CERTIFICATION OF APPROVAL

Mathematical Modelling and Simulation of Petrochemical Processes

by

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Approved by,

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CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

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ABSTRACT

The main objectives of this project is to set up the process model for Propane, C_3H_8 (Distillate) and Butane, C_4H_{10} (Bottom) distillation column, to build up MATLAB Simulink program for simulations of mentioned process and to analyze the process with parameters change. From this project, student will also be able to learn about the current crude oil distillation processes and the related factors that could improve the efficiency of the output products which are the Top product and Bottom product. Refineries are among the largest energy consumers in the chemical industries. It was evaluated that the energy requirement for the crude oil distillation plant is an amount of fuel equivalent to the 2% of the total crude processed. For this reason there is a great interest to identify ways to improve the energy efficiency of the existing plants.

The scope of study is to use the MATLAB software to simulate the petroleum distillation process base from the developed mathematical modeling done by fellow researcher. Then, analysis will be conducted base from the simulation. Modifications on the parameters of the simulation program could be done to improve the efficiency of the output products.

The methodology of the project would first start with the research study on current crude oil distillation processes and the mathematical modeling constructed. After that, use the developed mathematical modeling to simulate the processes using MATLAB software. Finally, analyze and modify the model to increase the efficiency of the output products.

There are several findings up until this report was produced. One of it is related with the design of the distillation column that could influence the percentage of the output products. As the number of tray increases, the purity of the Top product will also increases. But, there will be issues with the energy consume and economic cost. Besides, changes in parameters give different effects on the output products. Thus proper considerations need to be done for each situation.

ACKNOWLEDGEMENT

Towards the completion of my Final Year Project (FYP), I would like to express my greatest gratitude towards my FYP Supervisor, Dr. Vu Trieu Minh. Throughout the FYP, Dr. Vu provided lots of feedback that are related to the project as well as sharing his valuable experience on the subject. He also taught the aspects and methods required so that by the end of the course, the desired objectives could be achieved. Besides, Dr. Vu always encouraged me to do my best and stay on the correct path throughout the project.

Special thank you and appreciation are dedicated to all staff of Mechanical Engineering Department, my family, Mr Khoo Boo Kean and colleagues for their continued support, guidance and contribution to the success of the project whether direct or indirectly. It would be impossible to complete this Final Year Project without their help. I hope those personnel from Universiti Teknologi PETRONAS will continuously help and cater the needs of students in the future.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

CHAPTER 1

INTRODUCTION

1.1 Background Study

Distillation is a method of separating mixtures based on differences in their volatilities in a boiling liquid mixture. Usually it is done by applying heat to the mixtures until it reach a certain temperature or boiling point of the desired elements. Distillation is a unit operation, or a physical separation process, and not a chemical reaction. An example of distillation column with the output components can be seen in Figure 1 below.

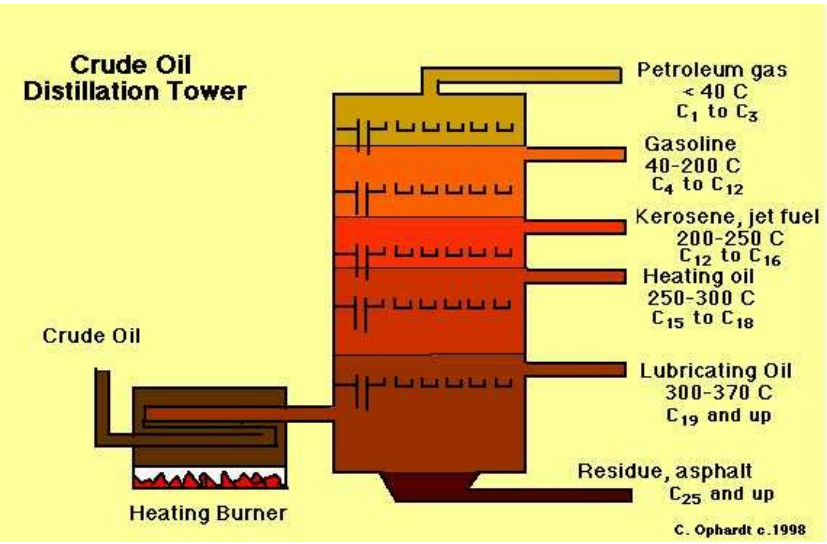

Figure 1: Distillation Column for Crude Oil

There are several types of distillation column designed to perform specific types of separations and each design different in terms of complexity. 2 major types of columns are Batch column and Continuous columns. In Batch column, the feed to the column is introduced batch-wise. The column is charges with a "batch" and then the distillation process is carried out. When the desired task is achieved a next batch of feed is introduced. While for Continuous column, it processes a continuous feed stream. No interruption occurs unless there is a problem with the column or surrounding process units. They are capable of handling high throughputs and are the more common of the two types. There are several types of continuous columns such as Binary column where

the feed contains only two components; Multi Product Column-feed that contains more than two components; and Multi Product Column-column which has more than two product streams (*Perry, E. S., and Weissberger, A., ed. (1965). Distillation, 2th ed. New York: Interscience Publishers, Inc*).

1.2 Problem Statement

Refineries are among the largest energy consumers in the chemical industries. It was evaluated that the energy requirement for these plants is an amount of fuel equivalent to the 2% of the total crude processed (*M. Bagajewicz, S. Ji, Rigorous, Part I: Targeting, Ind. Eng. Chem. Res. 40 (2001) 617–626*). For this reason there is a great interest to identify ways to improve the energy efficiency of the existing plants.

There are large numbers of alternative control models, thus the design for the control system of the distillation process shall satisfy all operational objectives in the presence of ever-changing external disturbances.

Parameters change in the distillation column system give different effects on the output product. Thus, proper manipulation of parameters must be determined to enhance the quality of the output products.

1.3 Objective And Scope Of Study

The objectives of this project are:

- To set up the process model for Propane, C_3H_8 (Distillate) and Butane, C_4H_{10} (Bottom) distillation column
- To build up MATLAB Simulink program for simulations of mentioned process
- To analyze the process with parameters change

The scope of study is to use the MATLAB software to simulate the petroleum distillation process base from the developed mathematical modeling done by fellow researcher. Then, analysis on the output products will be conducted base from the

simulation. Modification on the parameters involved in the system will be done to improve the efficiency of the output products.

This project is relevance with courses taken by student in previous semesters, for example the usage of MATLAB software which was learnt during Mechatronics course, transfer of heat during Heat Transfer course and matters related with design during Mechanical Engineering Design course. Besides, student is taking specialization in Petroleum Engineering, thus this project could improve student's understanding and become familiarize with petroleum industry.

This project is already completed by other researcher and been documented, thus there is high expectation that student could achieved the desired objective as mentioned above within the time frame which is totally about 32 weeks.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

The most common and famous method use to refine the crude oil is by using the distillation process. In this method, the crude oil is heated, pumped into a fractionating column and then separated into the major fractions such as Butane, Naphtha, Kerosene and residuum base from the boiling point of each component. The fractions of crude oil at respective temperatures, products recovered and usage of products in further processes can be seen in Figure 2 below.

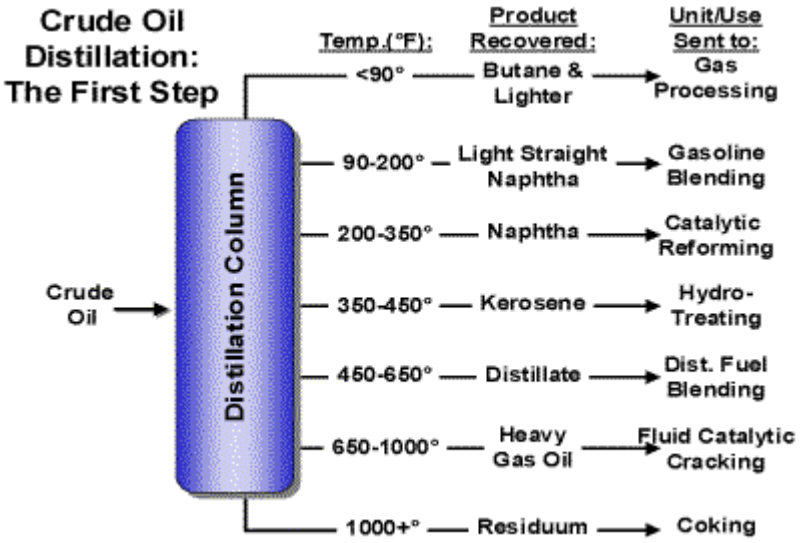

Figure 2: Output products from the crude oil distillation process

2.2 Distillation Principle

First of all, the feedstock is introduced usually somewhere near the middle of the column to a tray known as the feed tray. The feed tray divides the column into a top (enriching or rectification) section and a bottom (stripping) section. The feed flows down the column where it is collected at the bottom in the reboiler.

Heat is supplied to the reboiler to generate vapour. The source of heat input can be any suitable fluid, although in most chemical plants this is normally steam. In refineries, the

heating source may be the output streams of other columns. The vapour raised in the reboiler is re-introduced into the unit at the bottom of the column. The liquid removed from the reboiler is known as the bottoms product or simply, bottoms. The vapour moves up the column, and as it exits the top of the unit, it is cooled by a condenser. The condensed liquid is stored in a holding vessel known as the reflux drum. Some of this liquid is recycled back to the top of the column and this is called the reflux. The condensed liquid that is removed from the system is known as the distillate or top product (*James G Speight and Baki Ozum, "Petroleum Refining Process", 2002, Marcel Dekker, Inc*).

Thus, there are internal flows of vapour and liquid within the column as well as external flows of feeds and product.

2.3 Types Of Distillation

(Types of Distillation are taken from *Perry, E. S., and Weissberger, A., ed. (1965). Distillation, 2th ed. New York: Interscience Publishers, Inc*)

2.3.1 Azeotropic distillation

Azeotropic distillation usually refers to the specific technique of adding another component to generate a new, lower-boiling azeotrope that is heterogeneous (e.g. producing two, immiscible liquid phases). A common distillation with an azeotrope is the distillation of ethanol and water.

2.3.2 Extractive distillation

Extractive distillation is defined as distillation in the presence of a miscible, high boiling, relatively non-volatile component, the solvent, that forms no azeotrope with the other components in the mixture. The method is used for mixtures having a low value of relative volatility, nearing unity. Such mixtures cannot be separated by simple distillation, because the volatility of the two components in the mixture is nearly the same, causing them to evapourate at nearly the same temperature at a similar rate, making normal distillation impractical.

The method of extractive distillation uses a separation solvent, which is generally nonvolatile, has a high boiling point and is miscible with the mixture, but doesn't form an azeotropic mixture. The solvent interacts differently with the components of the mixture thereby causing their relative volatilities to change. This enables the new three-part mixture to be separated by normal distillation.

The original component with the greatest volatility separates out as the top product. The bottom product consists of a mixture of the solvent and the other component, which can again be separated easily because the solvent doesn't form an azeotrope with it. The bottom product can be separated by any of the methods available. It is important to select a suitable separation solvent for this type of distillation.

The solvent must alter the relative volatility by a wide enough margin for a successful result. The quantity, cost and availability of the solvent should be considered. The solvent should be easily separable from the bottom product, and should not react chemically with the components or the mixture, or cause corrosion in the equipment. A classic example to be cited here is the separation of an azeotropic mixture of benzene and cyclohexane, where aniline is one suitable solvent.

2.3.3 Fractional distillation

Fractional distillation is the separation of a mixture into its component parts, or fractions, such as in separating chemical compounds by their boiling point by heating them to a temperature at which several fractions of the compound will evapourate. It is a special type of distillation. Generally the component parts boil at less than 25 °C from each other under a pressure of one atmosphere (atm). If the difference in boiling points is greater than 25 °C, a simple distillation is used.

2.3.4 Steam distillation

Steam distillation is a special type of distillation (a separation process) for temperature sensitive materials like natural aromatic compounds. Many organic compounds tend to

decompose at high sustained temperatures. Separation by normal distillation would then not be an option, so water or steam is introduced into the distillation apparatus. By adding water or steam, the boiling points of the compounds are depressed, allowing them to evapourate at lower temperatures, preferably below the temperatures at which the deterioration of the material becomes appreciable. If the substances to be distilled are very sensitive to heat, steam distillation can also be combined with vacuum distillation. After distillation the vapours are condensed as usual, usually yielding a two-phase system of water and the organic compounds, allowing for simple separation.

2.3.5 Vacuum distillation

Vacuum distillation is a method of distillation whereby the pressure above the liquid mixture to be distilled is reduced to less than its vapour pressure (usually less than atmospheric pressure) causing evapouration of the most volatile liquid(s) (those with the lowest boiling points). This distillation method works on the principle that boiling occurs when the vapour pressure of a liquid exceeds the ambient pressure. Vacuum distillation is used with or without heating the solution.

2.4 Distillation Basic Component

*(*Distillation Basic Components is taken from *Nelson, W. L., 1982. Petroleum Refinery Engineering. Auckland: McGraw-Hill International Book Company)*

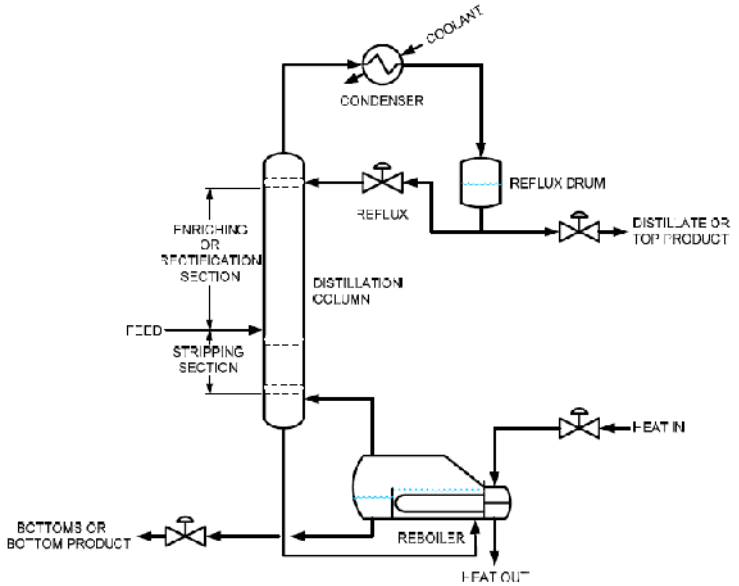

Figure 3: Basic components of a distillation

2.4.1 Feed stream (Distillation Column)

Usually in liquid form, consisting of a mixture of components to be separated, is fed into a vessel. This vessel is usually a tall cylinder in shape, standing vertically and is commonly referred to a "distillation column". Inside the vessel are structures designed for radial mixing (i.e. mixing at any given vertical level); but, not axial mixing (i.e. mixing along the length of the vessel) and the contact area between a stream of vapour are flowing up and a stream of liquid are flowing down. The purpose of all these different types of column internal structures is the same, to facilitate vapour/liquid contacting and mass transfer.

2.4.2 Enriching Section/Rectification Section. (Distillation Column)

The part is located inside the distillation column and above the feed point

2.4.3 Stripping Section. (Distillation column)

This part of the distillation column is below the feed point. Liquid trickles down the column, exits the bottom of the Stripping Section, and flows into the reboiler.

2.4.4 Reboilers

Reboiler is a special type of heat exchanger that uses steam or some other heat transfer fluid to heat the liquid in the reboilers to its boiling point. The vapour generated by this boiling liquid exits the reboilers and is fed back into the Stripping Section of the column.

2.4.5 Bottoms/Bottom Product

Excess liquid in the reboilers overflows and exits here. The vapour from the reboilers flows up the column, counter-current to the liquid flowing down the column. The components in the feed stream are separated according to their relative boiling points. Components with a lower boiling point tend to become enriched in the vapour traveling up the column. Components with a higher boiling point tend to become enriched in the liquid traveling down the column.

2.4.6 Enriching/Rectification Section. (Distillation column – Final column)

Eventually, the vapour enriched in low boiling components exits on the Rectification Section on the top of the distillation column or final stage of the column.

2.4.7 Condenser.

The condenser will then condense the vapour back to a liquid by cooling it in a heat exchanger.

2.4.8 Reflux drum

This area is where the condensed liquid is collected from the condenser. A portion of the condensed liquid is fed back into the Rectification Section to become the liquid flowing down the column as described previously.

2.4.9 Top Product/Distillate

This is the rest of the liquid that being collected in the Reflux Drum.

2.5 Mathematical

The mathematical model is established on dynamic continuity equations of mass and energy for each unit operation where mass and energy can accumulate. In general, the dynamic continuity equations state that the rate of accumulation of material (mass or energy) in a system is equal to the amount entered and generated, less the amount leaving and consumed within the system:

$$\begin{bmatrix} rate\ of\ accumulation \\ of\ mass\ (energy) \end{bmatrix} = \begin{bmatrix} mass\ (energy)\ flow \\ \text{int}o\ the\ system \end{bmatrix} - \begin{bmatrix} mass\ (energy)\ flow \\ out\ of\ the\ system \end{bmatrix} + \begin{bmatrix} mass\ (energy)\ flow \\ generated\ within\ the\ system \end{bmatrix} - \begin{bmatrix} mass\ (energy)\ flow \\ consumed\ within\ the\ system \end{bmatrix}$$

The accumulation term is a first order time derivatives of the total mass or energy. The flow terms are algebraic. The result is a first order ordinary differential equation that is usually non-linear. The liquid rate throughout the column will not be the same dynamically. They will depend on the fluid mechanics of the tray. Often a simple Francis Weir formula relationship is used to relate the liquid holdup on a tray to the liquid flow rate L_n over the outlet weir:

$$M_n = f(L_n)$$

The fundamental quantities are total mass and mass of the light component (the more volatile component).

2.5.1 Equations for Flows throughout General Trays

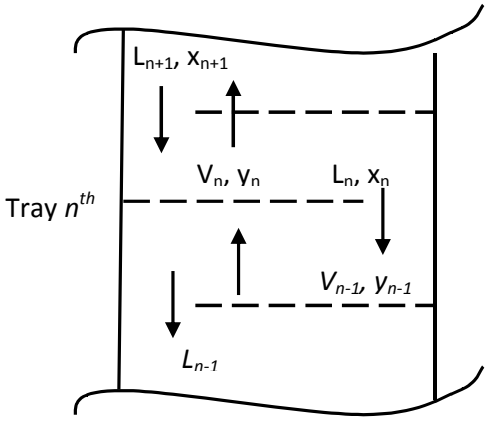

Figure 4: A General n^{th} Tray

	Phase	Flow rate	Concentration
INLET	Liquid	L_{n+1}	x_{n+1}
	Vapour	V_{n-1}	y_{n-1}
OUTLET	Vapour	V_n	y_n
	Liquid	L_n	x_n

Table 1: General notifications of flow rate and concentration

The total mole holdup in the n^{th} tray M_n is considered constant, but the imbalance in the input and output flows is accounted for in the component and heat balance equations (*see Figure 4*).

Total mass balance:

$$\frac{d(M_n)}{dt} = L_{n+1} - L_n + V_{n-1} - V_n \tag{1}$$

Component balance:

$$\frac{d(M_n x_n)}{dt} = L_{n+1}x_{n+1} - L_n x_n + V_{n-1}y_{n-1} - V_n y_n \tag{2}$$

By differentiating (2) and substituting for (1), we obtain:

$$\frac{d(x_n)}{dt} = \frac{L_{n+1}x_{n+1} + V_{n-1}y_{n-1} - (L_{n+1} + V_{n-1})x_n - V_n(y_n - x_n)}{M_n} \tag{3}$$

Energy balance:

$$\frac{d(M_n h_n)}{dt} = h_{n+1}L_{n+1} - h_n L_n + H_{n-1}V_{n-1} - H_n V_n \tag{4}$$

or

$$M_n \frac{dh_n}{dt} + h_n \frac{dM_n}{dt} = h_{n+1}L_{n+1} + H_{n-1}V_{n-1} - h_nL_n - H_nV_n \tag{5}$$

Because the term $\frac{dh_n}{dt}$ is approximately zero, substituting for the change of hold up $\frac{dM_n}{dt}$ in (5), and rearranging terms, we obtain:

$$V_n = \frac{h_{n+1}L_{n+1} + H_{n-1}V_{n-1} - (L_{n+1} + V_{n-1})h_n}{H_n - h_n} \tag{6}$$

where: n = tray nth

V = vapour flow

L = liquid flow

x = liquid concentration of light component

y = vapour concentration of light component

h = enthalpy for liquid

H = enthalpy for vapour

2.5.2 Equations for the Feed Tray (stage n = *f*) (*See Figure 5)*

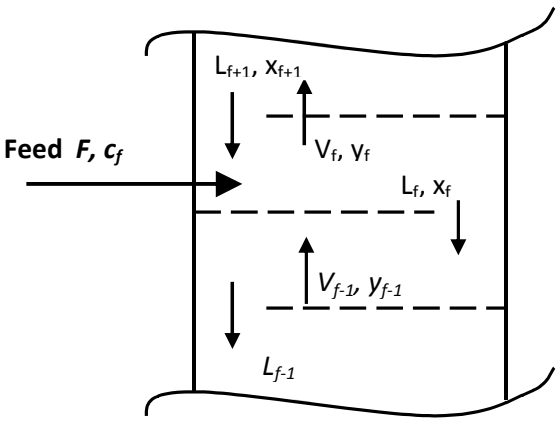

Figure 5: Feed Section

Total mass balance:

$$\frac{d(M_f)}{dt} = F + L_{f+1} + V_{f-1} - L_f - V_f \tag{7}$$

Component balance:

$$\frac{d(M_f x_f)}{dt} = Fc_f + L_{f+1}x_{f+1} + V_{f-1}y_{f-1} - L_f x_f - V_f y_f \tag{8}$$

$$\Rightarrow \frac{dx_n}{dt} = \frac{L_{n+1}x_{n+1} + V_{n-1}y_{n-1} - (L_{n+1} + V_{n-1})x_n - V_n(y_n - x_n)}{M_n} \tag{9}$$

Energy balance:

$$\frac{d(M_f h_f)}{dt} = h_f F + h_{n+1}L_{n+1} + H_{n-1}V_{n-1} - h_n L_n - H_n V_n \tag{10}$$

$$\Rightarrow V_n = \frac{h_F F + h_{n+1}L_{n+1} + H_{n-1}V_{n-1} - (L_{n+1} + V_{n-1})h_n}{H_n - h_n} \tag{11}$$

2.5.3 Equations for the Top Section (stage n=*N+1*) (*See Figure 6*)

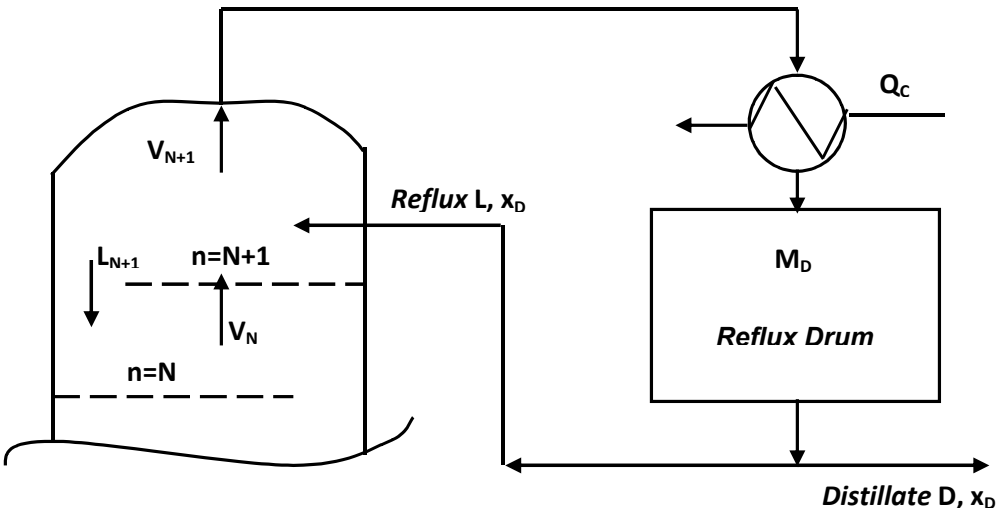

Figure 6: Top Section and Reflux Drum

Equations for the top tray (stage n=N+1)

Total mass balance:

$$\frac{d(M_{N+1})}{dt} = L + V_N - L_{N+1} - V_{N+1} \tag{12}$$

Component balance:

$$\frac{d(M_{N+1}x_{N+1})}{dt} = Lx_D + V_N y_N - L_{N+1}x_{N+1} - V_{N+1}y_{N+1} \tag{13}$$

Energy balance:

$$\frac{d(M_{N+1}h_{N+1})}{dt} = h_D L + H_N V_N - h_{N+1}L_{N+1} - H_{N+1}V_{N+1} \tag{14}$$

$$\Rightarrow V_{N+1} = \frac{h_D L + H_N V_N - (L+V_N)h_{N+1}}{H_{N+1} - h_{N+1}} \tag{15}$$

Equations for Reflux drum and condenser

Total mass balance:

$$\frac{d(M_D)}{dt} = V_{N+1} - L - D \tag{16}$$

Component balance:

$$\frac{d(M_D x_D)}{dt} = V_{N+1}y_{N+1} - (L+D)x_D \tag{17}$$

Energy balance around condenser:

The condenser duty, Q_C is equal to the latent heat required to condense the overhead vapour to bubble point:

$$Q_C = H_{in}V_{in} - h_{out}L_{out} = V_N(H_N - h_N) \tag{18}$$

2.5.4 Equations for the Bottom Section (stage n=2) (*See Figure 3.4*)

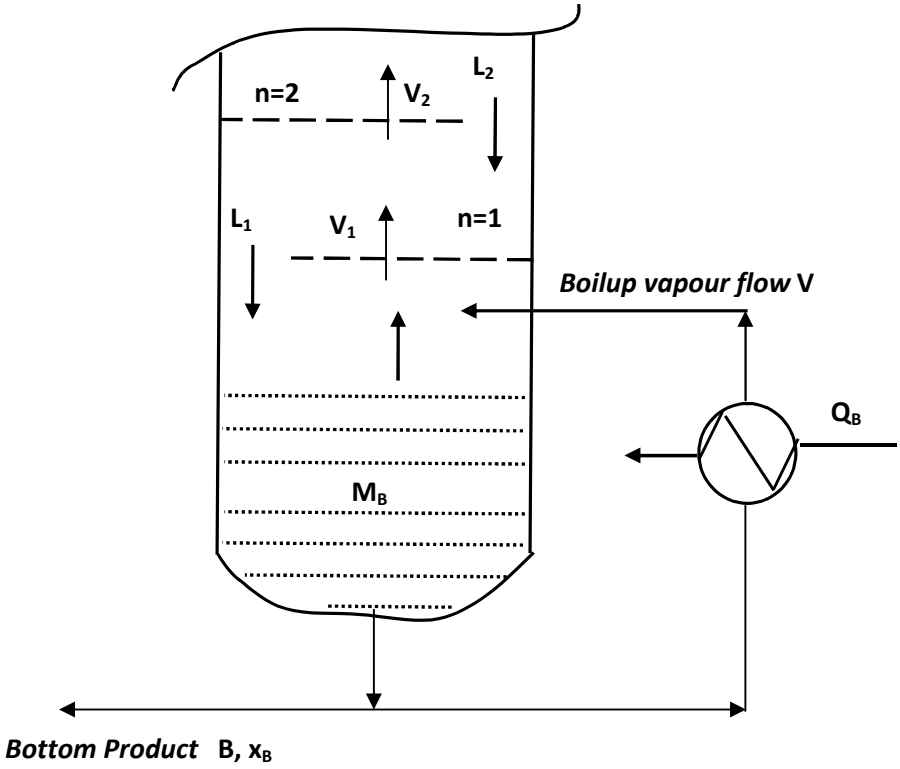

Figure 7: Bottom Section and Reboiler

Bottom Tray (stage n=2)

Total mass balance:

$$\frac{d(M_2)}{dt} = L_3 - L_2 + V_B - V_2 \tag{19}$$

Component balance:

$$\frac{d(M_2 x_2)}{dt} = L_3 x_3 - L_2 x_2 + V_B y_B - V_2 y_2 \tag{20}$$

Energy balance:

$$\frac{d(M_B h_B)}{dt} = h_3 L_3 + H_B V_B - h_2 L_2 - H_2 V_2 \tag{21}$$

$$\Rightarrow V_2 = \frac{h_3 L_3 + H_B V_B - (L_3 + V_B) h_2}{H_2 - h_2} \tag{22}$$

Reboiler and Column Bottoms (stage n=1)

The base of the column has some particular characteristics as follows:

- There is reboiler heat flux, Q_B establishing the boilup vapour flow, V_B
- The holdup is variable and changes in sensible heat cannot be neglected
- The outflow of liquid from the bottoms B is determined externally to be controlled by a bottoms level controller.

Total mass balance:

$$\frac{d(M_B)}{dt} = L_2 - V_B - B \tag{23}$$

Component balance:

$$\frac{d(M_B x_B)}{dt} = L_2 x_2 - V_B y_B - B x_B \tag{24}$$

Energy balance:

$$\frac{d(M_B h_B)}{dt} = h_2 L_2 + Q_B - h_B B - H_B V_B \tag{25}$$

$$\Rightarrow V_B = \frac{h_2 L_2 + Q_B - h_B B - M_B \frac{dh_B}{dt} - h_B \frac{dM_B}{dt}}{H_B} \tag{26}$$

All the equations above are state equations and describe the dynamic behavior of the distillation column. The state variables of the model are:

Liquid holdups: $M_1, M_2, \ldots\ldots, M_{N+2}$; $(M_1 = M_{Bottom}, M_{N+2} = M_{Reflux\ Drum})$

Liquid concentration: $x_1, x_2, \ldots\ldots, x_N, x_{N+1}$; $(x_1 = x_B, x_{N+1} = x_D)$

When all the modeling equations above are resolved, we find out how the flow rate and concentrations of the two product streams (distillate product and bottoms product) change with time, in the presence of changes in the various input variables.

2.5.5 Simplified Model

To simplify the model, we make the following assumption (*Dr. Vu Trieu Minh and Dr. Ahmad Majdi Abdul Rani (2009), Modeling and Control of Distillation Column in a Petroleum Process, Mathematical Problems in Engineering Volume 2009, Article ID 404702*):

- The relative volatility α is constant throughout the column. This means the vapour-liquid equilibrium relationship can be expressed by

$$y_n = \frac{\alpha x_n}{1+(\alpha-1)x_n} \tag{27}$$

where x_n: liquid composition on n^{th} stage (mole fraction of light component)
y_n: vapour composition on n^{th} stage (mole fraction of light component)
α: relative volatility

- The overhead vapour is totally condensed in a condenser
- The liquid holdups on each tray, condenser, and the reboiler are constant and perfectly mixed (i.e. immediate liquid response, ($dL_2 = dL_3 = ... = dL_{N+2} = dL$)
- The holdup of vapour is negligible throughout the system (i.e. immediate vapour response, $dV_1 = dV_2 = ... = dV_{N+1} = dV$).
- The molar flow rates of the vapour and liquid through the stripping and rectifying sections are constant:

$$V_1 = V_2 = ... = V_{N+1} \quad \text{and}$$
$$L_2 = L_3 = ... = L_{N+2}$$

- The column is numbered from bottom (n=1 for the reboiler, n=2 for the first tray, n=*f* for the feed tray, n=N+1 for the top tray and n=N+2 for the condenser).

Under these assumptions, the dynamic model can be expressed by the following equations:

Condenser (n=N+2):

$$M_D \dot{x}_n = (V + V_F) y_{n-1} - L x_n - D x_n \tag{28}$$

Tray n (n=f+2, …, N+1):

$$M\dot{x}_n = (V + V_F)(y_{n-1} - y_n) + L(x_{n+1} - x_n) \tag{29}$$

Tray above the feed flow (*n=f+1*):

$$M\dot{x}_n = V(y_{n-1} - y_n) + L(x_{n+1} - x_n) + V_F(y_F - y_n) \tag{30}$$

Tray below the feed flow (*n=f*):

$$M\dot{x}_n = V(y_{n-1} - y_n) + L(x_{n+1} - x_n) + L_F(x_F - x_n) \tag{31}$$

Tray n ($n=2, \ldots, f-1$):

$$M\dot{x}_n = V(y_{n-1} - y_n) + (L + L_F)(x_{n+1} - x_n) \tag{32}$$

Reboiler ($n=1$):

$$M_B\dot{x}_1 = (L + L_F)x_2 - Vy_1 - Bx_1 \tag{33}$$

Flow rate are assumed as constant molar flows as

$$L_F = q_F F \tag{34}$$

$$V_F = F - L_F \tag{35}$$

Assuming condenser holdup constant

$$D = V_N - L = V + V_F - L \tag{36}$$

Assuming boiler holdup constant

$$B = L_2 - V_1 = L + L_F - V \tag{37}$$

Composition x_F in the liquid and y_F in the vapour phase of the feed are obtained by solving the flash equations:

$$Fc_F = L_F x_F + V_F y_F \tag{38}$$

and

$$y_F = \frac{\alpha x_F}{1 + (\alpha - 1)x_F} \tag{39}$$

α is the relative volatility.

Although the model order is reduced, the representation of the distillation system is still *nonlinear* due to the vapour-liquid equilibrium relationship in equation (3.27) between y_n and x_n.

2.6 Model Simulation and Analysis

2.6.1 Model Dynamic Equations

It has been calculated for the distillation column with 14 trays with the following initial data (*Surinder Parkash, "Refining Processes Handbook", 2003. Gulf Professional Publishing*):

The feed mass rate of the plant: $F_{mass} = 15.47619 \ \ (tons / hour)$

The holdup in the column base: $M_B = 31.11 \ \ (kmole)$

The holdup on each tray: $M = 5.80 \ \ (kmole)$

The holdup in the reflux drum: $M_D = 13.07 \ \ (kmole)$

The gas percentage in the feed flow: $c_F = 38\%$

The internal vapour flow V_f selected by empirical: $V_f = 28\%$

The feed stream (m^3/h) with the density $d_F = 0.670$ (ton/m^3):

$$F = \frac{F_{mass}}{d_F} = \frac{15.47619}{0.670} = 23.0988 \quad (m^3 / h)$$

The calculated stream data summary is displayed in the table 4.1 below:

Stream	Formula	%	Volume flow (m^3/h)	Density (ton/m^3)	Mass flow (ton/h)	Molar weight $(kg/kmol)$	Molar flow $kmole/h$
Vapour rate in feed V_F	c_F+4	42	9.7015	0.591	5.7336	58.2	98.5152
Liquid rate in feed L_F	$100-V_F$	58	13.3973	0.726	9.7264	93.3	104.2491
Internal vapour rate V	V_f	28	6.4677	0.598	3.8677	58.3	66.3407
Internal liquid rate L	V_f+4	32	7.3916	0.615	4.5458	60.1	75.6380
Distillate flow rate D	c_F	38	8.7775	0.576	5.0554	54.5	92.7597
Bottoms flow rate B	$100-c_F$	62	14.3213	0.727	10.405	93.8	110.9235

Table 2: Stream Data Summary

Solving flash equation with the relative volatility ($\alpha = 5.68$) using MATLAB, we get:

$$\Rightarrow x_F = 0.26095; \quad y_F = 0.66728$$

Reference to equations from (28) to (39) we can develop a set of nonlinear differential and algebraic equations for the simplified model as:

$$13.07\dot{x}_{16} = 164.8559y_{15} - 75.6380x_{16} - 92.7597x_{16}$$
$$\Rightarrow \dot{x}_{16} = 12.6133y_{15} - 12.8863x_{16} \tag{40}$$

$$5.8\dot{x}_{15} = 164.8559(y_{14} - y_{15}) + 75.6380(x_{16} - x_{15})$$
$$\Rightarrow \dot{x}_{15} = 28.4234y_{14} - 28.4234y_{15} + 13.0410x_{16} - 13.0410x_{15} \tag{41}$$

$$5.8\dot{x}_{14} = 164.8559(y_{13} - y_{14}) + 75.6380(x_{15} - x_{14}) \tag{42}$$

$$\Rightarrow \dot{x}_{14} = 28.4234y_{13} - 28.4234y_{14} + 13.0410x_{15} - 13.0410x_{14}$$

$$5.8\dot{x}_{13} = 164.8559(y_{12} - y_{13}) + 75.6380(x_{14} - x_{13}) \tag{43}$$

$$\Rightarrow \dot{x}_{13} = 28.4234y_{12} - 28.4234y_{13} + 13.0410x_{14} - 13.0410x_{13}$$

$$5.8\dot{x}_{12} = 164.8559(y_{11} - y_{12}) + 75.6380(x_{13} - x_{12}) \tag{44}$$

$$\Rightarrow \dot{x}_{12} = 28.4234y_{11} - 28.4234y_{12} + 13.0410x_{13} - 13.0410x_{12}$$

$$5.8\dot{x}_{11} = 164.8559(y_{10} - y_{11}) + 75.6380(x_{12} - x_{11}) \tag{45}$$

$$\Rightarrow \dot{x}_{11} = 28.4234y_{10} - 28.4234y_{11} + 13.0410x_{12} - 13.0410x_{11}$$

$$5.8\dot{x}_{10} = 164.8559(y_{9} - y_{10}) + 75.6380(x_{11} - x_{10}) \tag{46}$$

$$\Rightarrow \dot{x}_{10} = 28.4234y_{9} - 28.4234y_{10} + 13.0410x_{11} - 13.0410x_{10}$$

$$5.8\dot{x}_{9} = 66.3407(y_{8} - y_{9}) + 75.6380(x_{10} - x_{9}) + 98.5152(0.66728 - y_{9}) \tag{47}$$

$$\Rightarrow \dot{x}_{9} = 11.4381y_{8} - 28.4234y_{9} - 13.0410x_{9} + 13.0410x_{10} + 11.3340$$

$$5.8\dot{x}_{8} = 66.3407(y_{7} - y_{8}) + 75.6380(x_{9} - x_{8}) + 104.2491(0.26.95 - x_{8}) \tag{48}$$

$$\Rightarrow \dot{x}_{8} = 11.4381y_{7} - 11.4381y_{8} - 31.0150x_{8} + 13.0410x_{9} + 4.8440$$

$$5.8\dot{x}_{7} = 66.3407(y_{6} - y_{7}) + 179.8871(x_{8} - x_{7}) \tag{49}$$

$$\Rightarrow \dot{x}_{7} = 11.4381y_{6} - 11.4381y_{7} + 31.0150x_{8} - 31.0150x_{7}$$

$$5.8\dot{x}_{6} = 66.3407(y_{5} - y_{6}) + 179.8871(x_{7} - x_{6}) \tag{50}$$

$$\Rightarrow \dot{x}_{6} = 11.4381y_{5} - 11.4381y_{6} + 31.0150x_{7} - 31.0150x_{6}$$

$$5.8\dot{x}_{5} = 66.3407(y_{4} - y_{5}) + 179.8871(x_{6} - x_{5}) \tag{51}$$

$$\Rightarrow \dot{x}_{5} = 11.4380y_{4} - 11.4381y_{5} + 31.0150x_{6} - 31.0150x_{5}$$

$$5.8\dot{x}_{4} = 66.3407(y_{3} - y_{4}) + 179.8871(x_{5} - x_{4}) \tag{52}$$

$$\Rightarrow \dot{x}_{4} = 11.4381y_{3} - 11.4381y_{4} + 31.0150x_{5} - 31.0150x_{4}$$

$$5.8\dot{x}_3 = 66.3407(y_2 - y_3) + 179.8871(x_4 - x_3)$$

$$\Rightarrow \dot{x}_3 = 11.4381y_2 - 11.4381y_3 + 31.0150x_4 - 31.0150x_3 \quad (53)$$

$$5.8\dot{x}_2 = 66.3407(y_1 - y_2) + 179.8871(x_3 - x_2)$$

$$\Rightarrow \dot{x}_2 = 11.4381y_1 - 11.4381y_2 + 31.0150x_3 - 31.0150x_2 \quad (54)$$

$$31.11\dot{x}_1 = 179.8871x_2 - 110.9235x_1 - 66.3407y_1$$

$$\Rightarrow \dot{x}_1 = -3.5655x_1 + 5.7823x_2 - 2.1325y_1 \quad (55)$$

and vapour-liquid equilibrium on each tray (n=1-16):

$$y_n = \frac{5.68x_n}{1 + 4.68x_n} \quad (56)$$

CHAPTER 3
METHODOLOGY

In order to fulfill the objectives of this project, the work has been allocated accordingly to suit both the semesters. So for FYP I, the related tasks include:

i. Literature Study
   -To search for, refer and study any related journal, books or conference papers on the proposed topic
ii. Study on the current distillation column and processes.
iii. Build up a mathematic modeling.
iv. Set up the Simulink simulation
v. Run simulations using MATLAB Software
vi. Analyze the output products with parameters change
vii. Provide recommendations from the analysis conducted

For this project, the only tool required is computer software which is the MATLAB software. This is due to the reliable of simulation provided by this software. This software can show the simulation of crude oil distillation process with the outputs which are the Top product and Bottom product. Besides, the representation of data such as plotted graphs, functions of equations, value indications, repeated and continuous calculations, and clearer observations through zooming application are pretty helpful so that greater understanding could be achieved. Any modification done on the program can be analyzed graphically and mathematically later on.

Key Milestone and Gant Chart for Final Year Project (FYP I and FYP II) are attached in this report as Appendix I and Appendix II.

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Matlab SIMULNIK

Based from the mathematical modeling, a Simulink function has been set up to represents the process involved. It starts with the main program of the column which consists of:

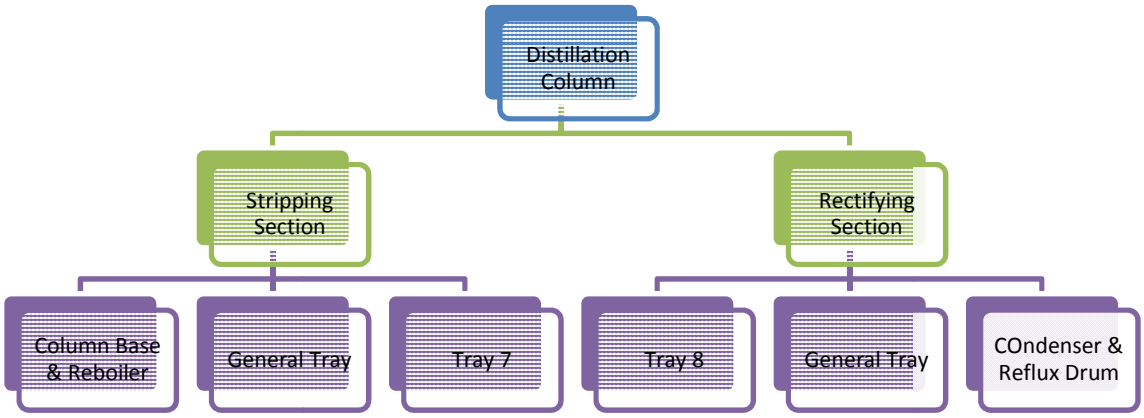

Figure 8: Main program/structure of the system

In Simulink function or module, the main program can be seen as:

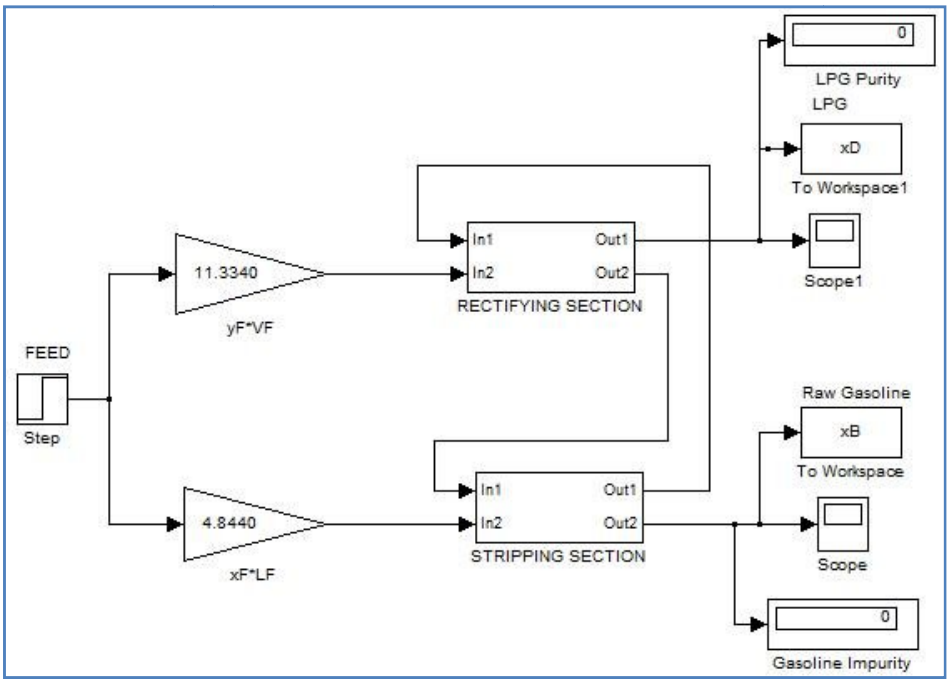

Figure 9: Main program in MATLAB Simulink

While for the Stripping and the Rectifying sections, they are a group of subsystem that consist the module for each tray of the respective sections.

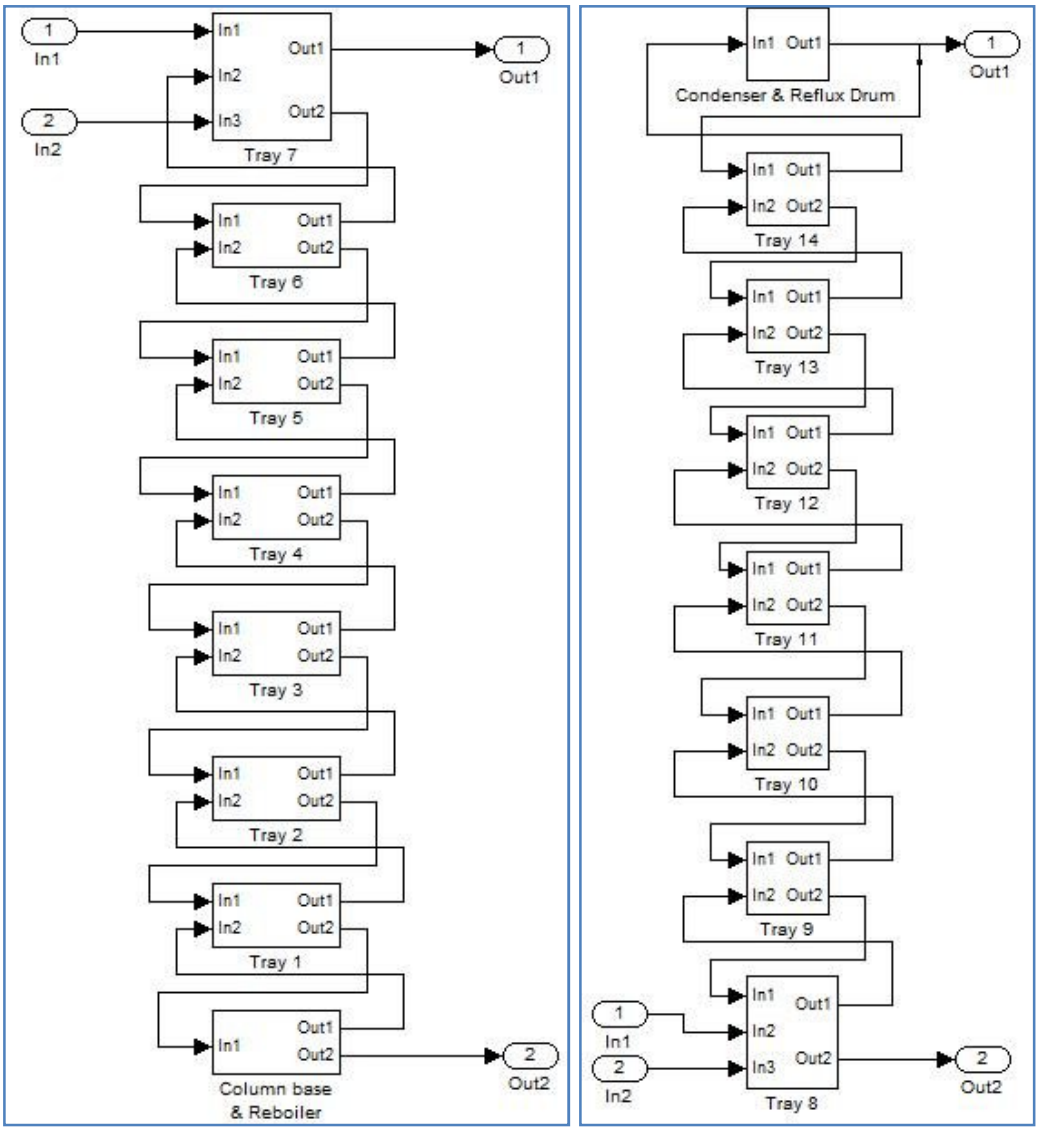

Figure 10: Subsystem of Stripping section (left) and Rectifying section (right)

At the bottom of the main program hierarchy, the most basic program represents each components existed in the distillation column which are Column Base, Reboiler, trays, Condenser and Reflux Drum. The module for each component can be seen below:

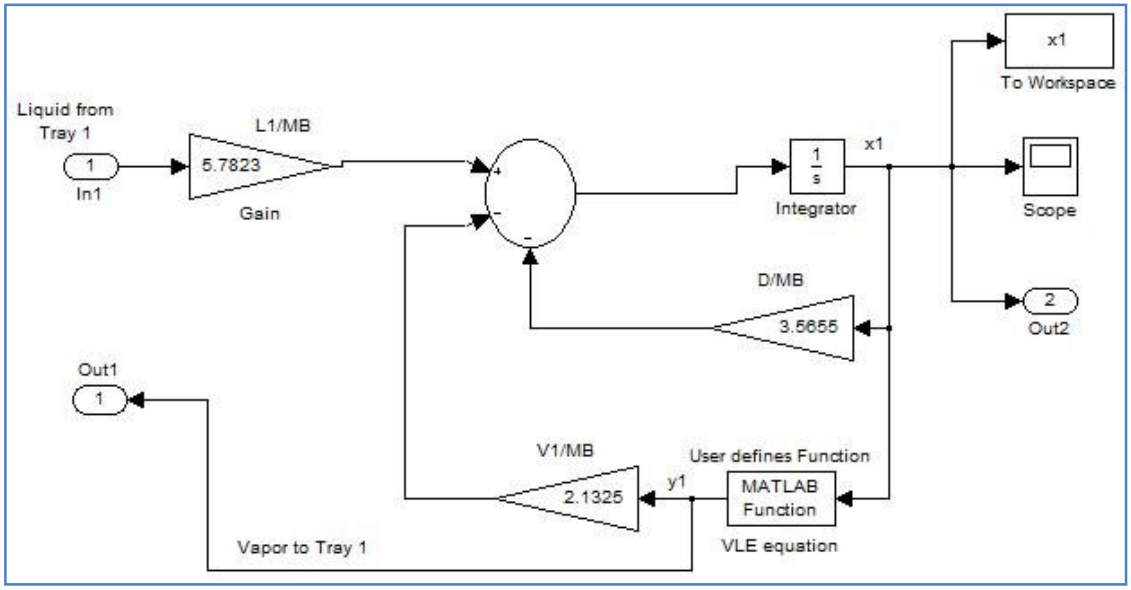

Figure 11: Module for Column Base and Reboiler

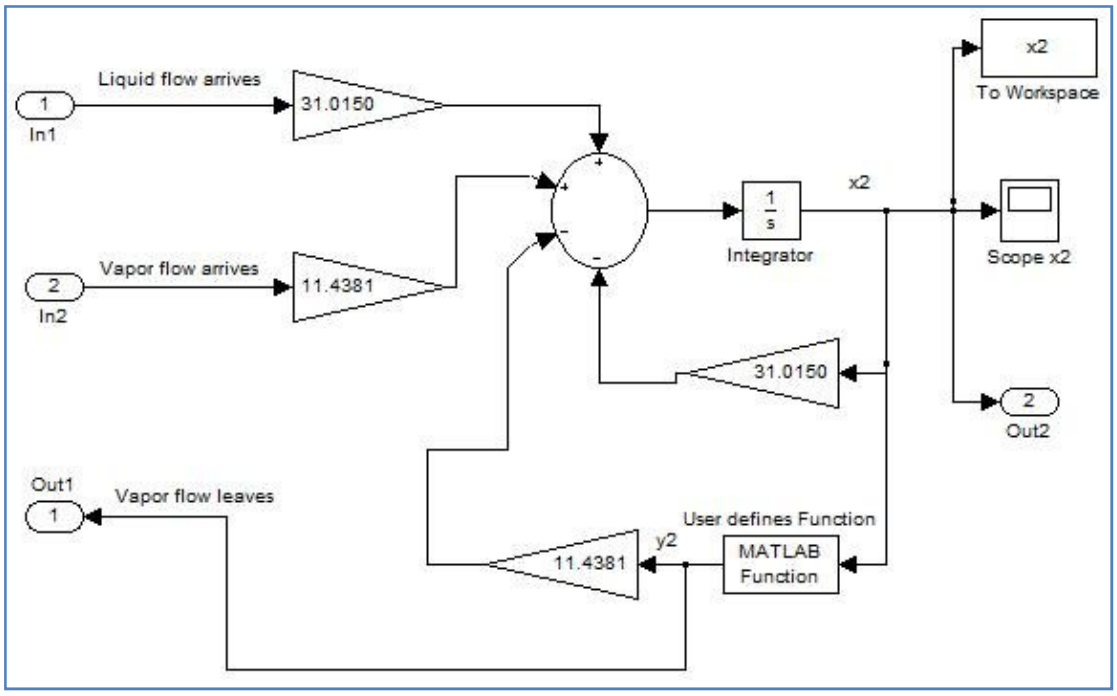

Figure 12: Module for General Tray of Stripping Section (example: Tray 1)

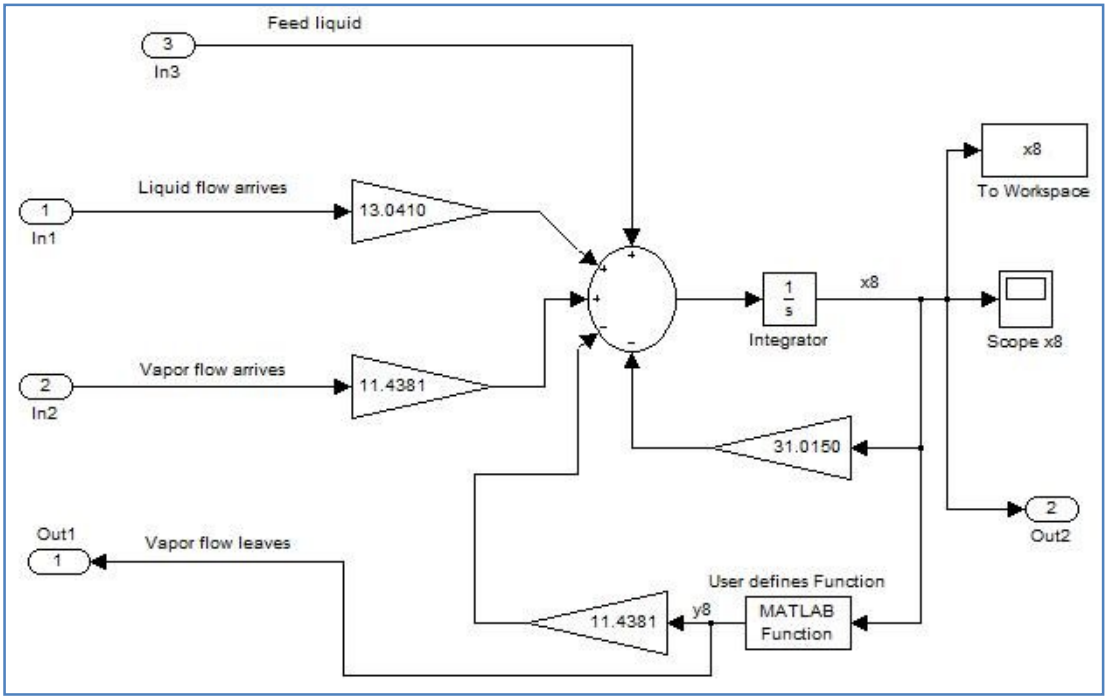

Figure 13: Module for Tray 7(Tray below the feed area)

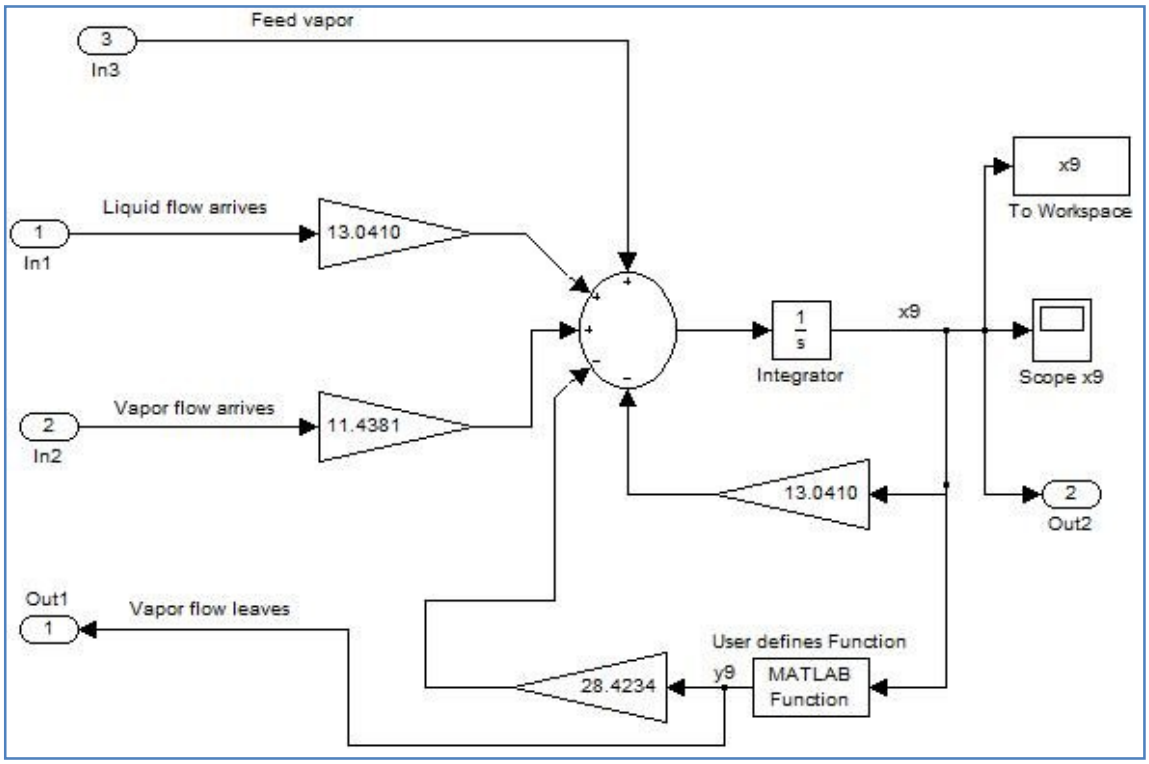

Figure 14: Module for Tray 8(Tray above the feed area)

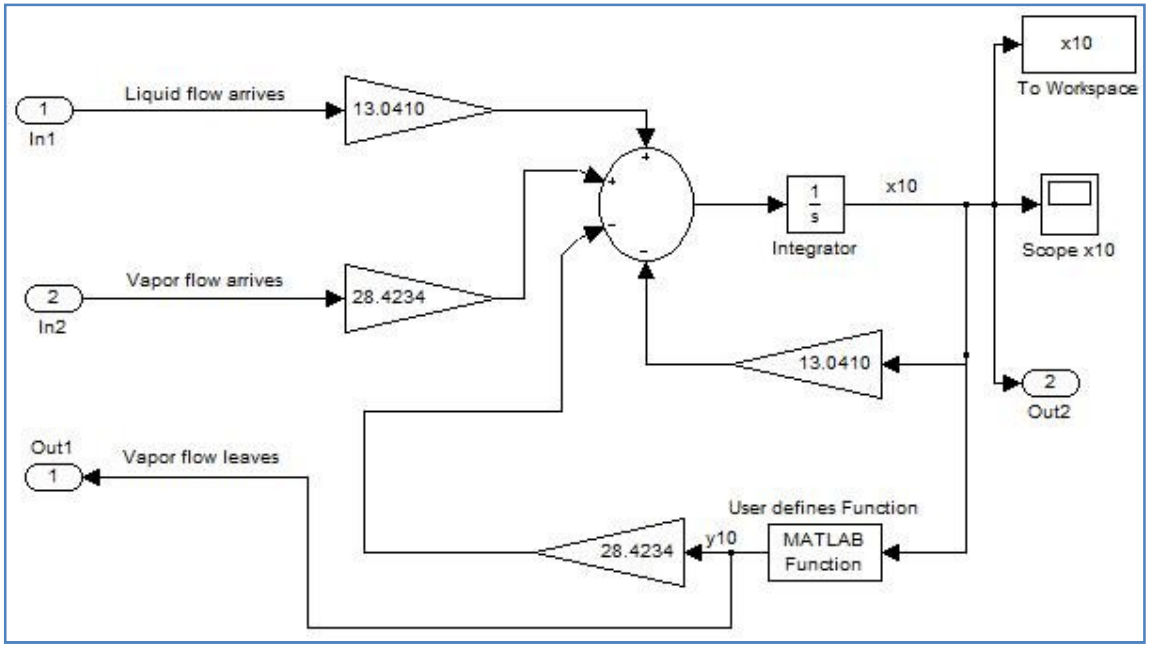

Figure 15: Module for General Tray of Rectifying Section (example: Tray 9)

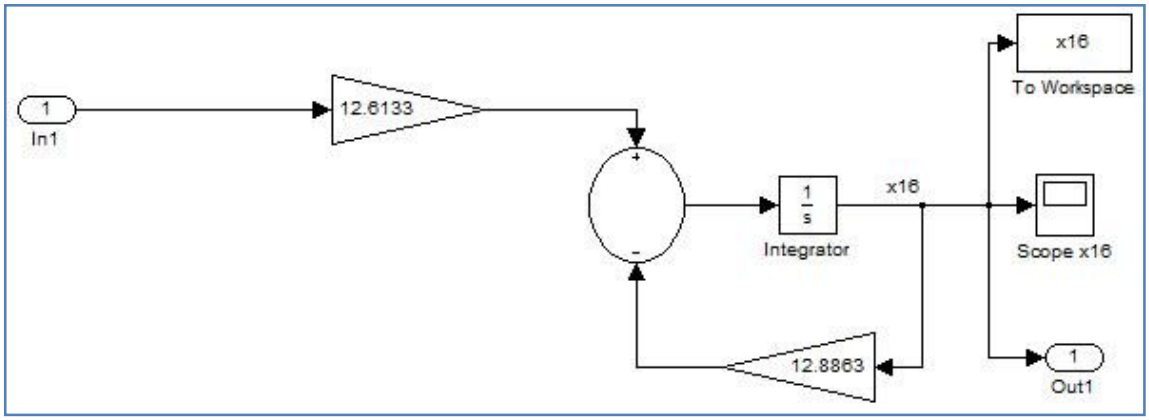

Figure 16: Module for Condenser and Reflux Drum

4.2 Analysis

From the simulations, the concentration of x_n (liquid composition) on each tray can be determined. This can be done by using the "Workspace" Menu and "Plot" function. Then, drag each variable from XB (Bottom Tray) up until XD (Distillate Tray) into the graph area to see the plot. While for y_n (vapour composition), "Display" block is required to determine the concentration on each tray. This method can also be applied to determine the value of x_n on each tray.

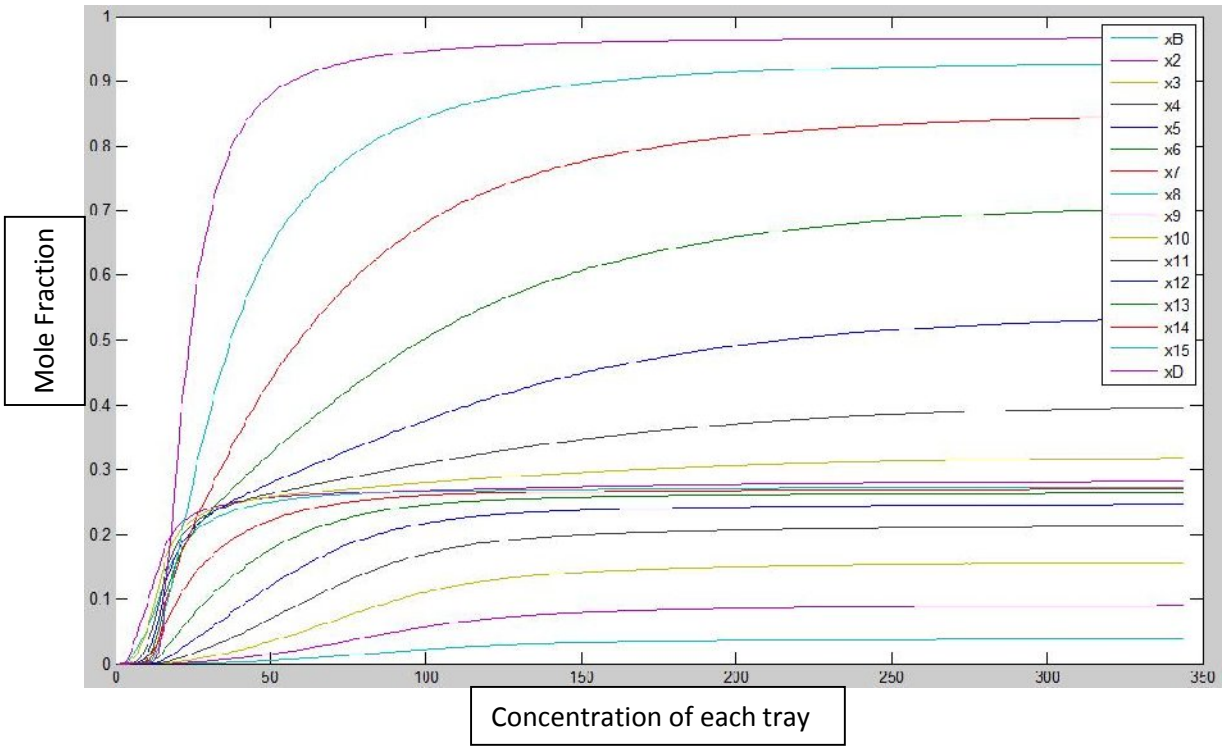

Figure 17: Steady State Values of Concentration x_n (liquid composition) on each Tray

	1	2	3	4	5	6	7	8
x_n	**0.0375**	0.0900	0.1559	0.2120	0.2461	0.2628	0.2701	0.2731
y_n	0.1812	0.3597	0.5120	0.6044	0.6496	0.6694	0.6776	0.6809
	9	**10**	**11**	**12**	**13**	**14**	**15**	**16**
x_n	0.2811	0.3177	0.3963	0.5336	0.7041	0.8449	0.9269	**0.9654**
y_n	0.6895	0.7256	0.7885	0.8666	0.9311	0.9687	0.9863	0.9937

Table 3: Summary of x_n and y_n concentration on each tray

4.3 Parameters Change

The datum for the distillation column of this project is by using 16 trays including the Column Base and Condenser. The specifications required are:

- Distillate purity ≥ 96%
- Bottoms impurity ≤ 4%

4.3.1 Different Number of Trays

For this part, the numbers of trays have been manipulated to observe the influence it would cause to the output products. This was done by reducing and adding 2 trays in the distillation column. The results can be seen as follows:

Number of Trays	Purity of the Distillate Product (%)	Impurity of the Bottoms Product (%)
14 (Reduced)	96.54	3.75
16 (Datum)	96.79	3.41
18 (Increased)	96.91	3.19

Table 4: Summary of manipulated number of trays

From the data obtained, a trend exists whereas the quality of the output product increase as the number of trays increases. This shows that trays manipulating can be considered as a potential option to improve the efficiency of the existing plants. But the economic factor also needs to be put into consideration as the cost will also increase by introducing more trays into the distillation column.

4.3.2 Noise Disturbance

Feed flow rate is assumed to be constant throughout the process for the ease of calculations part. So for this part, it is assumed that disturbance occurred in feed flow rate due to noise. The noise disturbance is being manipulated in terms of percentage with range of ±10% to observe the effects to the output products.

Feed Flow Rate	Purity of the Distillate Product (%)	Impurity of the Bottoms Product (%)
Reduced (90%)	90.23	0.66
Datum (100%)	96.54	3.75
Increased (110%)	97.30	11.66

Table 5: Summary of manipulated feed flow rate

From the results obtained, it was observed that noise disturbance does give effects to the output product. The disturbance may occur by reduced or increased in the feed flow rate. For the first situation which is reduced feed flow rate, the quality of the Bottom Product increased but the quality of the Distillate Product reduced. While for the second situation of increased feed flow rate, the quality of Distillate Product increased but the quality of the Bottom Product reduced. This means that it is important to avoid disturbance in the feed flow rate to obtain an optimum output from the processing plant. The source of noise may be due to upstream process or improper maintenance conducted on the feed piping.

4.3.3 Fluctuate Feed Flow Rate

Sometimes, there are possibilities that the feed flow rate fluctuate during the process. To represents the situation, "Signal Generator" Block will be introduced into the Simulink function.

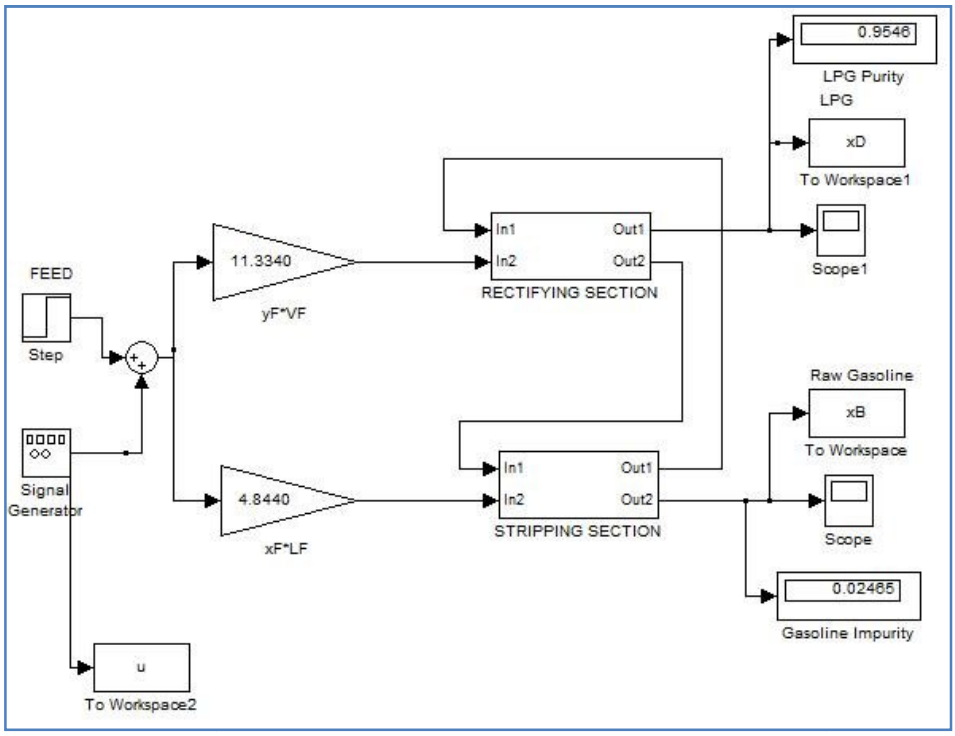

Figure 18: Signal Generator Block introduced into the Simulink function

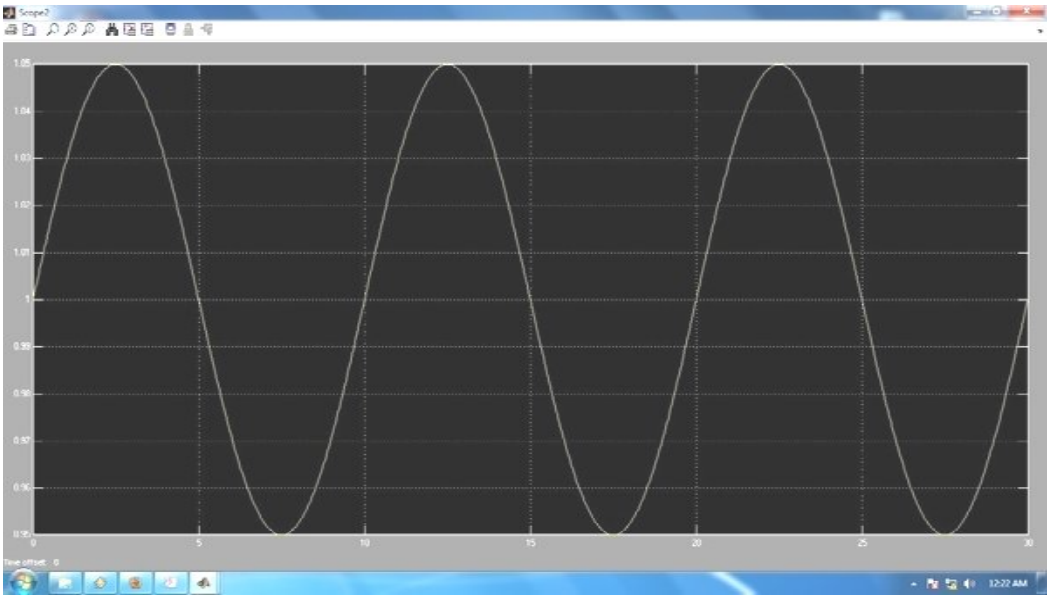

Figure 19: Feed flow rate fluctuate in a sine wave by ±5%

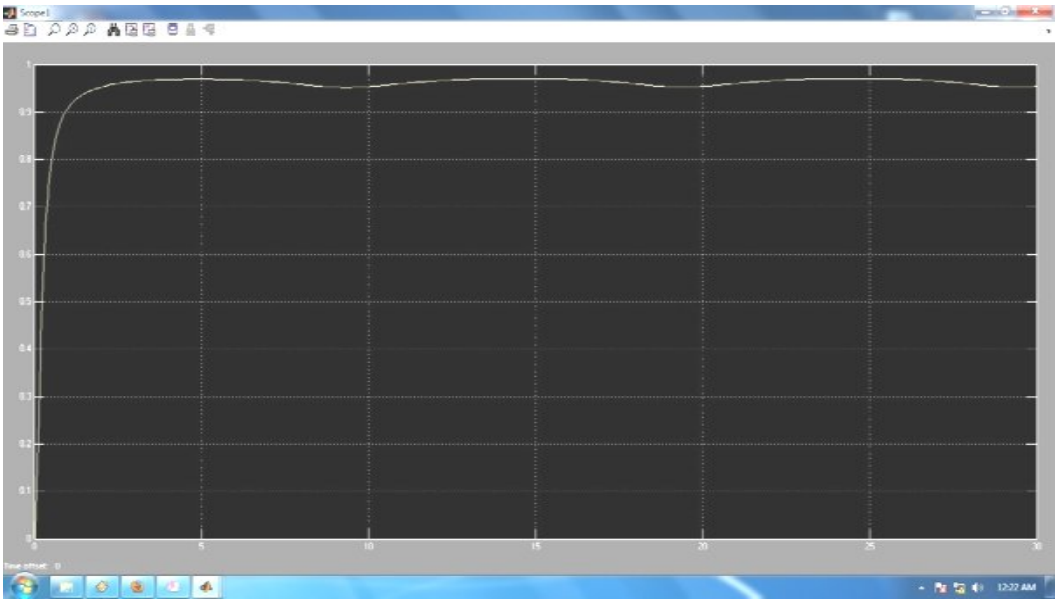

Figure 20 Distillate product fluctuated

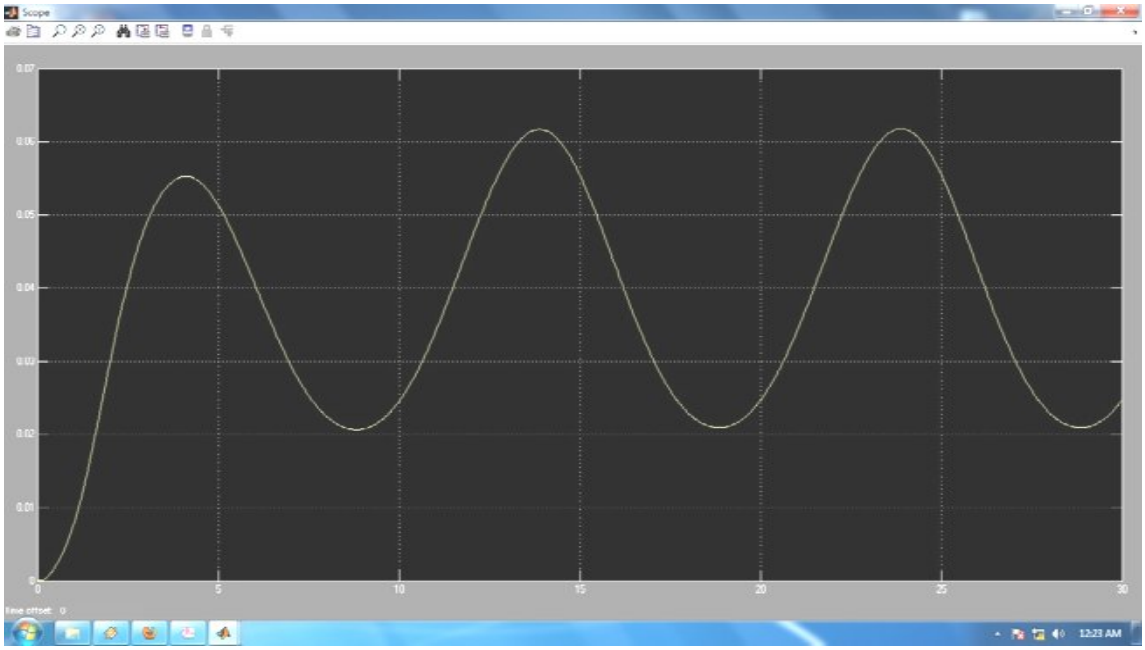

Figure 21: Bottom product fluctuated

Results	Feed Flow Rate (%)	Distillate Purity (%)	Bottoms Impurity (%)
Max Value	105	96.92	5.53
Min Value	95	95.26	2.06

Table 6: Product Quality Depending on the Input Sine Wave Fluctuation

From the simulations conducted, it was observed that the output product also fluctuate if the feed flow rate fluctuates by ±5%. This means that the quality of the output product also affected but not as much as manipulating the number of trays and disturbance in the feed flow rate. Again, such situation must be avoided in real life in order to fully utilize the processing plant for optimum output.

CHAPTER 5
CONCLUSION AND RECOMMENDATION

As a conclusion, simulations of a typical petroleum distillation process can be done by using the Simulink function of the MATLAB software. First of all, current petroleum distillation process needs to be learnt to obtain a brief view of the process. After that, mathematical model will be built base from the developed mathematical modeling done by fellow researcher. By having sufficient data, Simulink functions can be set up by referring to the mathematical model. Then, analysis on the process will be conducted from the simulations and any possible parameters that could affect the quality of the output products could be manipulated. From the parameters change, recommendations could be provided for future enhancement.

Throughout the project, better understanding on Propane, C_3H_8 and Butane, C_4H_{10} distillation column and modeling have been achieved. This could improve student's understanding and help them to be familiarized with petroleum industry. Besides, student has acquired basic knowledge in one of the Chemical Engineering field which is Separation Process.

Changes in parameters give different effects on the output products. For example, by having a greater number of trays in the distillation column, the quality of Distillate and Bottom product could be improve. This phenomena act proportionally with the increased number of trays. Another example is by manipulating the feed flow rate due to noise disturbance. It was seen that the quality of Distillate product reduced while the quality of Bottom product increased when feed flow rate reduced. But the situation will be vice versa if the feed flow rate increased. This shows that disturbance of feed flow rate give great influence to the output products, thus it is important to make sure that the process operates at the optimum flow as modeled.

The manipulation of parameters represents certain situations in real life for distillation process. The increase number of trays could be an improvement method for better

output product while the change in the feed flow rate could be occurred due to disturbance in the feed system. Thus proper considerations need to be done for each situation. For example by adding more trays to the distillation column, the investment and maintenance cost will also increase. While for the issue of feed disturbance, scheduled maintenance should be conducted to make sure that the process runs at the optimum performance.

As a recommendation, further improvements could be done on the Simulink functions by having a feedback loop to the distillation process. As a comparison, the produced Simulink function is only in open loop process, which gave the output without having feedback. By having feedback, we can analyze the output more efficiently. For example, in the case of manipulating the number of trays used in the distillation column. The feedback loop can be used to determine the maximum allowable number of trays to be added as it could affect the cost of operating the plant, increase number of trays will also increase the cost.

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APPENDIX

Appendix 1: Final Year Project (FYP 1) Schedule Semester July 2009

No	Detail/Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	Selection of project topic																	
2	Preliminary research work																	
	Introduction to the project																	
	Methodology development																	
	Research/study on basic knowledge and principles																	
3	Submission of Preliminary Report																	
4	Project work																	
	Study about current distillation process																	
	Study of the developed mathematical modelling																	
5	Submission of Progress Report																	
6	Seminar																	
7	Project work continues																	
	Study & research about MATLAB Simulink modules																	
8	Submission of Interim Report																	
9	Oral Presentation																	

Appendix 2: Final Year Project (FYP II) Planned Schedule Semester Jan2010

No	Detail/Week	1	2	3	4	5	6	7	Mid-semester Break	8	9	10	11	12	13	14
1	**Project work continues** Literature studies Run simulations using developed mathematical modeling Determine possible parameters to be manipulate															
2	**Progress Report I submission**															
3	**Project work continues** Literature studies Manipulate parameters (no of trays, flow rate speed) Run simulations Analysis and compare with the datum															
4	**Progress Report II submission**															
5	**Seminar (compulsory)**															
6	**Project work continues** Literature studies Manipulate other possible parameters (feed disturbance) Run simulations Analysis and compare with the datum															
7	**Poster exhibition**															
8	**Dissertation Final Draft Submission**															
9	**Oral Presentation**									During study week						
10	Dissertation submission (hard bound)									7 days after oral presentation						