors affecting yield results and optimization of atmospheric distillation by the manipulating variables are also contented.

**Chapter 5** concludes all the findings achieved in this research study. Recommendations for future studies on this research topic are included as well.

# CHAPTER TWO

# LITERATURE REVIEW

## 2.1 Crude Refinery

### 2.1.1 Evolution of Crude Refinery

Crude oil was first commercially refined by Samuel Kier producing lamp oil in Pennsylvania. The refined products then varied as time passed by. Different end product properties were necessary based on constantly changing world market demand. Refinery operation in the early days took place in an absolute different method. For example, distillation of crude oil involved fractional distillation at high temperature and pressure, crude tank or distillation tower was more of barrel by look and longer in longitudinal arrangement.

Distillation of crude was also less efficient at its early stage of invention before being developed. In 1890s, kerosene and heavy fuel oils were more in demand by the global market rather than lighter crude products. Thus, the crude processing manner differed especially temperature of distill fraction set and steam flowrates. Also, at early 20$^{th}$ century, crude refinery plant saw distillation product streams in liquid phase only before the LPG use and vapor storage was well utilized by downstream petroleum industries. Then, after 1910, light crude products were more in demand such as kerosene, gasoline and naphtha (Bobby, 2009). Also, around 1932, researches were conducted to determine optimized process of column and membrane separation as it was an era which had crude distillation done in batch not continuously as we have now, in industry (Fenske et al., 1932).

Crude refinery saw lots of changes since then. Fractional distillation at atmospheric pressure was standardized by all oil and gas companies. In the further upstream, catalyst use became an innovative upgrade to product forming, different cracking methods and purifying of end products of crude refinery took place as well (John et al., 2018).

## 2.2 Current Industrial Crude Distillation

Crude refinery operations can be described in 4 basic stages: Desalting pre-treatment, distillation, conversion and blending post-treatment. Desalting involves removal of certain metals and other suspended solids from crude before entering the distillation stage. Distillation unit stands from 2 sections: atmospheric distillation and vacuum distillation. This is the stage where crude fractionates into various, desired hydrocarbon products. Conversion stage involves reshaping and breaking down of product molecules increasing product yield and quality. Finally, post-treatment is all about product specification. Product processing such as removal and mixing of elements take place to meet the desired product properties at end of refinery (Fahim et al., 2010).

The current refinery industrial companies are always on duty, working on ways to optimize the distillation unit and crude processing as overall. One widespread methodology of optimization practiced by trending companies is the pinch analysis or technology (China National Petroleum Corporation, 2015). The technology focuses more on optimizing design and energy consumption at intermediate sections of the atmospheric distillation using advanced computer simulation software. Refinery field successors also never neglect the potential of biomass in contributing and portraying properties similar to the fossil fuel based crude. Industry now also owns process flow with bio-touch producing bio-fuels. For example, petroleum refinery and downstream processing of crude involves use of biocatalyst and biochemical treating substance vastly now. This is due to their environmental friendly and sustainable nature (Speight, 2011).

### 2.2.1 Features of Atmospheric Distillation Column

The atmospheric distillation unit (ADU) is made of furnace followed by atmospheric distiller tower. The tower also has side-stripping product streams: naphtha, kerosene and atmospheric gas oil. The distillation column unit has pressure around 101325 Pa, thus, it is known as atmospheric distillation. However, the distillation occurring at atmospheric pressure do have a pressure profile within the column. The column experiences significant pressure drop at every stage within column while heated vapour get fractionated out as product flow (Sloley, 2014). These side-stripping product streams may be varied based on desired demand. Besides side streams, the tower also produces a bottom product, atmospheric residual stream and an overhead flow producing column residue water and light petroleum gas. The side-stripping streams are fitted with pumparounds to ensure that the pressure in side-stripping pipes and their flowrates are not lowered (More et al., 2010). Side-stripper functions to regulate and set desired temperature profile in the column. Not to be forgotten, the stripping steam streams are all at superheated condition where, the flow temperature is higher than boiling point of water at absolute pressure. This criteria of steam allows stripping stream to eliminate the light end components from the side-product flow about to be leaving distillation column at its pour point (Seo et al., 2000). This feature increases butane and lighter hydrocarbon absorbed into the LPG stream cumulatively. Similarly, pumparound functions to regulate and set desired pressure profile within column (Sotelo et al., 2017).

Pumparound draws liquid from the distillation tower, cools the stream as pumped around and then return the flow, back into the column at a tray stage above the stage at which liquid was earlier drawn (Sloley, 2014). The atmospheric residue would be the inlet for vacuum distillation column unit.

## 2.3 Previous Works on Optimizing Crude Distillation

Previous studies carried out to maximize production were more concern on optimizing crude refinery as whole rather than a single processing unit optimization (Lin et al., 1997). Optimization is a subsisting research path in petroleum refinery to overcome crisis like diminishing fossil fuels, alarming greenhouse gases release rate and growth in renewable energy in various economic driven fields (Benali et al., 2012a). Previous works by researches varied vastly, some compared experimental results of crude distillation to simulated distillation process results (Gu et al., 2014) while another category of researchers worked their research papers wholly based on simulation results (Al-Muslim et al., 2005). Research paper by Waheed and Oni (2015) focused on economic analysis of overall design of CDU, energy-saving capability of simulated process and optimization of the desired outlets. Re-designing of flowsheet was done time-to-time so that the modification was efficient to be practiced for real applications. This made simulation run an important channel of problem-solving. Husain and Ibrahim's journal : Thermodynamic analysis of crude oil distillation systems (2005) on thermodynamic analysis also worked on simulation and thermodynamics modelling equation of CDU for optimum performance of process. Simulation was a familiar technique of setting away operating condition and equipment design problems as it is all computerized and does not involve prototype building in real space. Real prototype would definitely be a costly option.

Therefore, different designs of distillation column were tested to identify the most efficient set of atmospheric distillation column equipment (Alattas et al., 2011). For example, distillation process was optimized for number of pumparound fitted to column (Bagajewicz et al., 2001). Also, every possible parameters of materials and equipment of crude distillation simulation model were also optimized based on previous research literatures (García-Herreros et al., 2013).

Other than crude distillation, various works on pre-treatments and post-treatments of distillation were fitted in the petroleum refinery process to increase lighter products of refinery which are higher in demand. For an example, de-butanizer and de-ethanizer towers were proposed to increase the LPG yield. Similarly, further downstream processes such as thermal cracking, hydrocracking and fluidized catalytic cracking were intended to increase light atmospheric distillation products including LPG. These modification to refinery or known better as post-treatment processes also favour distillation optimization (John et al., 2018).

Below is a table of previous researches on factors affecting and optimization of atmospheric crude distillation:

Table 2.1: Previous Researches of CDU

| **Case** | **Reference** | **Research Purpose** | **Parameters Measured** |
|---|---|---|---|
| **1** | Al-Muslim et al., 2005 | Effect of distillation unit operating conditions (Temperature, Pressure) on energy efficiencies | Product flow, yield<br>Energy loss |
| **2** | Anitha et al., 2011 | Comparative study of various crude type effect on ADU and CDU Aspen Plus simulation | Product flow and yield |
| **3** | Benali et al., 2012a | Effect of preheating unit installation on energy consumption by CDU | Exergy analysis,<br>Product flow |
| **4** | Liau et al., 2004 | Optimization of input crude oil conditions affecting CDU process | Side stripping product flowrate |
| **5** | More et al., 2010 | Optimization of CDU using AspenPlus software and effect of binary feed on distillation process | Product flowrate<br>Case study cost profit |
| **6** | Sotelo et al., 2017 | Effect of control strategy on distillation column product quality | Temperature and flow variables |

## CHAPTER THREE

## MATERIALS AND METHODOLOGY

A process simulation model for atmospheric distillation of crude oil is generated with the Aspen Plus V8.8 simulator software. This is to study the relationship between the column operating conditions: furnace temperature, number of trays in column, ratio of steam to crude feed flowrate and yield of LPG.

### 3.1 Distillation Model

This research project involves the simulation and optimization of the crude atmospheric distillation using Aspen Plus Version 8.8 and Design Expert software (Liu, 2012). Aspen Plus software was utilized as a tool to conduct simulation and analysis of factors of atmospheric distillation of crude oil on the production of butane and other lighter hydrocarbons in the form of LPG (More et al., 2010). Then, Design Expert was used to commence optimization of factors of distillation process using RSM. The figure below shows process flow diagram (PFD) of the atmospheric distiller equipment in the CDU:

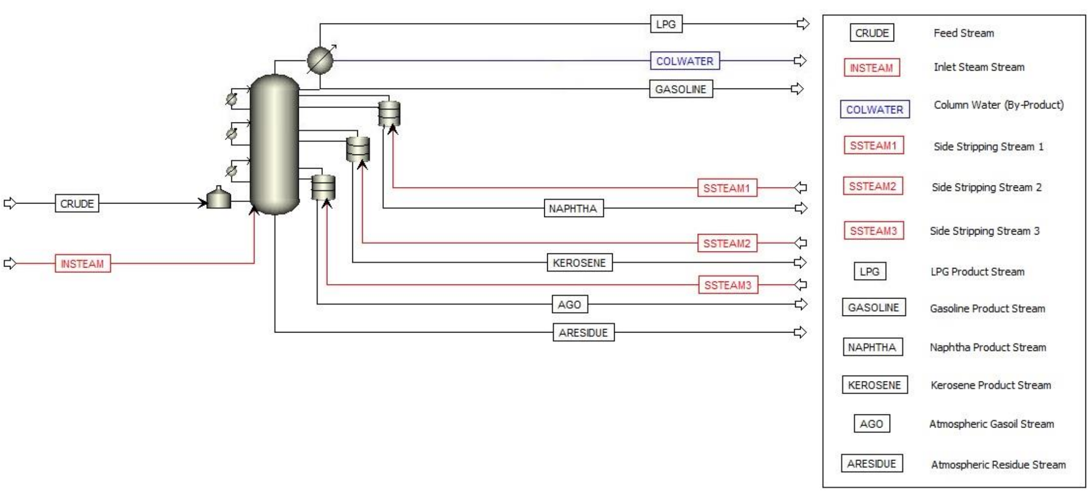


Figure 3.1: Atmospheric Distiller PFD

After pre-heating, crude enters the ADU. The journey in the unit starts at furnace. Then, the hot crude flows to column tower and for heat balancing, pressure and temperature regulation to occur in the distillation tower, processed crude flows through pumparounds across side-strippers fractioning desired products at their specified stages (Gary et al., 2001). Tray or stage numbering starts from topmost tray and ends at bottom tray in increasing number order. The PFD diagram above shows usage of 3 pumparounds and side-strippers since there was only 3 side products formed, in presence of more side products, equal number of pumparounds and side-strippers would be suggested in the flowsheet drawing.

In order to conduct simulation of the atmospheric distillation, firstly, a suitable distillation column block from Aspen Plus was chosen based on the assigned type of data with appropriate assumptions.

Assumptions made in the simulation of the crude atmospheric distillation process model:

1. No accumulation of mass in the distiller tower.
2. Heat loss and recycle streams effects are negligible.
3. Unit model is portraying maximum efficiency of distillation process.
4. No unreacted feed present in tower model.
5. Heat capacity of all streams and column content are constant.

The process model was then developed. The correlation between the parameters and desired product yield was studied and compared with a previous case studies mentioned in Table 2.1. Then, factors affecting LPG yield pattern were identified and recorded. The simulated distillation model was saved for further use. Design Expert 6.06 software was used to design a simulation layout:

Table 3.1: Design Expert Simulation Analysis Table

| **Std** | **Run** | **Block** | **Factor 1: Furnace Temperature (K)** | **Factor 2: Number of Stages** | **Factor 3: Steam to Feed Flowrate Ratio (%)** | **Response: LPG Yield (%)** |
|---|---|---|---|---|---|---|
| 14 | 1 | Block 1 | 630.50 | 35.00 | 3.27 | |
| 5 | 2 | Block 1 | 603.00 | 25.00 | 2.50 | |
| 3 | 3 | Block 1 | 603.00 | 45.00 | 0.25 | |
| 2 | 4 | Block 1 | 658.00 | 25.00 | 0.25 | |
| 16 | 5 | Block 1 | 630.50 | 35.00 | 1.38 | |
| 17 | 6 | Block 1 | 630.50 | 35.00 | 1.38 | |
| 20 | 7 | Block 1 | 630.50 | 35.00 | 1.38 | |
| 7 | 8 | Block 1 | 603.00 | 45.00 | 2.50 | |
| 11 | 9 | Block 1 | 630.50 | 27.00 | 1.38 | |
| 6 | 10 | Block 1 | 658.00 | 25.00 | 2.50 | |
| 15 | 11 | Block 1 | 630.50 | 35.00 | 1.38 | |
| 18 | 12 | Block 1 | 630.50 | 35.00 | 1.38 | |
| 9 | 13 | Block 1 | 584.25 | 35.00 | 1.38 | |
| 19 | 14 | Block 1 | 630.50 | 35.00 | 1.38 | |
| 10 | 15 | Block 1 | 676.75 | 35.00 | 1.38 | |
| 13 | 16 | Block 1 | 630.50 | 35.00 | 0.52 | |
| 12 | 17 | Block 1 | 630.50 | 44.00 | 1.38 | |
| 4 | 18 | Block 1 | 658.00 | 45.00 | 0.25 | |
| 8 | 19 | Block 1 | 658.00 | 45.00 | 2.50 | |
| 1 | 20 | Block 1 | 603.00 | 25.00 | 0.25 | |

The layout consists of a few columns, the most left representing the factors or controllable variables that shall be input into the Aspen simulation model. The other column in the most right shall be the factor or yield computed by the model. The model generates the results and the results are transferred into the response columns to enable optimization of the process parameters using RSM.

This study on factors affecting yield is a sensitivity analysis made at a range of minimum to maximum value of factors. Lastly, using the optimization facility in the software, optimization of atmospheric distillation process is done by maximizing the yield of LPG and identify the optimized factors contributing to it. In order to validate the resulting Aspen Plus simulation model, experimental data from journal studied earlier was compared to the simulation data. Further process model sensitivity analysis in Design Expert software was conducted only after the validation of the data (Anitha et al., 2011). A general flow of the methodology is shown in Figure 3.1.

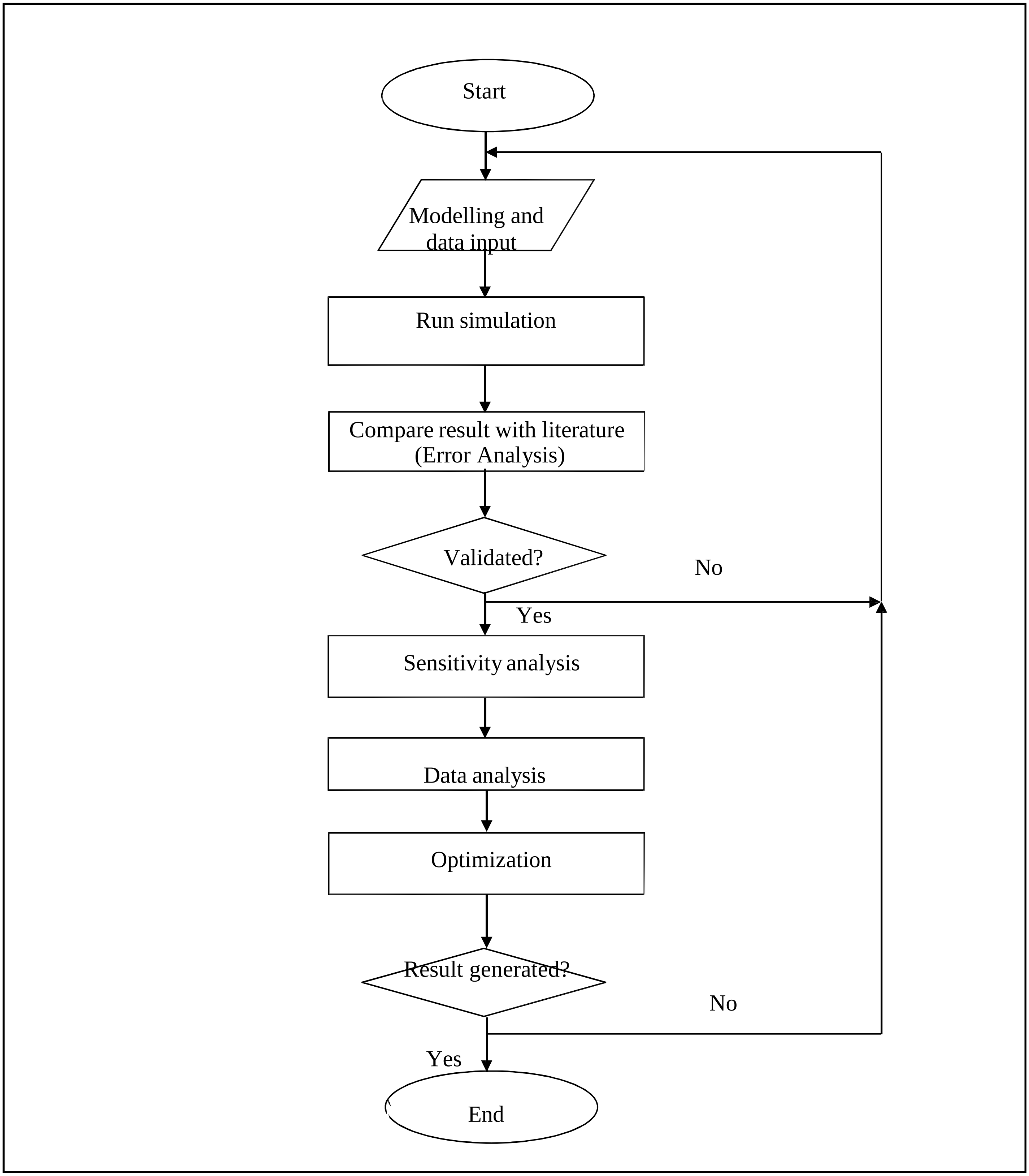

Figure 3.2: Methodology Flowchart

## 3.2 Crude Assay and Default Values

Crude assay analysis is important before distillation process can begin because it contains the characteristics of the crude oil such as API gravity, viscosity, percentage of cut at different boiling points when it is exposed to heat under different operating conditions. It is a type of property model which is crucial to be defined in order to run the properties of Aspen Plus simulation. The analysis can estimate the amount and types of products that will come out from the distiller. The simulation was conducted starting from the following crude petroleum analysis (Speight, 2015) :

Table 3.2: Crude Assay 53016 (McKinney et al.,1959)

**CRUDE PETROLEUM ANALYSIS**

Bureau of Mines Bartlesville Laboratory
Sample 53016

**IDENTIFICATION**

Hastings Field

Texas
Brazoria County

**GENERAL CHARACTERISTICS**

Gravity, specific, 0.867 Gravity, ° API, 31.7 Pour point, ° F., below 5
Sulfur, percent, 0.15 Color, brownish green
Viscosity, Saybolt Universal at 100° Nitrogen, percent,

**DISTILLATION, BUREAU OF MINES ROUTINE METHOD**

STAGE 1—Distillation at atmospheric pressure, 751 mm. Hg
First drop, 84 ° F.

| Fraction No. | Cut temp. ° F. | Percent | Sum, percent | Sp. gr., 60/60° F. | ° API, 60° F. | C. I. | Refractive index, $n_D$ at 20° C. | Specific dispersion | S. U. visc., 100° F. | Cloud test, ° F. |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 122 | 0.8 | 0.8 | 0.673 | 78.8 | | | | | |
| 2 | 167 | 1.0 | 1.8 | .685 | 75.1 | 15 | | | | |
| 3 | 212 | 3.0 | 4.8 | .725 | 63.7 | 24 | 1.39574 | 127.7 | | |
| 4 | 257 | 3.4 | 8.2 | .755 | 55.9 | 29 | 1.41756 | 128.6 | | |
| 5 | 302 | 3.1 | 11.3 | .777 | 50.6 | 32 | 1.42985 | 135.4 | | |
| 6 | 347 | 3.9 | 15.2 | .798 | 45.8 | 35 | 1.44192 | 137.8 | | |
| 7 | 392 | 4.9 | 20.1 | .817 | 41.7 | 38 | 1.45217 | 139.9 | | |
| 8 | 437 | 6.8 | 26.9 | .833 | 38.4 | 40 | 1.46057 | 140.3 | | |
| 9 | 482 | 8.0 | 34.9 | .848 | 35.4 | 41 | 1.46875 | 148.0 | | |
| 10 | 527 | 10.9 | 45.8 | .864 | 32.3 | 44 | 1.47679 | 149.8 | | |
| STAGE 2—Distillation continued at 40 mm. Hg | | | | | | | | | | |
| 11 | 392 | 7.3 | 53.1 | 0.873 | 30.6 | 45 | 1.48274 | 155.2 | 42 | Below 5 |
| 12 | 437 | 7.8 | 60.9 | .879 | 29.5 | 44 | 1.48474 | 156.2 | 50 | do |
| 13 | 482 | 6.2 | 67.1 | .889 | 27.7 | 45 | 1.49058 | 152.7 | 71 | do |
| 14 | 527 | 5.7 | 72.8 | .901 | 25.6 | 48 | | | 125 | 10 |
| 15 | 572 | 6.9 | 79.7 | .916 | 28.0 | 52 | | | 280 | 20 |
| Residuum | | 20.3 | 100.0 | .945 | 18.2 | | | | | |

Carbon residue, Conradson: Residuum, 4.7 percent; crude, 1.0 percent.

From the assay analysis, some of the important information such as the atmospheric distillation pressure of 101325 Pa, API of crude (31.7) and distillation curve type - True Boling Point (Liquid Volume Basis), are necessary in the Aspen program and shall be used to setup the distillation model.

Based on these data, more relevant inputs, necessary for simulation model were also collected from existing literaturacy. PETROFRAC distiller model was chosen during simulated study because the program is embedded in the software to simulate crude refinery. The choice of distiller model helps to increase efficiency of problem solving. The modeling was based on Peng-Robinson (Peng-Rob) method. The base method is suitable for mixtures of real heavier hydrocarbons being processed at low pressure temperature ranging to 703.15 K (Bagajewicz et al., 2001).

Input setup is data such as light end components of crude which were defined based on the journal by Bagajewicz and Ji, 2001. The light crude of assay 53016 is likely to have properties similar to crude from the journal as it had light crude as well. Thus, crude hydrocarbon components were adapted from that journal. The input setup for the PETROFRAC distiller block in ASPEN simulation are adapted from references (literature of case study) stated in Table 2.1. As prime default, operating data of distillation unit and stream conditions of journals More et al., 2010 and Sotelo et al., 2017 were used. The parameters were changed relevantly for each journal case of Table 2.1 before simulation was done. The parameters from the two journals mentioned earlier were used as prime default values because, those were the journals providing all necessary values to run simulation. The table below shows light end components and their relevant percentages in crude.

Table 3.3: Light End Percentage in Crude

| Compound | Volume Percent in Crude (%) (Bagajewicz and Ji, 2001) | Volume Percent in LPG (%) (Chang et al., 2001) |
|---|---|---|
| Ethane | 0.13 | 1.00 |
| Propane | 0.78 | 82.8 |
| Isobutane | 0.49 | 4.70 |
| n-butane | 1.36 | 11.30 |
| Isopentane | 1.05 | - |
| n-pentane | 1.30 | - |

Input setup includes information for equipment parameters and value details of streams involved in a process simulation as well. Based on the atmospheric distiller PFD, the column setup can be defined according to few segments: furnace, atmospheric distillation column and few more. The sub-chapters below show definitions of different segments of atmospheric distillation column configured to generate results from the Aspen Plus simulation.

### 3.2.1 Case 1

Tables 3.4 and 3.5 show operation values of different segments of ADU used in Case 1.

Table 3.4: Case 1 Definitions of Atmospheric Distillation Column

| Segment | | Condition | Operation |
|---|---|---|---|
| Distillation Tower | | Number of stages | 27 (including condenser) |
| | | Bottom flowrate | 260.1879 kg/s |
| | | Feed Stage | 23 |
| | | Top Tray Pressure | 96 kPa |
| | | Valid phases | Vapour-Liquid-FreeWater |
| Condenser | | Type | Partial-Vapor-Liquid |
| | | Temperature | 343.15 K |
| | | Duty | 43.4 MW |
| Furnace | | Type | Single stage flash |
| | | Pressure | 160 kPa |
| | | Temperature | 616.48 K |
| Pumparound | 1 | Drawoff type | Partial |
| | | Flowrate | 0.1 $kg/s$ |
| | | Temperature | 323.15 K |
| | | Duty | 22.3 MW |
| | | Draw stage | 5 |
| | | Return stage | 3 |
| | 2 | Drawoff type | Partial |
| | | Flowrate | 0.4 $kg/s$ |
| | | Temperature | 398.15 K |
| | | Duty | 33.7 MW |
| | | Draw stage | 10 |
| | | Return stage | 7 |
| | 3 | Drawoff type | Partial |
| | | Flowrate | 0.3 $kg/s$ |
| | | Temperature | 493.15 K |
| | | Duty | 8.8 MW |
| | | Draw stage | 17 |
| | | Return stage | 13 |
| Stripper | 1 | Number of stages | 4 |
| | | Stripper product | Naphtha |
| | | Liquid draw | 3 |
| | | Overhead return | 5 |
| | | Stripping steam | Side stripping steam 1 |
| | | Main column draw flowrate | 5 $kg/s$ |
| | 2 | Number of stages | 4 |
| | | Stripper product | Kerosene |