OPTIMAL OPERATION AND CONTROL OF FOUR PRODUCT DIVIDING-WALL (KAIBEL) DISTILLATION COLUMN

BY

FARRUKH ILYAS ABID

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This thesis, written by **FARRUKH ILYAS ABID** under the direction his thesis advisor and approved by his thesis committee, has been presented and accepted by the Dean of Graduate Studies, in partial fulfillment of the requirements for the degree of **MASTER OF SCIENCE IN CHEMICAL ENGINEERING.**

Dr. Abdallah Al-Shammari
(Advisor)

B.H.

Dr. Housam Binous
(Co-Advisor)

Dr. Mohammed Ba-Shammakh
(Member)

Dr. Abdulhadi Al-Juhani
(Member)

Shain

Dr. Mohammad Shamsuzzoha
(Member)

Dr. Mohammed Ba-Shammakh

Department Chairman

Dr. Salam A. Zummo
Dean of Graduate Studies

5/1/16

Date

The thesis work is dedicated to my beloved parents whose support and prayers make possible this achievement.

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“In the name of Allah, The Most Merciful and The Most Gracious”

All praise and thanks to Almighty, the Creator of all worlds for giving me the courage to accomplish this work sincerely and successfully. May there be every peace and blessings upon the holy prophet Muhammad (SAW), his family and his companions.

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LIST OF ABBREVIATIONS

DWC : Dividing Wall Column

FTCDC : Fully Thermally Coupled Distillation Column

MPC : Model Predictive Control

Vmin : Minimum Vapor Flow rate

SIMC : Simple / Skogestad Internal Tuning Rules

TAC : Total Annualized Cost

R_L : Liquid Split Ratio

R_V : Vapor Split Ratio

RGA : Relative Gain Array

PID : Proportional Integral Derivative

ABSTRACT

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Due to the globalization and increased market competition, the process industry is trying to maximize the productivity at minimal operational cost. According to the literature, the distillation operation mainly used in oil refineries and petrochemical industries is consuming 3% of total world’s energy consumption. The energy consumption can be reduced appreciably by using complex distillation column arrangements i.e. fully thermally coupled distillation column, divided wall column etc. The operation and control of four product divided wall distillation column was studied with the help of simulation software package i.e. Aspen HYSYS. Three different feed stocks are introduced to divided wall column one by one in order to compare the energy consumptions with conventional distillation column. In order to achieve optimal operational parameters, the effect of degree of freedom on operation of distillation column was studied. It has been observed that divided wall distillation column has capability of saving about 20 – 30% energy consumption. Finally, a feasible control strategy have been implemented in order to study the control behavior of distillation column, dynamic simulation of kaibel distillation column has been carried out and system was tested by giving some disturbances from the feed. It has been observed that the implemented control strategy has an ability to reject disturbance and track the given set points values.

ملخص الرسالة

الاسم الكامل: فاروق إلياس عابد

عنوان الرسالة: العملية المثلى والسيطرة على عمود تقطير(كايبيل) ذو جدال فاصل لتقطير أربعة مركبات كيميائية

التخصص: هندسة كيميائية

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بسبب العولمة والمنافسة المتزايدة في الأسواق الصناعية تسعى كثيراً من الشركات لزيادة الأنتاجية مع خفض تكاليف التشغيل. و وفقاً للأبحاث، تستهلك أعمدة التقطير في معامل تكرير النفط والصناعات البتروكيماوية 3% من استهلاك الطاقة الإجمالي في العالم. استهلاك الطاقة في عمود التقطير يمكن تقليصه بستخدام تقنيات حديثة مثل أعمدة التقطير ذات الجدار الفاصل. في هذة الدراسة تم إستخدام برنامج محاكاة للعمليات الصناعية (هايسس HYSYS) وتم دراسة تشغيل و التحكم بهذا النوع الحديث من أعمدة التقطير لفصل أربعة مركبات كيميائية. تمت دراسة ثلاثة مخاليط مختلفة لتحديد مستوى خفض الطاقة المستخدمة و تبين أنه يمكن خفظ الإستهلاك بنسبة تتراوح بين 20 و 30 بالمائة مقارنة بإعمدة التقطير التقليدية. كذلك تم دراسة التحكم بهذة الأعمد و تبين قدرة طرق التحكم على غزل أثر المتغيرات على نظام التشغيل و الحفاظ على تشغيل سلس

CHAPTER 1

INTRODUCTION

This chapter presents a brief introduction about the most widely used unit operation i.e. distillation in almost all the chemical process industries all over the world. Although distillation operation techniques are considered to be well matured and established but it is responsible for consuming immense amount of heat energy for the separation of components. This is why, it is very important to consider both the benefits and drawbacks of the current distillation technology. Here, brief introduction to different distillation column arrangements are studied when number of components to be separated are greater than two. The advantages and disadvantages of all the configurations will also be considered. Along with, different control strategies of distillation column are also studied.

1.1 Introduction to Distillation Operation

The distillation operation can be defined in few words as;

“Distillation is a unit operation (physical phenomenon) that separates the component substance from a liquid mixture on the basis of their boiling points. Upon achieving the boiling point temperature, components get boil and their vapors rise up and then separated in a separate pot to condense the vapors and pure liquid product can be obtained”.

It is very interesting to study about the history of distillation technique or why the old human beings feel the requirement of such physical separation. The petroleum matter present beneath the earth crust consists of complex mixture of hydrocarbons that can be found in liquid, gaseous and solid states. But the word “petroleum” is generally used for the liquid form, but it also contains natural gas and the solid bitumen. Small reserves of natural gas and oil seeps have been known since ancient time. The crude oil and asphalt is used by ancient Sumerians, Assyrians and Babylonians about 5000 years ago. Early in the Christian era, Egyptians used crude oil in the wars as weapon. The Arabs and Persians obtained flammable products by processing (distillation) of crude oil; and as a result of the Arab invasion of Spain, distillation got introduced in Western Europe by 12th century [1].

There was no commercial use of crude oil before the 19th century, because there was no setup of markets and a steady supply could not be continued. In 1846, Abraham Gesner developed a process for preparing a liquid fuel from coal, which he said as “Kerosene” (or coal oil) and sold out for lightening purposes [2]. Before this discovery, whale oil was a primary fuel used for lamps etc. In 1854, Benjamin Silliman Jr. analyzed the crude oil as a possible alternate for whale oil in Pennsylvania. Silliman noticed that on boiling and distilling crude oil at different temperatures, a fraction (Kerosene) could be obtained which is high quality illuminating oil. The early refineries utilized the existing coal oil refineries to process the crude oil and were located where oil was found.

Early refineries were very simple and they used large horizontal tanks to process crude oil to get volatile components. In 1856, the first oil refinery of the world started its operation in Ploiesti, Romania. While in the United States the first oil refinery opened in 1861. Later on with the development of electricity and internal combustion engine, the demand of refined oil products got increased. Airplanes and World War II realized the demand of high octane gasoline and jet fuel [3]. Today, petroleum refinery is a well-established industry with developed infrastructure and technology base, who convert crude oil into valuable products that fulfill the consumers demand.

There are various industrial examples of distillation process like fractionation of crude oil into some useable fractions (e.g., naphtha, kerosene, diesel, light diesel oil and furnace oil etc.), production of alcoholic beverages having high alcohol content (Frobes, 1970), purification of organic solvents, water desalination and purification, splitting of air to get its components (e.g., oxygen, nitrogen and argon) and in many other petrochemical processes.

Figure 1 illustrates the schematics of a binary distillation column with feed as input stream and two output streams i.e. one top product called as distillate product (D) obtained from the top of the column and one bottom product (B) obtained from the bottom of the distillation column. Please remove the texts in red which is given only as a guide.

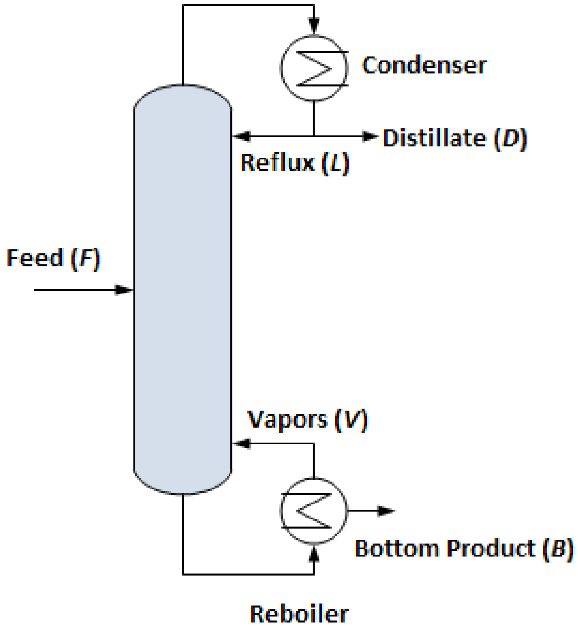


Figure 1: Process Flow Diagram (PFD) of a Binary Distillation Column

This binary distillation column consists of two heat exchangers, one is “condenser” at the top of the column and other is known as “reboiler” at the bottom of the distillation column. Actually, vapors coming from the top of the column are directed towards the condenser to absorb their heat energy and provide top liquid product and reflux (L). Reflux is the cool liquid that sent back to the distillation column to maintain the heat balance of the column and to improve the top product purity. The reboiler is used to provide the necessary heat energy to boil the liquid present in the bottom of the column. The long column shown in the above figure usually consists of trays or stages in it. The quantity of trays, types of trays and distance between each tray are calculated during the design of distillation column. There are another option of using packing of different types like raschig rings, ceramic berl saddle, metal fleximax and many more depending upon the conditions and product requirements.

A distillation column consists of number of stages and it is assumed that vapor-liquid equilibrium (VLE) is occurring at each stage of column. It reflects that at any particular tray, the amount of liquid phase and vapor phase are equal for the given temperature and pressure conditions at that tray. The concept of VLE can be elaborated by the equation given below.

$$[y_1, y_2, \dots, y_{Nc-1}, T] = f(P, x_1, x_2, \dots, x_{Nc-1}) \tag{1.1}$$

Here, N_c is the number of components to be separated and ‘y’ is showing the vapor phase mole fraction of all the components, similarly ‘x’ is denoted the liquid phase mole fraction of all the components present in the feed mixture and ‘T’ and ‘P’ denote the temperature and pressure respectively (Halvorsen, 2001). Figure 2 is giving a general idea of inlet and outlet streams (liquid and vapor) from the trays of distillation column.

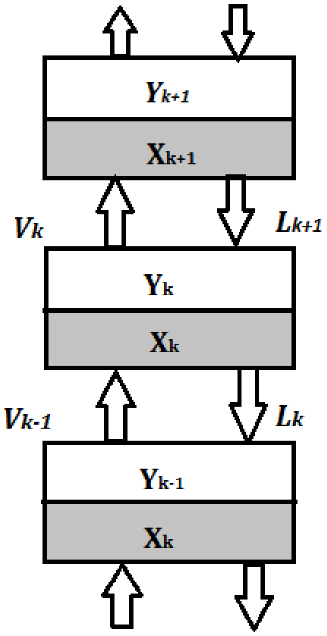


Figure 2 : Three Equilibrium Stages of a Distillation Column

In the above figure, it is clear that there are two streams entering the stage "K" (one vapor stream from the lower stage and one liquid stream from the upper stage) and two streams are leaving the same stage. This mechanism applies on all the stages of the distillation column [4]. It is also worthy to mention here that there is a simultaneous heat and mass transfer operations occurs on each stage of the distillation column. The counter-current contact of vapor and liquid streams results in the development of a temperature profile across the distillation column. The peak temperature will always found to be at the bottom of the column and the lowest temperature will be at the top of the distillation column.

A distillation column is usually divided in two sections i.e. rectifying and stripping section. The portion or area of column above the feed tray is known as “rectifying section”. Because in this section the concentration of lighter components (more volatile components) increases in both liquid and vapor phases. While the section below the feed stage is known as “stripping section”. As in this section, the concentration of more volatile components decreases or concentration of heavier components increases in both phases. Actually the lighter components get heat energy (provided by the reboiler) to move upward in the column. There is also another zone known as “flash zone”, which includes the tray at which distillation column feed is charged. Actually the pressure drop occurs when the feed enters the flash zone and it get split into two phases i.e. vapors and liquid immediately.

The ideal stages of a distillation column should meet the three criteria given below (Kister, 1992a):

i. The column will operate at steady state and it has both a liquid product and vapor product.
ii. All liquid and vapors streams entering the stage should be contacted properly and mixed perfectly.
iii. The total amount of liquid leaving the stage should be in equilibrium with the total vapor leaving that stage.

Total number of ideal stages can be calculated by multiplying the stage efficiency with number of non-ideal stages. The non-ideal tray may decrease or increase the separation - if it is increasing the separation then stage efficiency may approach to 100%. The idea of "stage efficiency" is used to calculate about the non-ideality of a stage.

1.2 Material Balance on Distillation Column

It is very easy to apply overall material balance on any distillation column either it is binary, ternary or multi product distillation column. The overall material balance for the distillation column shown in Figure 1 can be written as;

According to steady state material balance, we have;

Input = Output + Accumulation

$$Feed = (Distillate + Bottoms) + 0 \tag{1.2}$$

According to above material balance equation, there are only two streams leaving the binary distillation column i.e. one from the top (Distillate product) and other from the bottom (B). Now, let's suppose there are only two components i.e. P and Q in the feed of the distillation column. The component balance on each component can be applied in the similar way as shown below [5];

Component Balance on P:

$$\left(x_{F,P}\right) * \mathrm{F} = \left(x_{D,P}\right) * \mathrm{D} + \left(x_{B,P}\right) * \mathrm{B} \tag{1.3}$$

Component Balance on Q:

$$\left(x_{F,Q}\right) * \mathrm{F} = \left(x_{D,Q}\right) * \mathrm{D} + \left(x_{B,Q}\right) * \mathrm{B} \tag{1.4}$$

Where;

F = mass flow rate of feed stream

D = mass flow rate of distillate stream

B = mass flow rate of Bottom stream

X_F = mass fraction of component in feed

X_D = mass fraction of component in distillate

X_B = mass fraction of component in bottom

Similarly, the material balance for each stage of a distillation column can be made. Let's apply the material balance on the k^{ith} tray of a distillation column shown in Figure 1.2. If $N_{i,k}$ is the number of moles of component 'i' on tray k, L_k is showing the liquid flow coming from k^{th} tray to k-1 and V_k is representing the vapor flow coming from k^{th} tray to k+1. So, the material balance equation can be written as;

$$\frac{dN_{i,k}}{dt} = \left(L_{k+1}x_{i,k+1} - V_k y_{i,k}\right) - \left(L_k x_{i,k} - V_{k-1}y_{i,k-1}\right) \qquad (1.5)$$

Beside the material balance equations, there are also some other useful equations should be mentioned here. For example, the partial pressure of a component can be determined with the help of Raoult's law.

This law can be stated as "the partial pressure (p_i) of a component 'i' is equal to the product of the liquid mole fraction (x_i) and vapor pressure at that temperature $p_i^o(T)$".

Mathematically it can be written as;

$$p_i = x_i * p_i^o(T) \qquad (1.6)$$

To find the vapor pressure $p_i^o(T)$, the *logarithmic Antoine equation* can be used at any temperature. The values of Antoine coefficients i.e. A, B, C etc. can be taken from any chemical handbooks. The mathematical expression for the equation is given below;

$$lnp^o(T) = A + \frac{B}{C+T} + D * ln(T) + E * T^f \qquad (1.7)$$

Usually the constants *D* and *E* of Antoine equation are equal to zero. To relate the partial pressure with the total pressure in the vapor phase for a closed system, Dalton's law gave a simple mathematical equation to serve in the field of distillation.

$$p_i = y_i * P \qquad (1.8)$$

Here "*P*" denotes the total pressure in the vapor phase for an isolated system. It is important to mention here that both *Raoult's* and *Dalton's* laws are obeyed by only ideal mixture. This is a very brief theory regarding the distillation and its governing laws. Now we will discuss the technology advancement in the field of this unit operation.

Till yet, only the binary distillation column was considered above. But the real problem is to handle and operate multi-product distillation columns. Now, have some look on different distillation columns arrangements for multi-product purposes.

1.3 Different Configurations for Distillation Column

With the increase in the degree of globalization, it's become very important to run a process plant so as to minimize the loss and maximize the profit. Along with, development in the field of process modeling as well as achievements in computational power and advanced numerical methods in the field of chemical engineering made process intensification possible. Process intensification in the field of chemical process engineering has increased awareness towards the limited energy resources of the modern society (Huang et al., 2007). There are number of stages before the erection and commissioning of an industrial production plant. For example, there are design calculations, project feasibility analysis, process simulations and especially cost analysis (which includes capital investment, operational cost, payback period etc.) against each unit operation and unit processes involved in the process. Similarly, industrial distillation unit technology is also very well matured and developed. This is why it is being used by almost all the petrochemical plants and oil refineries all over the world. But with the passage of time, it has been realized that there is still need of modification of this process. The key reasons of development in the technology will be discussed here.

As shown in the above Figure 1, we have noticed that only one distillation column is needed for the separation of a binary feed mixture into its components. But for the separation of multi component mixtures, the number of distillation columns increases and a particular sequence should be applied. For example, at least two or three columns are needed for the separation of three and four components respectively. But the arrangement or sequence of the distillation columns depends upon the nature of the components and required product purities. The distillation column arrangements are divided into two main categories i.e. simple column configuration (Kiss, Kenig and Yildirim, 2011) and complex column configuration (Petlyuk, Slavinskii and Platonov, 1965). The further classification of each configuration is shown in Figure 3 below.

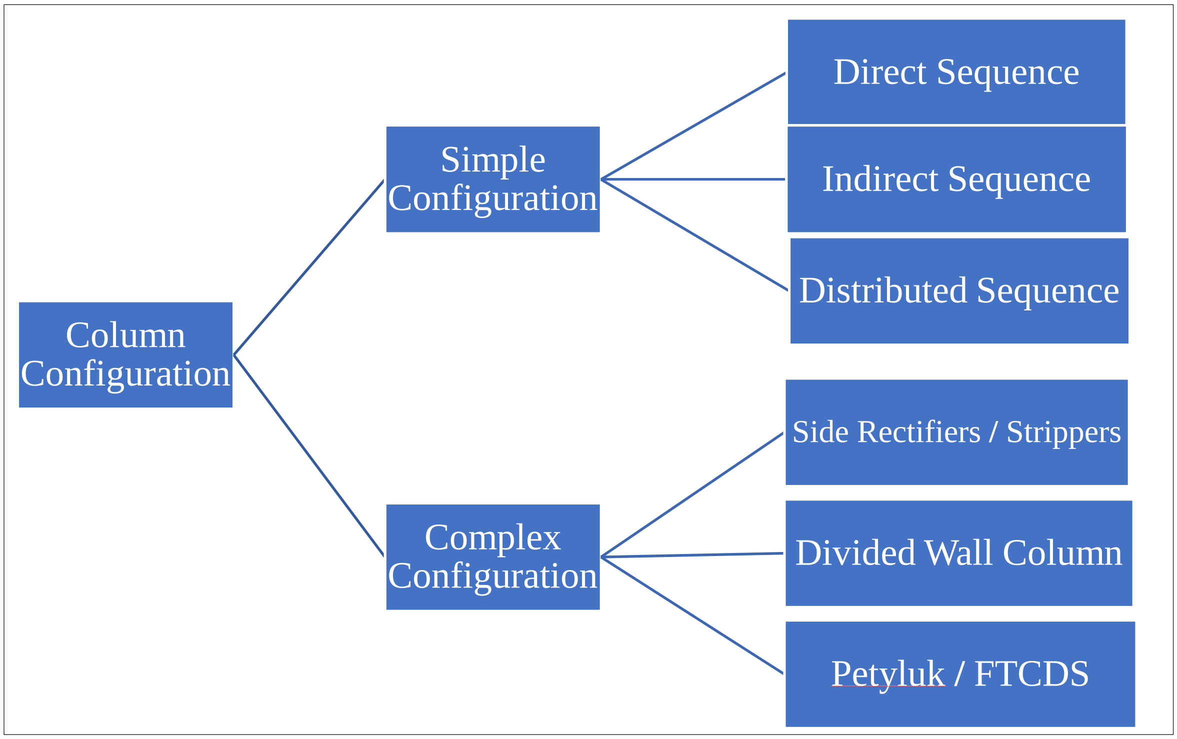


Figure 3: Block Diagram showing different configurations of distillation column

The complex configuration is very energetic alternative of the previously used sequence in many ways like energy consumption and capital investment. Actually in this column configuration, there is a thermal coupling between prefractionator and the distillation column (Petlyuk et al.). While the condenser and reboiler are attached to the main distillation column. This integrated configuration is known as “fully thermally coupled distillation column (FTCDC)”. Here we will discuss briefly the advantages and disadvantages of all the sequences one by one with the help of process flow diagram.

1.3.1 Simple Column Configuration

Simple column arrangement is generally divided into three patterns i.e. direct sequence, indirect sequence and distributed sequence. All these patterns consists of two or more distillation columns (each distillation column contains single feed and two products) depending upon on the number of components in the feed mixture. There is a condenser to condense the top product of the column into liquid and a reboiler is there to provide heat energy at the bottom of the column.

In the direct sequence, the feed is introduced to the first distillation column and lighter product is obtained from the top of first column. While the bottom product of the first column is charge to second column to give two more pure products i.e. one from the top and one from the bottom of the column, as shown in Figure 4.

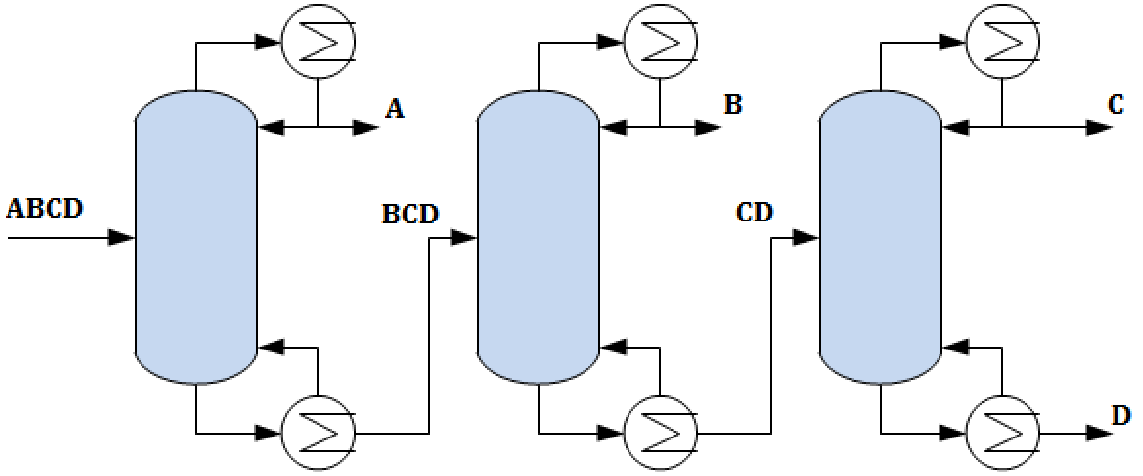


Figure 4: Direct Sequence for Distillation Columns

The above figure is showing the direct arrangement of distillation columns when the feed mixture contains four components. This sequence is used when the feed contains high concentration of lighter component (in this case lightest component is ‘A’) or the separation between middle components i.e. between ‘B’ and ‘C’ is relatively more difficult than between ‘A’ and ‘B’. In simple way, we can say that the relative volatility $\alpha_{A/B}$ is greater than $\alpha_{B/C}$.

While in the indirect sequence, the top product from the first column becomes the feed of the second distillation column and the top product of second column becomes the feed of third distillation column as shown in Figure 5. Unlike from the direct sequence, the pure products are obtained from the bottom of each column. This sequence is used when the feed contains larger concentration of middle components (like ‘C’ in the above figure) or the separation between ‘A’ and ‘B’ is relatively tougher than the separation of ‘B’ and ‘C’ [6]. The second and third columns are usually operated at a pressure lower than that of their preceding column to provide a natural flow of vapors without using an external aid like compressor.

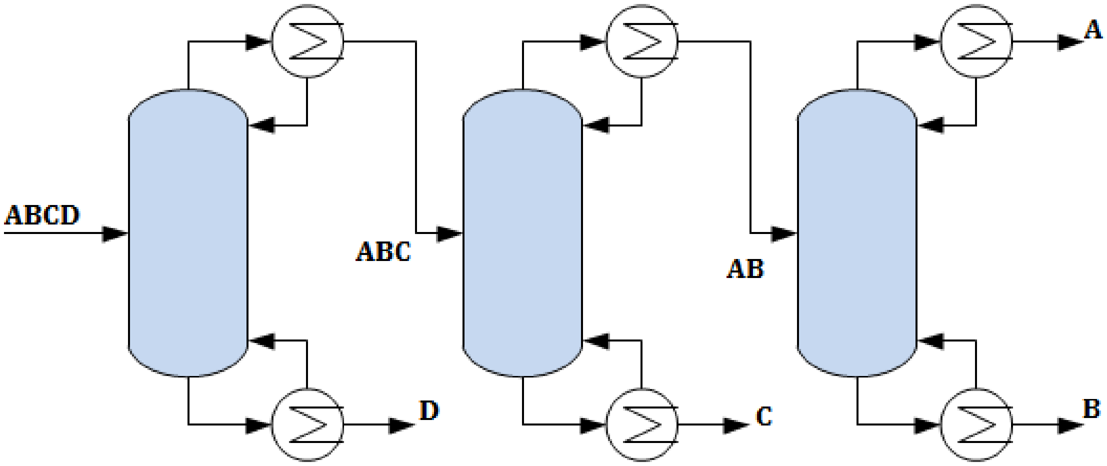


Figure 5: Indirect Sequence for Distillation Columns

There is another sequence of distillation column which consist of both direct and indirect arrangement for the separation of four components. The arrangement of distillation columns are shown in Figure 6.

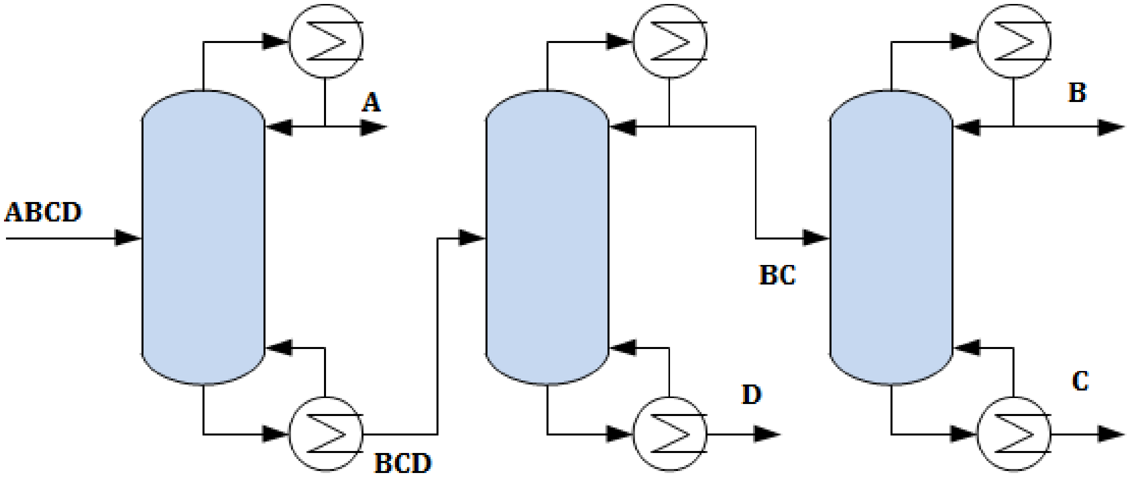


Figure 6: Direct-Indirect Sequence for Distillation Columns

There is another sequence of simple column configuration, where the first column distributes the feed components in such a way that there is a very low concentration of lighter components appears in the bottom and heavier in the top of the first column. The distillate of the first column becomes the feed of the second column to give two pure products and the bottom stream of the first column becomes the feed of the third column to give the heavier component i.e. ‘C’ and ‘D’ of the feed as pure products, as shown in Figure 7.

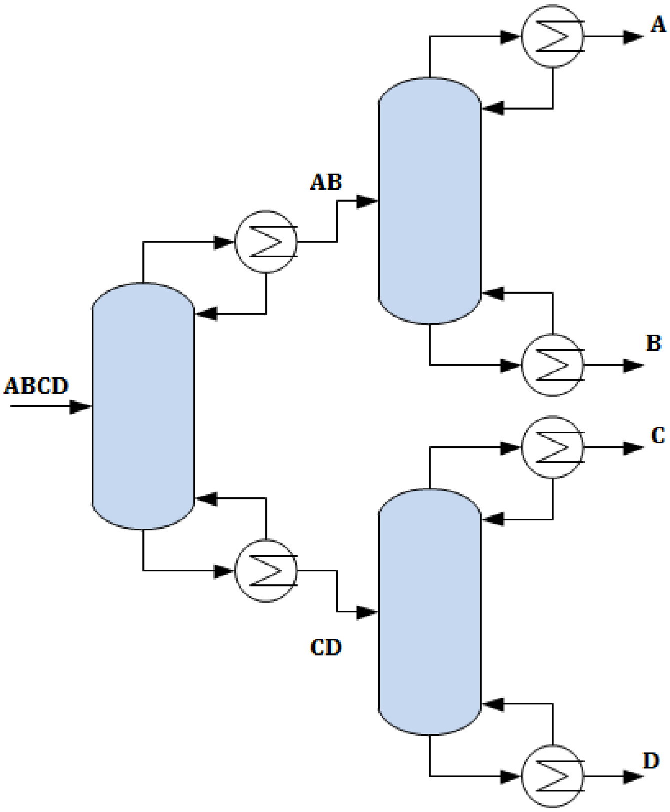


Figure 7: Distributed Sequence for Distillation Columns

This configuration of distillation columns is higher in its separation efficiency when the first column uses a partial condenser at its top [7]. This sequence is usually used when the feed contains a high concentration of ‘B’ or the both splits are tough. In other words we can say that the relative volatility of A/B and B/C are approximately equal but lower than 1.50.

1.3.2 Complex Column Configuration

Although distillation is the most widely used unit operation for the fluid separation in the chemical process industry, but it is estimated that it consumes about the 3 % of the total world's energy [8]. It is also calculated that more than 70 % of the operational cost includes only energy expenses of the process [9]. The key drawbacks of using simple distillation column arrangements are higher operational cost, higher investment cost and high energy requirements to do the required separation. The reason of higher investment cost and higher energy consumption can be seen in the above figures of simple distillation column arrangements that they require three condensers, three reboilers and three distillation columns to get four pure products. The basic reason of inefficiency of multi-component conventional distillation columns is the irreversible mixing of non-identical streams. The concentration of the middle components once reached to maximum in middle section of distillation column and then ultimately decreases to maintain the overall material balance. Actually this remixing effect decreases the efficiency of the separation.

But with the development of process integration and intensification techniques, energy efficient distillation columns like heat integrated distillation column (HIDiC), reactive distillation, thermally coupled distillation columns and divided wall distillation columns (DWC) get introduced. All these configurations are known as "complex column configurations". These complex configurations contains direct coupling of vapor and liquid stream between the pre-fractionator and the main distillation column which results in the minimum energy consumption for the required separation. Kolbe and Wenzel [10] report that about 25 % investment cost, 35 % operating cost and 40 % space requirement can be saved by using divided wall distillation column. These complex column configurations have an ability to reduce mixing losses, energy consumption and investment cost. They may contain other column like side rectifier to reduce remixing of components and pre-fractionator to reduce mixing losses at feed tray location. The thermal coupling in the complex column arrangements results in the improvement of the component separation efficiency, reduction in the column duties and a better temperature spread. A condenser and a reboiler can be eliminated by using thermal coupling between two distillation columns to obtain side stripper and side rectifier arrangements, respectively. These two arrangements of side stripping and side rectifying are also known as “partial thermally coupled distillation columns”. Fidkowski [11] proved that by employing the side stripper or side rectifier will results in a reduction of energy consumption. To separate the ternary feed mixture by partially thermally coupling of distillation columns are shown in the below Figures 8 and 9. In the side rectifier, the reboiler of the second distillation column is removed and two streams are added in place of it. One of them is the liquid stream going towards the first distillation column and second is the vapor stream coming from the first distillation column to provide the necessary heat energy in the second distillation column.

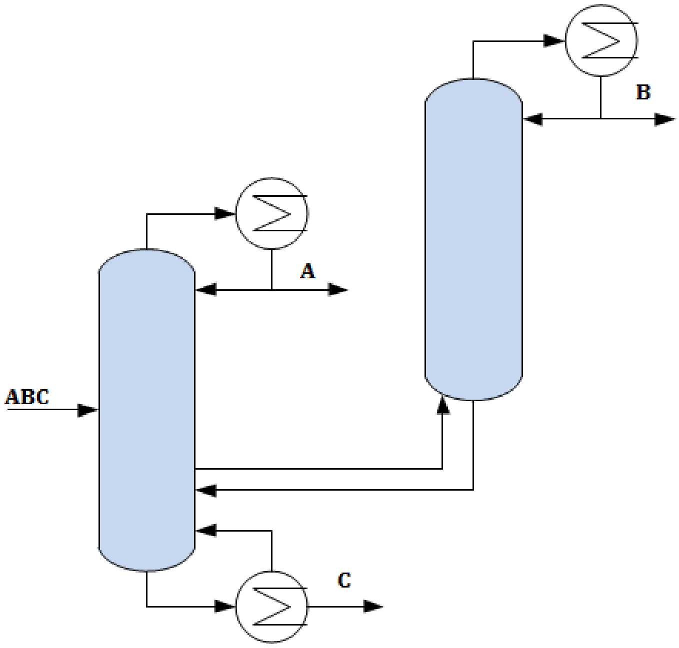


Figure 8: Side Rectifier Arrangement

In the side stripper configuration, the condenser of the second distillation column is replaced by the thermal coupling of the first and second column with vapor and liquid streams. These both arrangements lead to save the cost of a heat exchanger and also reduce the energy consumption to do the require separation.

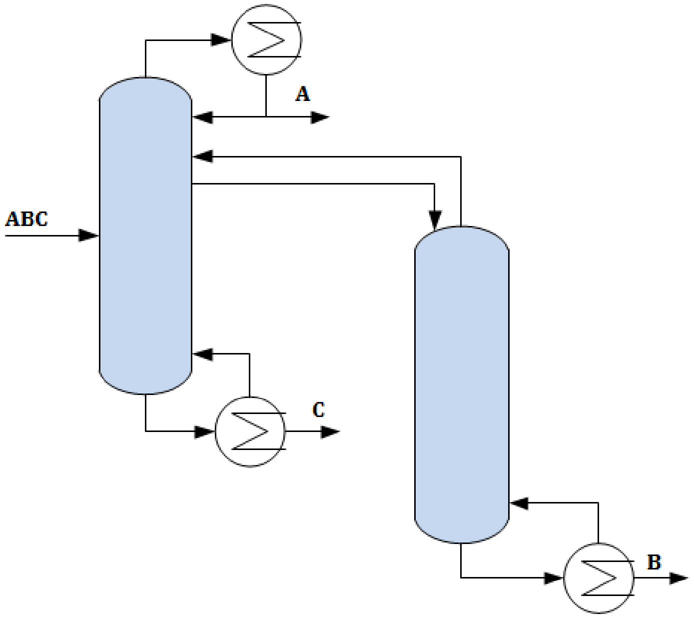


Figure 9: Side Stripper Arrangement

Now we will focus on complex column arrangements (FTCDC & DWC) for the separation of four components. In 1930, Brugma [12] was the first who gave the concept of thermally coupled distillation column. This unit operation configuration was re-studied and introduced by Wright [13] and also studied by Petlyuk [14] in 1965. They researched that energy requirements of the distillation operation can be minimized by employing direct thermal coupling of columns with process streams instead of using condenser and reboiler between the two columns, while the necessary condenser and reboiler are connected with the main column. This so called Petlyuk arrangement is implemented and proved to be very energy efficient in cryogenic processes [15]. This configuration is usually known as "fully thermally coupled distillation columns", which have replaced the condenser and reboiler of the first column (prefractionator) with the direct thermal coupling with the second distillation column as shown in Figure 10. This modification results in reduced capital investment, mixing losses and improved vapor-liquid contact in all the areas of the both distillation columns. This configuration requires less amount of energy to strip vapors or to rectify the liquid among all the configurations discussed above in simple columns configuration. But there is a difficulty in design and control of such distillation arrangements because it has greater number of degree of freedom (numbers of parameters should be specify to completely define the system) as compared to conventional column configuration.

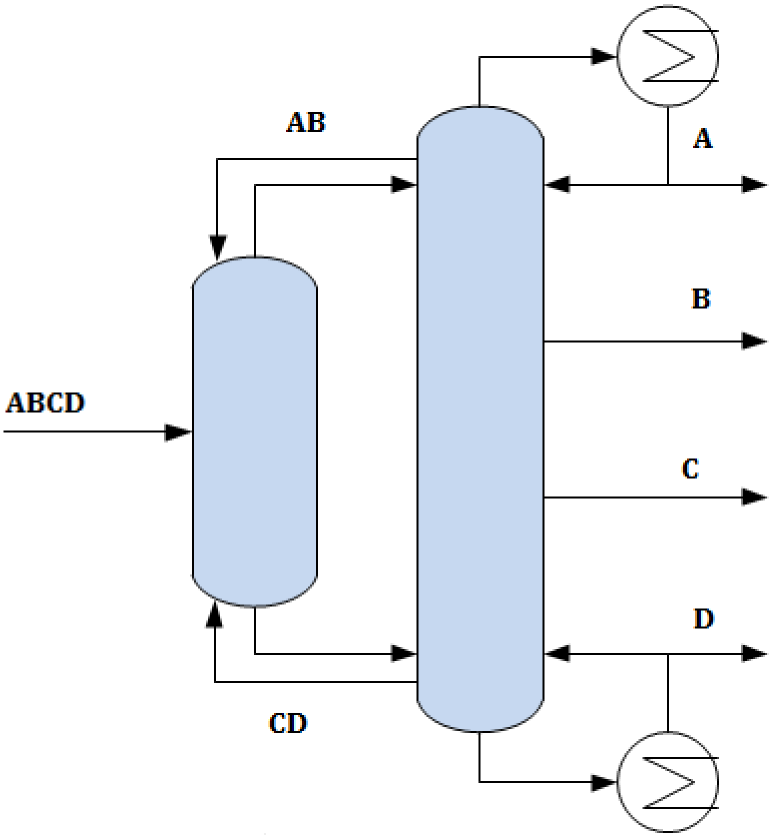


Figure 10: Fully thermally coupled distillation column

The pre-fractionator does a sharp split between light boiling component (A) and heavy boiling component (D) as shown in the above figure, whereas the middle boiling components i.e. B & C are also get separated to a great extent in the top and bottom streams respectively.

Dividing-wall distillation column (DWC)

If the two columns of the petlyuk configuration are merged or integrated into one distillation column, then the further energy and cost saving can be done. This configuration is known as "divided wall column" (DWC) and shown in Figure 11 (Kaibel, 1987; Yildrim, Kiss 2011).

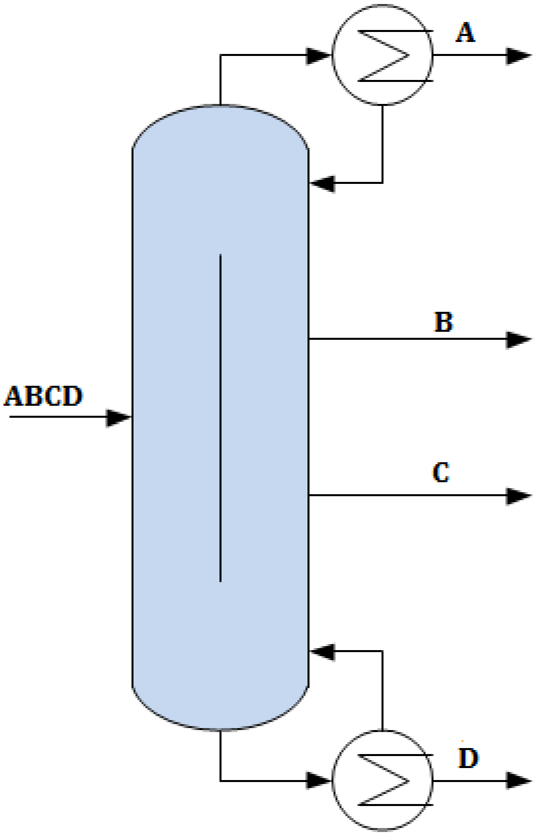


Figure 11: Divided -wall distillation column

This type of distillation column consists of an adiabatic wall inside the column shell. It also may contain packing material or trays similar to the conventional distillation column depending upon the operating conditions. The only difference between dividing-wall distillation and petlyuk column is the transfer of heat energy across the partition wall. This column arrangement is thermodynamically equal to the petlyuk configuration discussed above. Dividing wall column has an ability to produce high purity side draw products from a single column. Kaibel (1987) was the first who extended the idea of multi component separation into four and more products by using only one shell. The first industrial implementation of the packed DWC was seen in 1985 by BASF, Germany.

The major benefits which can be achieved from dividing-wall distillation column are as follows;

i. Appreciable energy savings
ii. Notable capital cost reduction by installing less number of equipment like less number of heat exchangers will be used as compared to other configuration etc.
iii. Less operational cost
iv. Less plot area required for installation which makes it suitable for offshore units
v. Small flare system due to low load

Premkumar et al. (2009) also did successful research for retrofitting of conventional distillation columns to dividing-wall columns for taking advantages of different savings.

1.4 Control Strategies for Distillation Column

During the operation of a distillation column, some variables are very necessary to be controlled at its optimal value to get the optimal product. These variables are known as "control variables" of the distillation column. They are usually flow rate, pressure, or temperature values measured by a sensor to give an input to the controller. For example, the controlled variables in the distillation column are as follows;

i. Pressure of distillation column
ii. Liquid level of reflux tank
iii. Bottom level of distillation column
iv. Bottom Temperature of distillation column
v. Composition of product streams
vi. Continuous supply of required heat energy

Actually all the above variables are very important to control at their given set point values in order to get required product specifications. There are some strategies discussed below to control the above parameters without disturbing the operation of the distillation column.

Pressure control of distillation column

The reflux drum mounted at the top of the distillation column separates the low pressure gas from the liquid product. Now, this LP gas can be released or trapped inside the drum depending upon the situation. In general, to control the pressure of distillation column this gas is usually vented to flare. In winters, the pressure of the distillation columns gets low due to the raining, storming. In such cases, an inert gas like nitrogen can be injected before the vent line of the reflux drum to maintain the pressure of the distillation column. If the required phase of the distillate is vapor, then the condenser should be partial with controlled temperature of its cooling medium.

Temperature Control with Distillate Rate

In this strategy, the temperature controller controls the temperature of the distillation column by manipulating the distillate flow rate. In simple words, here the process variable is temperature that should be controlled to a given set point and the controller output is the input for the control valve mounted at the distillate line. Upon increasing or decreasing the flow rate of the distillate product will definitely affect the level of the reflux drum. Then the level controller of the reflux drum manipulates the opening of the valve at the reflux line. In the startup of distillation column, the column is operated initially at full reflux by closing the control valve at distillate stream. The controller at reflux drum controls the level of drum by manipulating the reflux rate to the distillation column. For startup conditions, this strategy of controlling temperature by manipulating the flow rate of distillate product is suitable where the column run at higher reflux ratio like greater than 5 or total reflux. Sometimes, the temperature controller is not tuned well for the manipulation of distillate flow rate; in such cases plant operator is contacted to do operate manually the control valve of the distillate stream.

Temperature control with Reflux rate

In this control scheme, the temperature controller of the distillation column adjusts or manipulates the control valve installed at reflux line. While the control valve at distillate stream is manipulated according to the signal coming from the level controller of the reflux drum and the column bottom level is controlled by the flow rate of the bottom product. The manipulation of reflux rate scheme is a little bit difficult for the startup conditions of the distillation column. Because in the start there is not enough light components accumulated in the reflux drum and tower temperature may get too high. In the result of this, the level of reflux drum may get very low. This problem can be handled with computer control by setting the loop at low-level constraint. This type of strategy is recommended where the reflux ratio is less than 0.8.

Temperature control by boilup rate

The reboiler at the bottom of the distillation column provides the heat energy required for the desired separation. There is a hot process stream (in some cases saturated steam can also be used) passing continuously through a reboiler to pass its heat energy to the liquid of distillation column. So, in this scheme the temperature of the distillation column is controlled by manipulating the flow rate of hot stream to the reboiler. Regarding the others control loops; the reflux drum level is controlled by the distillate flow rate and the column bottom level is controlled by manipulating the flow rate of the bottom product. This boilup scheme is an old strategy used when the feed flow rate and reflux rate is controlled with the help of manual valves and rotameters are used to measure the flow rates at the control room.

CHAPTER 2

OBJECTIVES

The objectives of this research work includes the study of four product dividing-wall distillation (kaibel) column from an operability and control point of view. The motivation of research behind the study of this particular complex configuration of distillation column is the appreciable reduction in energy consumption for a specified separation, as well as less operational cost and investment cost as compared to conventional column configuration.

Regarding the optimal operation of kaibel distillation column, the objectives consists the study of distillation column in two different modes. First, the operation of kaibel distillation column at minimum available heat energy by specifying the product purities at fixed values. After this, to operate the column with a fixed heat energy to achieve maximum product purities.

The second target is to implement a feasible control strategy to operate the kaibel distillation column economically optimal and stable in the presence of disturbances which might be occur during the operation.

CHAPTER 3

LITERATURE REVIEW

Asprion et al. (2010) studied the fundamentals of divided wall distillation column to show the potential benefits of this new technology in the field of unit operations. They also discussed the challenges in the design of divided wall column (DWC), its technical applications and the limitations of divided wall distillation column. To do this study, they presented a comprehensive comparison between simple column configuration and complex column configuration. For example, they have shown that greater number of distillation columns and heat exchangers are required in using direct, indirect or distributed column configuration for the separation of multi component mixture. While complex column configuration (side strippers, side rectifiers, fully thermally coupled distillation column and divided wall column) requires less number of column shell and heat exchangers to do the same separation. Along this, another advantage of using complex column configuration is to save energy consumption and capital investment to an appreciable extent. But the design of DWC is more challenging than a conventional distillation column. As, number of parameters required to completely specify a four product divided wall column are eighteen (18). In which six (06) operational variables, ten (10) structural design variables and two (02) control variables are included. The limitations in the use of divided wall columns are as follows; 1) only one pressure range is possible 2) column height are usually higher than the other column configuration 3) feed mixtures should be near to ideal behavior and 4) divided wall columns are avoided if reactions in the bottom lead to low boiling components and high boiling components at the top of the distillation column [16] [17].

Dejanovic et al. (2010) studied comprehensively the simulation of three and four product dividing wall column. They have shown the internal configuration of the three product dividing wall column with three different respects. One is the simple one, which contains the partition wall in the center of the distillation column. But the others configurations may contains the dividing wall in the extreme bottom or top of the distillation column. In the later configuration, the temperature difference across the DWC is higher as compared to the first configuration containing the partition wall in the middle. All positions of partition wall have their own advantages and disadvantages and used for specific purposes. More potential advantages and investment savings can be approached if the column is designed for obtaining four pure products from a mixture of feed. The reason of investment savings and potential benefits is that this arrangement will replace the three conventional columns with a single dividing wall column. Afterwards, they focused on the design and simulation of multi component dividing wall distillation column. Regarding the design approach of the DWC, the initial are similar with the design of conventional column. Further the establishing the column configuration, short-cut or comprehensive (detailed) design i.e. number of stages, reflux calculations, optimization, column sizing and design of control system is considerable different from the later one. They also have shown the fully extended petlyuk sequence for four product dividing wall column containing multiple wall partitions in it. This arrangement proved to be more energy efficient as compared to the distillation column having single partition wall. Along this, they discussed the optimization, column dimensioning and the difficulties in controllability of such distillation columns. With the success of process intensification, reactive dividing wall columns are also described. Such configurations consist of catalyst packing in the pre-fractionator part of the DWC [18].

Halvorsen et al. (2011) elaborated the concept of energy saving distillation columns configuration like divided wall column (DWC), internally heat integrated columns (HIDiC) etc. and shown the methodology to calculate minimum energy requirements distillation column internal flow distribution for a fully thermally coupled distillation column. They also shown the arrangements for fully thermally coupled distillation columns (Petlyuk column) and divided wall columns that can be used as an alternative of conventional column configuration. They used the concept of minimum energy or minimum vapor flow diagram (V_{min} diagram) to calculate the energy consumption in the distillation column. Basically, V_{min} diagram is a graph plotted between vapor rate above the feed (V/F) and net distillate flow to the top (D/F) per unit feed. All other parameters of the distillation system like component recoveries, internal flow rates and product composition can be specified against any point (D/F, V/F) of the graph. In this research study, they have shown the V_{min} diagram for three, four and five products divided wall distillation columns. The diagram looks like a mountain pattern having many peaks and valleys depending upon the numbers of components in the feed. The overall required energy can be estimated by the value of highest peak in the diagram. As, this highest peak is representing the most difficult product split occurring in the whole column. We will waste energy if the energy provided to the distillation column is excess than this peak value. Basically the vapor flow diagram (V_{min} diagram) tool is invented by Halvorsen in 2001. They also discussed a little bit research regarding control of divided wall column. Actually, drift is usually avoided to stabilize the column profile of a distillation column. For a two product divided wall column, it is easy to manipulate the reflux in order to maintain the temperature between feed stage and product stage. But for a divided wall distillation column, it is a little bit complicated and challenging to control the all the parameters. Because a four product divided wall distillation column (kaibel) have 9 dynamic degree of freedom (feed rate, distillate rate, bottom rate, side draw-1, side draw-2, reflux rate, liquid split, vapor split, vapor flow rate and condenser duty) for stabilizing the control of divided wall distillation column [19].

Ghadrdan et al. (2011) studied the kaibel distillation column from operational point of view. They studied both mode of optimal operation of kaibel distillation column in this piece of research i.e. minimizing the boilup rate or energy consumption at fixed product purities and other is to get the maximize product purities by keeping the boilup rate as constant. They formulated the objectives functions for both of the modes which based on the operational degree of freedom. The conclusion obtained from the research study was that more difficult to operate the kaibel distillation column with fixed product purities from control point of view. Here they tried to operate the column as optimum as possible but did not studied the dynamic issues of the distillation column. First they proved that the energy consumption for a four product kaibel distillation column is less than the all the arrangement i.e. direct sequence, indirect sequence, direct–indirect sequence, indirect–direct sequence and pre-fractionator configurations. They took help of V_{min} diagram to accomplish these calculations of energy consumption to get 95 % recovery of each component. Regarding the cost function, the cost function (J) is to be minimized for the mode-1 is therefore set equal to boilup rate (V). For mode-2, the cost function (J) is also to be minimized and can be equated as the sum of the impurities in the products. The feed mixture consists of first four alcohols i.e. methanol, ethanol, 1-propanol, 1-butanol. The simulation study is done in a commercial software known as “UNISIM” [20].

Dejanovic et al. (2011) studied the separation of multi component aromatic mixture through dividing wall column. They also compared the energy consumption of simple column configuration and dividing wall column for the given aromatic mixture. The “V_{min} diagram” is used as tool to design the distillation column. Actually in the petroleum refinery, benzene has to be removed as a heart cut in the platforming process. Benzene is carcinogenic component and a certain amount is allowable in the petroleum products. For this case, they studied the energy consumption, cost analysis for the four product dividing wall distillation column (kaibel distillation column). They illustrated the schematic study of two alternative configuration for kaibel distillation column i.e. one contains only one partition wall inside the column shell and other consists of multi partition in it. It has been shown that the multi partition dividing wall column (fully extended Petlyuk arrangement) is more energy efficient than other dividing wall column and simple column arrangements. They recover about 62.9 % benzene as second draw product of distillation column. The “V_{min} diagram” played a key role to find out the internal flow rates of vapor and liquid streams for all the configurations mentioned in the study. They also studied the equipment, utility and total annualized cost (TAC) for conventional sieve tray column, single partition divided wall column (“2-4”) and multi partition four product divided wall column (“2-3-4”) containing structured packing in it. It also has been shown that cost savings can be done by using single partition DWC and multi partition DWC about 40.1 % and 48.2 % respectively as compared to conventional column [21].

Ghadrdan et al. (2012) did a comprehensive research on optimal operation and control of kaibel distillation column. In this study, they designed a control structure for a four product divided wall distillation column. While the control structure based on plant wide procedure, developed by Skogestad (2000). They presented the approach of self-optimizing control for optimal control the parameters for four product divided wall distillation column. The basic concept behind self-optimizing control is to fix a parameter or variable which can defines the optimum operation of the column and the optimum value of this variable should be very less sensitive to variations in disturbance as compared to the others degrees of freedom. Here, they used different process simulation software (MATLAB and UNISIM) to operate the four product divided wall distillation column at its optimum value. As it is also reviewed in the previous literature review that there are two approaches to run the distillation column at its optimum value; one is to specify the product purities and manipulate the other degree of freedom to minimize the boil up rate, which is the motivation of using thermally coupled distillation column. The second approach is to fix the column boil up rate at and get the product specification as much as possible. The later approach is used when the energy is very cheap and the operational cost of the process is not considerably increasing by the energy consumption. But here they studied the second approach for the optimal operation of distillation column [22].

Dwivedi et al. (2013) illustrated the detail study of the control structure for four product extended Petlyuk distillation column. The components of the feed mixture required to be separate have almost similar relative volatilities like methanol, ethanol, propanol and n-butanol. They reported about 50 % of energy savings in using extended Petlyuk configuration distillation column as compared to direct and indirect conventional column configuration. They assumed that there is ten degree of freedom available for the optimal control of composition. The three vapor split valves are considered as manipulated variables. Again, here “V_{min} diagram” is used to find out the energy required to separate the most difficult binary split. In this research study, they presented four decentralized control structures and then described their performance regarding control. These control structures are studied for a wide range of disturbances variables like feed flow rate, composition fluctuations and vapor fractions in it. As a whole, the extended Petlyuk column can be viewed as seven sub columns. For the first control structure (CS1), they set the basic 2 point LV structure on each sub column. In this control structure, the reflux controls the amount of key impurity in the top and vapor controls the key impurity in the bottom. The second control structure (CS2) is almost similar to the first one except it involves the reboiler loop also in it. The third control structure (CS3) employs the temperature data to find out the composition there. The last and fourth control structure is just the modification of the third one. Along this, they have shown different result of all the control structures when a disturbance comes in the feed. The SIMC (Simple / Skogestad internal tuning rules) tuning rules are used to do tuning of decentralized control structures [23].

Khanam et al. (2014) studied the optimal operation and control of three product divided wall column. Different researchers studied the optimal operation of divided wall column with different objectives and constraints. In this study, they discussed possible modes for optimal operation of DWC keeping the energy consumption as an objective. Also, they studied self-Optimizing control structure for three product divided wall column. The research study consists of the number of assumptions like equilibrium stages, constant relative volatilities, constant pressure, constant molar flow throughout the column, total condenser and linearized flow dynamics. The feed is considered here as disturbance, then they have left five steady state degree of freedom i.e. vapor flow rate (V), side stream flow rate (S), reflux rate (R), liquid split (R_L) and vapor split (R_V). The main four constraints are to achieve the desired product purities of all the three products and to keep the energy consumption as low as possible. As we have two different modes of operation of column i.e. Mode-I and Mode-II and four different constraints. So, they have shown that the optimal operation of three product divided wall column is possible in sixteen ($2^4=16$) different ways. In the mode-I, the objective is to minimize the energy requirements for all the given constraints. This mode will be optimal, when all the three product purities are active to give maximum product and the available energy is expensive. If the energy is expensive but the three products purities are not active constraints then the operation is done to minimize the impurities and energy. The second mode will be known as optimal when the energy is cheap and we operate the column with maximum supply of energy to get the maximum product purities. This mode is used when the product of purity is much important and energy price is cheap. Here, the price of the product is directly related with its purity. By applying the self-optimizing control structure, they have shown that regulatory control layer of the distillation column is same as the economic self-optimizing control layer [24].

Kvernland et al. (2010) studied the control of four product kaibel distillation column by model predictive control (MPC). The advantages of kaibel distillation column have been discussed above by energy consumption point of view. As distillation operation is multivariable process so, it offers a multivariable control problem. This is why, the control of four product divided wall distillation (Kaibel) column offers some challenges and energy consumption cannot be achieved if the distillation column is not operated near its optimal operating conditions. Model predictive control basically gives the optimal inputs to the system with the help of mathematical optimization which based on the mathematical model of the system (process). The process model taken is a pilot plant of four product divided wall distillation column built at Department of Chemical Engineering, NTNU. The feed mixture contains methanol, ethanol, 1-propanol, and 1-butanol. They took distillate rate (D), bottom product rate (B), side stream-1 rate (S_1), side stream-2 rate (S_2), reflux rate (L) and liquid split (R_L) as manipulated variables. While the composition of methanol, ethanol, 1-propanol in the feed, feed condition, feed flow rate, column vapor flow rate and vapor split (R_V) are considered as disturbance variables. The level of condenser and reboiler are controlled by the flow rate of top and bottom product streams respectively. These manipulated variables are controlled at a particular set point by the PI-controllers. The remaining manipulated variables (input) are adjusted to control the temperature. They developed two different configuration or MPCs; a single layer model predictive control that is responsible for controlling the process inputs and second is supervisory MPC which controls the set points of decentralized control layer. The simulations are done in MATLAB by employing MPC Toolbox in the Simulink library. They also conclude that MPC strategy get successful to achieve less impurity flow in the presence of disturbance and avoid the interactions in the process as compared to decentralized controller [25].

Kim et al. (2014) studied the application of divided wall column in offshore floating LNG plant. As the offshore process plants require compactness in equipment design and optimal operation due to the harsh environment conditions. They got decrease in heating duty as well as cooling duty up to 35 % and 18% respectively by using divided wall distillation column as compared to conventional distillation arrangement. Also, the utility cost also has been reduced up to 16 % by using proposed design of DWC. The raw natural gas is charged as feed to the distillation column. This gas contains minute amount of liquid i.e. oil, water etc. which is separated in the pre-treatment units [26].

Wolff et al. (1995) studied the operation and control of integrated three product distillation column. Almost half a century ago, Wright (1949) presented a consolidating design of a distillation column for separating mixture consisting of three components known as ternary feed. His design contains a simple column shell having feed and giving side streams (products). But the column consists of a vertical wall having appropriate dimensions and it divides the column into two sections. The vertical wall inside the column shell works as a prefractionator. This design gives savings in capital cost, energy requirement as well as operating cost as compared to the simple distillation column configuration. This structure is generally known as Petlyuk column after the name of Petlyuk et al. (1965). Many researchers worked on the design of such columns but research in the field of operation and control of such columns were not studied very much. The reason behind the limited installation of such columns in industries is the greater degree of freedoms than an ordinary distillation column and a little bit difficult design and control. In this research work, they have shown the dynamic behavior of a Petlyuk distillation column and suggested feasible controller structure. But the result reveals us that there exist serious difficulties regarding the steady-state behavior which are going to offer problems in practical operation [27].

Strandberg et al. (2006) studied the separation of four components by utilizing fully thermally coupled distillation column (FTCDS). Their objective was to save considerably degree of cost as compared to conventional configuration of columns. Actually Kaibel column was introduced in 1987 (Kaibel, 1987) which gives four products from a single column shell and utilizes only a single re-boiler and condenser and the kaibel column is the extended form of petlyuk column. This column also has a potential to save enormous amount of energy. One of the leading industrial company BASF, have operated first kaibel column (Kaibel et al., 2004) successfully many years ago. In this research work, they have successfully shown the control loops for the stabilized operation of column and manipulated degree of freedom also in order to run the distillation column at optimal value. After that the results of different control scheme are compared obtained from dynamic simulations. Along this, the system was tested by giving disturbances and some set point changes also [28].

Ghadrdan et al. (2013) studied the effect of manipulation of vapour split in the kaibel column on energy and cost savings. In this piece of work, they researched two different approaches: First they used a very helpful tool known as V_{min} diagram to estimate the effect of vapor split on the energy consumption. Secondly, they compared the results with the rigorous simulation using UNISIM software. At the end they have shown that on line manipulation of the vapor split is necessary to maintain minimum energy operation in the presence of feed property fluctuations [29].

In another research paper Ghadrdan and her team used a shortcut method to design a four product divided wall column. They studied the profile of four components which are methanol, ethanol, 1-propanol and 1-butanol. They also first sketched the Vmin diagram for the components discussed. Because Vmin diagram give guess about the impurities in the product. For example, the highest peak in the diagram tells us the component that might be come as unwanted component in the product during the normal operation. They also calculated the minimum flowrates through all parts of the column. Underwood equation helped out to calculate minimum number of plates. And Fenske equation is utilized to calculate plates in section between two side streams. In short, very helpful work done to minimize energy requirements in the kaibel distillation column for four components [30].

As discussed above about the utilization of V_{min} diagram, Skogested and his team members done an extensive work in this field. In this research work, they also do their best effort to show the practical prove of minimization of energy in using kaibel distillation column. Actually V_{min} diagram is introduced by Halvorsen and this technique is best to execute the performance of a kaibel distillation column. Here, they showed the energy saving of 33% as compared to simple column configuration (direct sequence) for a mixture of four components having relative volatilities of 6:4:2:1. They elaborate the simplicity of finding analytical expressions for minimum energy of the kaibel distillation column [31] [32].

Kumari et al. (2014) objectives of their work was to show the difficulties in the development of a control strategy which are able to handle effectively number of disturbances, while the purities of all the products are maintained at their target values with reduced reboiler duty. The focus of the research work is on the design of control strategy for optimal operation of the column which already exists. The results of closed loop dynamics are shown to quantify the reboiler duty reduction benefit [33].

Ghadrdan et al. (2010) studied the operation of thermally coupled kaibel distillation column with the help of process simulation software i.e. HYSYS. They studied and compared the results of two steady state simulation case with the following objectives; first simulation is converged with the objective of constant product purities at minimum vapor flow rate (boil up rate) and second simulation is studied under fixed boil up rate with maximum product purities. This research study is very helpful for the column control structure design and it's inside behavior. The values of minimum flow rates and other necessary data for the simulation is obtained from the V_{min} diagram. In the first case, the vapor and liquid splits are manipulated against the boil up rate. The minimum boil up rate (V) of 157.77 (Kmole/hr) was chosen at liquid & vapor split values of 0.41 and 0.623, respectively. [34]

Rewagad et al. (2012) studied the dynamic optimization and advanced control of DWC based on model predictive control (MPC). In addition to control loops typically found in distillation systems, an extra optimization loop for controlling the heavy component in the top of the feed side of the column is added. Implicit energy minimization is achieved in this loop by using the liquid split as its manipulated variable. The techniques proposed as applied to separation of the mixture benzene–toluene–xylene (BTX) in a DWC and the results are compared with those contained in literature for the same application.

As a means of stating the motivation for this work, the paper makes a brief and critical review of advanced control techniques on DWC of the few works that are found in literature. It states that of these works, MPC is the only one with a significant industrial impact because of the advantages associated with the technique, which include good handling of multivariable control problems while taking actuator constraints into account and providing robust optimization procedure even with input and output constraints. Other advantages include simultaneously taking the effect of all manipulated variables on controlled variables and allowing ample online computation time. This is desirable especially in industrial applications where control update rates are low. Therefore, the application of MPC to DWC can possibly augment the benefits of both systems in terms of process stability, improved and optimal performance.

In this study, MPC and the best multi-loop PID control strategy on a BTX separation system are compared. The internal prediction model used by MPC is derived from the linearization of the nonlinear distillation model rather than from step-response experiments because the former yields a more accurate representation of system states. A description of MPC is given and then adapted to the derived DWC model. MATLAB-MPC toolbox was used to simulate the adaptation.

Sensitivity analysis of the MPC model was carried out. This was done by performing open loop simulations on the linear model where disturbances are applied to it in order to determine the optimal values of its characteristic variables that correspond to minimum energy requirements and to characterize the quality of linearized prediction model with respect to the nonlinear model. In doing this, a V_{min} (minimum vapor flow based on underwood Eqs.) diagram was plotted with the help of simulation software. Controller tuning – using trial and error method for the MPC and direct synthesis method for the PID – were also done. Dynamic simulations were done on the model controlled by MPC, PID and MPC + PID, where the dynamic responses were tested for regulatory and inventory control, and stability.

Based on results obtained from the methodology of this work, it was concluded that overall, for DWC, MPC gives a remarkable, industrial-grade performance in disturbance handling and set point tracking in the presence or absence of measurement noise. It was also found that the combined MPC and PID control configuration gives a similar performance to use only the MPC, and therefore, in practice, either of the methods could be used to achieve a similar control goal [35].

Serra et al. (1999) objective of this work is to extend feedback diagonal control strategies in literature to DWC control design in detail. The impact of optimizing the energy usage of a DWC on its controllability is also studied. The boilup flow rate is taken as objective function and its minimization is considered to be energy optimization of the DWC with a fixed number of trays.

The concept of DWC is introduced and reasons for its lower energy consumption when compared with conventional distillation arrangements for ternary separations are stated. These reasons are its thermal coupling and also, only one component is distilled out in each section of the DWC. A literature review of works based on decentralized feedback control of DWC is presented, stating the work done and conclusion reached in each work. Based on the results from these works, it was inferred that feedback control of the DWC appears practicable and the decentralized feedback control was to be investigated here. The principal objective of the paper is to consider all the possible control configurations for a DWC given its complexity and compare them using a simulations and frequency-dependent analysis of the transfer functions. This comparison was carried out for both optimal and non-optimal operation in order to study the effect of the energy optimization on the controllability of a DWC.

Using assumptions from literature that allow ease of modeling but do not significantly impair accuracy, a non-linear symmetric DWC was modeled. This model was implemented in MATLAB and SIMULINK, and the “Ode15” function was used to solve differential equations. Numerical linearization was applied to the non-linear model to obtain a linear model and a transfer function was obtained by applying step inputs. The linear model obtained had 120 states and a model reduction was carried out to get a model of 16 states whose frequency response can be satisfactorily approximated to model with 120 states.

Using the resulting model and stated required specifications, two cases were studied – non-optimal operation and optimal operation. For non-optimal operation, nominal values of control input variables that fulfill required specifications were obtained. These control input variables that characterize the system include Reflux rate (kmol/min), Boilup (kmol/min), Distillate flow rate (kmol/min), Bottoms flow rate (kmol/min), and Side stream flow rate (kmol/min). In the second case, the optimal nominal operation characteristics are found. Here, using perfect control in the condenser and reboiler, the steady state operation with minimum boilup flow rate is obtained. It is found that the boilup flow rate of the optimal nominal operation is 25% lower than the boilup flow rate of the non-optimal nominal operation.

The paper goes on to present an inventory control of the column which is reduced to the control of the tank liquid levels. Different inventory control structures were proposed – proportional controllers were often used because only a maximum-minimum type control is often required. For each of the inventory control structures, an analysis of the composition control structures was developed using Single Value Decomposition (SVD) and Relative Gain Array (RGA). The method of tuning of these controllers is also presented.

Separation control was then analyzed over the stabilized DWC and some optimization control aspects were considered. The optimization control problem was defined as how to know the values of the manipulated variables which bring the process to optimal operation in the presence of disturbances from the optimal operating conditions. After mentioning several techniques proposed in literature, the self-optimizing control technique was adopted and shown to be having a good behavior in the presence of step disturbances. The authors however state that further work should be done to obtain a control structure capable of handling all possible disturbances and sources of uncertainty.

In summary, this work uses SVD, RGA, frequency analysis and other tools for linear control analysis and simulations to compare various control configurations for DWC under performance and robustness considerations. It was concluded that self-optimizing control presents a good control behavior for DWC and that a compromise must be reached between energy efficiency and control efficiency of the DWC. The work also states the need for further work in order to find the best control strategy for a DWC in different operating conditions [36].

CHAPTER 4

DESIGN OF DIVIDED WALL DISTILLATION COLUMN

The most commonly used unit operation in the chemical process industry for the thermal separation of the liquid mixture is “distillation”. Despite of its widespread applications and advantages, it has one important drawback of utilizing excess amount of energy. It is also estimated that operational cost of a distillation plant consists of about 50 % of energy cost provided to the distillation column (Taylor and Kooijman, 2003). We can adjust the requirement of energy by manipulating the different design parameters of distillation column. For example, total number of actual trays, location of feed tray, identification of side draw location, number of pump around provided to the distillation column, reflux ratio and column diameter etc. are the most important key parameters in the designing of column. Which are adjusted in an allowable limit to get the required product specification and other factors. This is why, design of any distillation column is very important to get the required result. If distillation column is not properly designed than the results will be in the form of low product purity (useless product can also come), high energy consumption and some other process safety issues.

The design of distillation column is a little bit complex as compared to the other unit operations equipment. As the design variables are greater than any other equipment like operating pressure of the column, total number of stages, location of feed tray, reboiler duty, composition of the products, reflux ratio and many more. Regardless of the design complexities, many effective heuristic methods have been developed to give the optimal design. Here, we are more concerned with the design of divided wall distillation column by different effective methods. Presence of a partition wall inside the column shell of divided wall distillation column made the designing of divided wall column more difficult and complex as compared to simple distillation column. Because the number of design parameters in case of DWC got increased and we need more variables to completely specify the system. It is important to mention that DWC may contain two or more than two partition wall to achieve the requirements. They are more complex columns and need more attention and care to study. The wall configuration varies for tray and packed column distillation column. The construction of a tray divided wall column is easier than the packed column. As in the case of tray column, the divided wall is welded inside the column that gives more stability to the column shell.

4.1 Design of Divided-Wall Distillation Column

BASF, Germany was the first chemical company to introduce the valuable technology of divided wall column to reduce energy requirements of the distillation operation. Till 1999, no one have enough information and technical aspects related to the design and construction of DWC except BASF. But after a year or so, divided wall distillation column was also built for the first time outside the BASF. That was a tray distillation column and installed in a chemical plant in South Africa. The objective of this DWC was to recover valuable petrochemicals from Fischer-Tropsch synthesis products. This gave attractive recovery and the dimension of the column was also very feasible. This practical example became the attraction of other chemical companies and research centers. It was also tested for other feed and results were published by many researchers in the past decade. In 2004, Petlyuk reached to the following conclusions after comprehensive analysis of distillation column having a partition wall inside the column shell;

i. In each section of distillation column, the components having extreme volatilities (i.e. the heavier one and lighter one) will be taken as key components.
ii. Regardless of the number of products, only a single reboiler and condenser are enough to get the required specifications.
iii. High purity can be achieved for all products.
iv. Capital investment and operations cost can be reduced to a great extent.

The optimal design of divided wall distillation column needs suitable models and process simulation to be done with the help of commercial simulator. But these simulation software do not have sub details of divided wall distillation columns. A decomposition method developed by Smith and Triantafyllou in 1992 resolves the design problem to some extent. In the literature, the mostly discussed design methods of DWCs are of just three products. However, it can be extended to four or more products. But for more four products degree of freedom of the column will be higher as compared to simple four product distillation column.

4.2 Heuristic Rules of Divided-Wall Distillation Column Design

The design of divided wall distillation column requires accurate initial guess of design parameters and some guidance to obtain converged simulation. The following are some heuristics points to get good initial values for short-cut and other process simulations. These rules are proposed by Kreis, Godorr and Becker in 2001.

i. Design a base case of conventional two product distillation column system (e.g. Indirect / direct or distributed sequence).
ii. Find out the total number of trays for divided wall column, as 80% of the total number of stages in the conventional distillation column are required in the divided wall column sequence: NDWC = 0.8*(N1+N2+N3).
iii. Install a partition or dividing wall in the middle third of the distillation column e.g., 33-66% of height of distillation column.
iv. Estimate the internal vapor and liquid flow rates inside the divided wall distillation column from the reboiler and condenser heat duties.
v. Take both the liquid and vapor splits as 0.5, just for initial guess.

CHAPTER 5

OPTIMAL OPERATION OF FOUR PRODUCT DIVIDED WALL (KAIBEL) DISTILLATION COLUMN

The core objective of any distillation column is to separate a given feed mixture into its respective fractions which satisfy the customer requirements and other environmental regulations. But this will not be a core objective, if the required product specifications are obtained while the distillation unit is running at financial loss. After this, two other goals emerges – first is that the operation of distillation unit should be profitable and secondly it should be capable of giving the required product specifications. For the sake of general estimate, number of steady-state simulations have been done in order to get specific set of conditions which are satisfied by the column operation. As the simulation is a helpful tool for analyzing the operating efficiency of distillation process as well as the initial estimated required for the design. Distillation column simulation can be steady state (time independent) or dynamic simulation (time dependent). Actually steady-state simulation are done to study the energy consumptions in different schemes, like the trends of heat exchange from one unit to another or fractionation efficiency. But here, the focus was to study the operation of complex distillation column i.e. DWC rather than simple distillation column. The enormous advantages like capital saving, appreciable reduction in energy consumption of dividing-wall distillation columns for the separation of multi-components are the key reason for industrial implementation. Here, first of all some key results published by the some researchers regarding the operation of dividing-wall distillation column are presented. For example, dividing wall distillation columns are best especially for mixtures having three or more components and also where the middle components are in the higher concentration (Olujic and Dejanovic, 2010). But when the composition of heaviest component is the highest in the given feed then thermally coupled distillation columns are not suitable according to Emtir et al. (2001) and Mizsey et al. (1998). After a comprehensive research, it has been shown that energy savings is very dependent to the composition of feed. On the other hand, Suphanita et al. (2007) have shown that if heat transfer is there across the partition wall of the column then the operation of dividing-wall distillation column can be improved.

However, we have to sacrifice some parameters in front of the advantages of dividing wall columns like a little bit tough optimal control and difficult operation of distillation columns as compared to conventional distillation column configurations (Harmsen, 2010). Actually controllability factor is very important because this property has disturbance rejection capability and leads the system to new admissible operating conditions (Luyben, 1997). This is why, best control structure design is very important for achieving optimal operation of dividing wall distillation column. Due to the thermal coupling of pre-fractionator and main distillation column, the degrees of freedom becomes greater than as compared to other simple arrangements.

When the optimal operation is objective then it is usually considered that the product purities should be achieved as required and energy consumed should be minimum as possible. Operation of DWC can be studied under two different modes as follows;

i. To achieve the defined product purities by providing minimum energy
ii. To achieve the maximum product purities with a fixed available energy value

The requirement of first mode is to specify all the required product purities and it should be obtained at minimum available energy. While in the second mode the available energy should be specified and maximum product purities should be obtained at this available energy. To study the optimal operation of divided wall distillation column, three different case studies were simulated in steady-state way. The first case study consists of a feed mixture of first four alcohol. The second case study consists of a mixture of first eight hydrocarbons as a feed and need to be separate as some valuable products like LPG etc. while the last case study is related to an aromatic stream exiting from an oil refinery plant and also needs to be separate to give some valuable products like benzene, toluene etc. Before going towards the steady-state simulation, it is very necessary to obtain the optimal parameters for the accurate convergence of distillation column. This is why, some graphs are plotted to get an estimate or choose optimal values of operational parameters. For example, effect of liquid and vapor split ratio on reboiler duty, product composition etc., as shown in figures below.

As described above that the excess number of operational degree of freedom in case of dividing wall distillation column are liquid and vapor split ratio (R_L & R_V, respectively), which should be used in an energy efficient way for optimal operation of column. It is very important to proper suggest these values along with the many others parameters. Because only the optimal values of these variables will gives us the required product purities at minimum energy consumption.

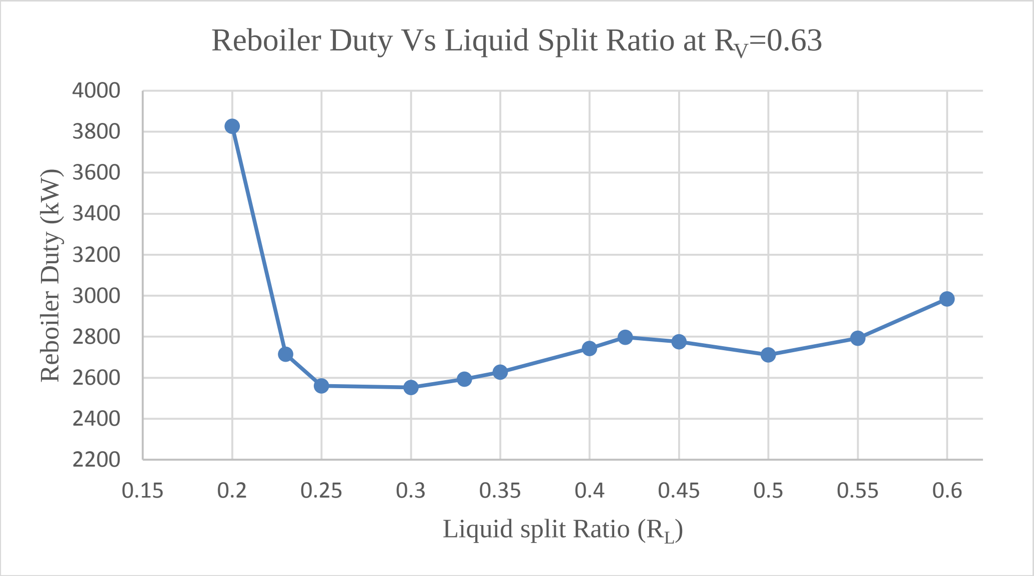


Figure 12: Effect of liquid split ratio on reboiler duty

As shown in the above graph, energy consumption is almost decreasing with the increase of liquid split ratio at fixed vapor split ratio of 0.63. Now we have to select one optimal value of liquid split ratio at which the required product purities can be achieved. After trying all the values of liquid split ratio, it has been observed that "0.42" will be the optimal value for alcohol case. It may be noted from the above graph that values ranging from 0.25 – 0.40 are employing less amount of energy, but they are not providing the required product specifications. Also it may happens that minimum energy requirements for optimal operation gets change due to disturbance in the feed composition or in the product purity targets. Regardless of the normal disturbances in the column operation, liquid split ratio can be controlled or manipulated for ensuring that energy savings is there. Similarly, the effect of liquid split ratio on product composition also can be seen in below Figure 13.

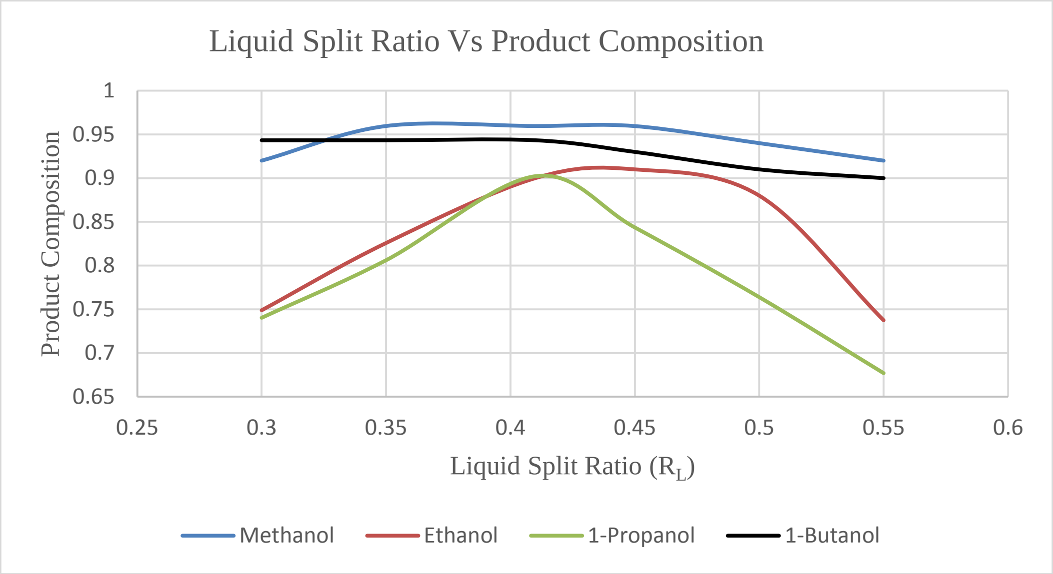


Figure 13: Effect of liquid split ratio on product composition

It is now clear that with the manipulation of liquid split ratio, product composition are also get disturbed especially the side draw products. The graph was plotted by keeping the vapor split ratio at a constant value of 0.63. These are some parameters which cannot be manipulated online in an industrial plant. This is why, all the parameters for the below case studies are determined and then simulation is done under optimal variables.

Similarly, the effect of vapor split ratio (R_V) on product composition is also studied for alcohol case. The graph trends are shown in the below Figure 14. It may be noted that at low values of vapor split ratio, the product specifications are not acceptable. The compositions of side draw products are very sensitive to manipulation of vapor split ratio as compared to top and bottom product composition.

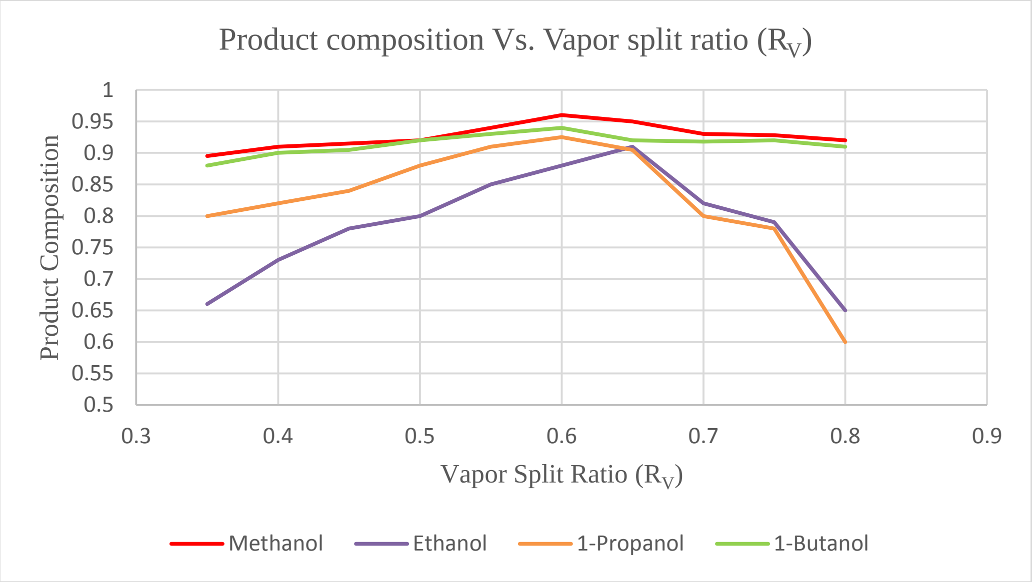


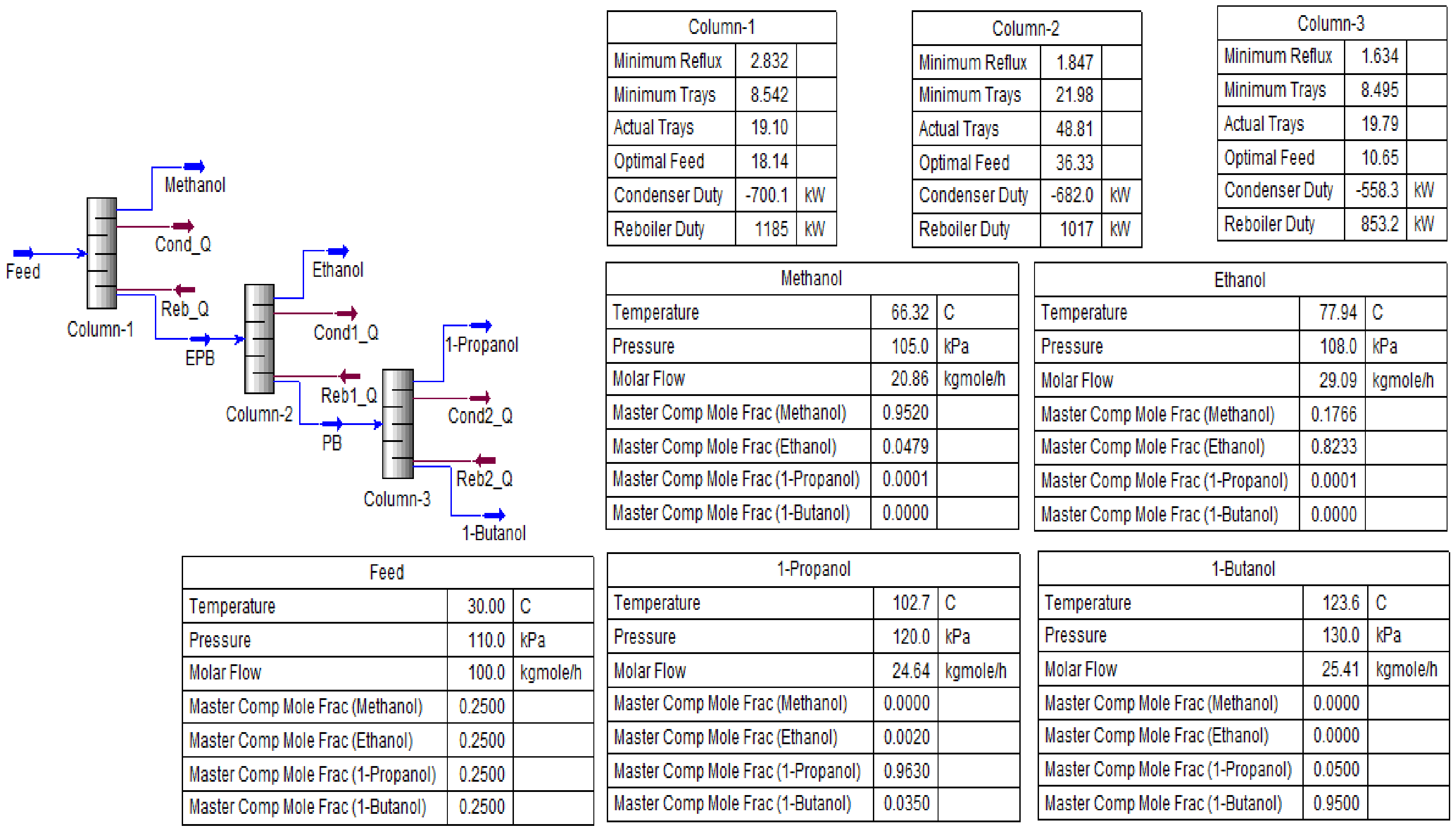
Figure 14: Effect of vapor split ratio on product composition

The above figure is plotted at a fixed value of liquid split ratio to study the behavior of product composition with the manipulation of vapor split ratio. An optimum value of vapor split ratio around 0.63 can be taken to specify in the simulation. Because at particular this value of vapor split ratio, desired product specifications at minimum supplied energy can be achieved.

5.1 Alcohol Mixture as Feed

In the very first case study, the problem is to separate the alcohol mixture into its respective components by using distillation technique. The process simulation software i.e. Aspen HYSYS was used to accomplish the task of steady-state simulations. The dividing wall distillation column was used to reduce the energy consumption and to get almost pure products. Our feed consists of four equimolar components i.e. methanol, ethanol, 1-propanol and 1-butanol [37]. Just for comparison, four different possible arrangements of distillation columns having the same feed conditions are simulated and shown below. For example, Figures 15, 16 and 17 are showing the direct, indirect and distributed sequence of distillation columns respectively. The reboiler duty required for achieving the required product purities and other necessary results are also shown in the snapshot of simulation window. The thermodynamic model used to converge the simulation is Wilson equations or model.

Figure 18 is showing the simulation result of four product kaibel distillation column and Figure 19 is showing the column environment made under the distillation column in HYSYS. The initial estimates (feed tray location, number of theoretical stages, minimum reflux ratio etc.) to converge this simulation is taken from the simulation result of distributed sequence. Four product dividing wall distillation column (Kaibel) is also converged in another possible way as shown in Figure 23. The available symbol of simple distillation column is used for the simulation of divided wall distillation column (DWC). As there is no available equipment tool present for DWC in the object palette of Aspen HYSYS. But it can be simulated in different ways as shown below in the figures.



Column-1		
Minimum Reflux	2.832	
Minimum Trays	8.542	
Actual Trays	19.10	
Optimal Feed	18.14	
Condenser Duty	-700.1	kW
Reboiler Duty	1185	kW

Column-2		
Minimum Reflux	1.847	
Minimum Trays	21.98	
Actual Trays	48.81	
Optimal Feed	36.33	
Condenser Duty	-682.0	kW
Reboiler Duty	1017	kW

Column-3		
Minimum Reflux	1.634	
Minimum Trays	8.495	
Actual Trays	19.79	
Optimal Feed	10.65	
Condenser Duty	-558.3	kW
Reboiler Duty	853.2	kW

Feed		
Temperature	30.00	C
Pressure	110.0	kPa
Molar Flow	100.0	kgmole/h
Master Comp Mole Frac (Methanol)	0.2500	
Master Comp Mole Frac (Ethanol)	0.2500	
Master Comp Mole Frac (1-Propanol)	0.2500	
Master Comp Mole Frac (1-Butanol)	0.2500	

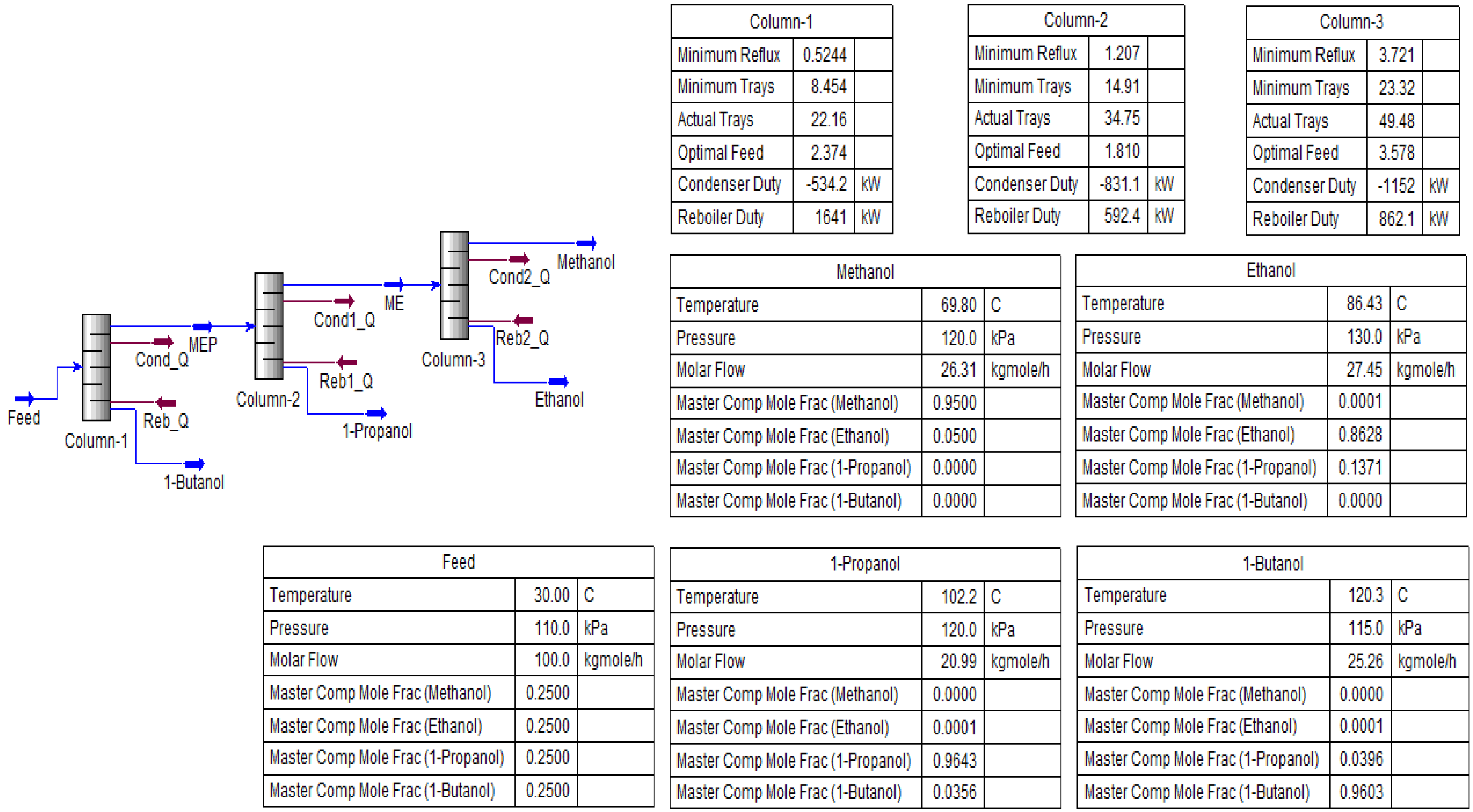
Methanol		
Temperature	66.32	C
Pressure	105.0	kPa
Molar Flow	20.86	kgmole/h
Master Comp Mole Frac (Methanol)	0.9520	
Master Comp Mole Frac (Ethanol)	0.0479	
Master Comp Mole Frac (1-Propanol)	0.0001	
Master Comp Mole Frac (1-Butanol)	0.0000	

Ethanol		
Temperature	77.94	C
Pressure	108.0	kPa
Molar Flow	29.09	kgmole/h
Master Comp Mole Frac (Methanol)	0.1766	
Master Comp Mole Frac (Ethanol)	0.8233	
Master Comp Mole Frac (1-Propanol)	0.0001	
Master Comp Mole Frac (1-Butanol)	0.0000	

1-Propanol		
Temperature	102.7	C
Pressure	120.0	kPa
Molar Flow	24.64	kgmole/h
Master Comp Mole Frac (Methanol)	0.0000	
Master Comp Mole Frac (Ethanol)	0.0020	
Master Comp Mole Frac (1-Propanol)	0.9630	
Master Comp Mole Frac (1-Butanol)	0.0350	

1-Butanol		
Temperature	123.6	C
Pressure	130.0	kPa
Molar Flow	25.41	kgmole/h
Master Comp Mole Frac (Methanol)	0.0000	
Master Comp Mole Frac (Ethanol)	0.0000	
Master Comp Mole Frac (1-Propanol)	0.0500	
Master Comp Mole Frac (1-Butanol)	0.9500	

Figure 15: Direct Sequence for Distillation Columns



Column-1		
Minimum Reflux	0.5244	
Minimum Trays	8.454	
Actual Trays	22.16	
Optimal Feed	2.374	
Condenser Duty	-534.2	kW
Reboiler Duty	1641	kW

Column-2		
Minimum Reflux	1.207	
Minimum Trays	14.91	
Actual Trays	34.75	
Optimal Feed	1.810	
Condenser Duty	-831.1	kW
Reboiler Duty	592.4	kW

Column-3		
Minimum Reflux	3.721	
Minimum Trays	23.32	
Actual Trays	49.48	
Optimal Feed	3.578	
Condenser Duty	-1152	kW
Reboiler Duty	862.1	kW

Methanol		
Temperature	69.80	C
Pressure	120.0	kPa
Molar Flow	26.31	kgmole/h
Master Comp Mole Frac (Methanol)	0.9500	
Master Comp Mole Frac (Ethanol)	0.0500	
Master Comp Mole Frac (1-Propanol)	0.0000	
Master Comp Mole Frac (1-Butanol)	0.0000	

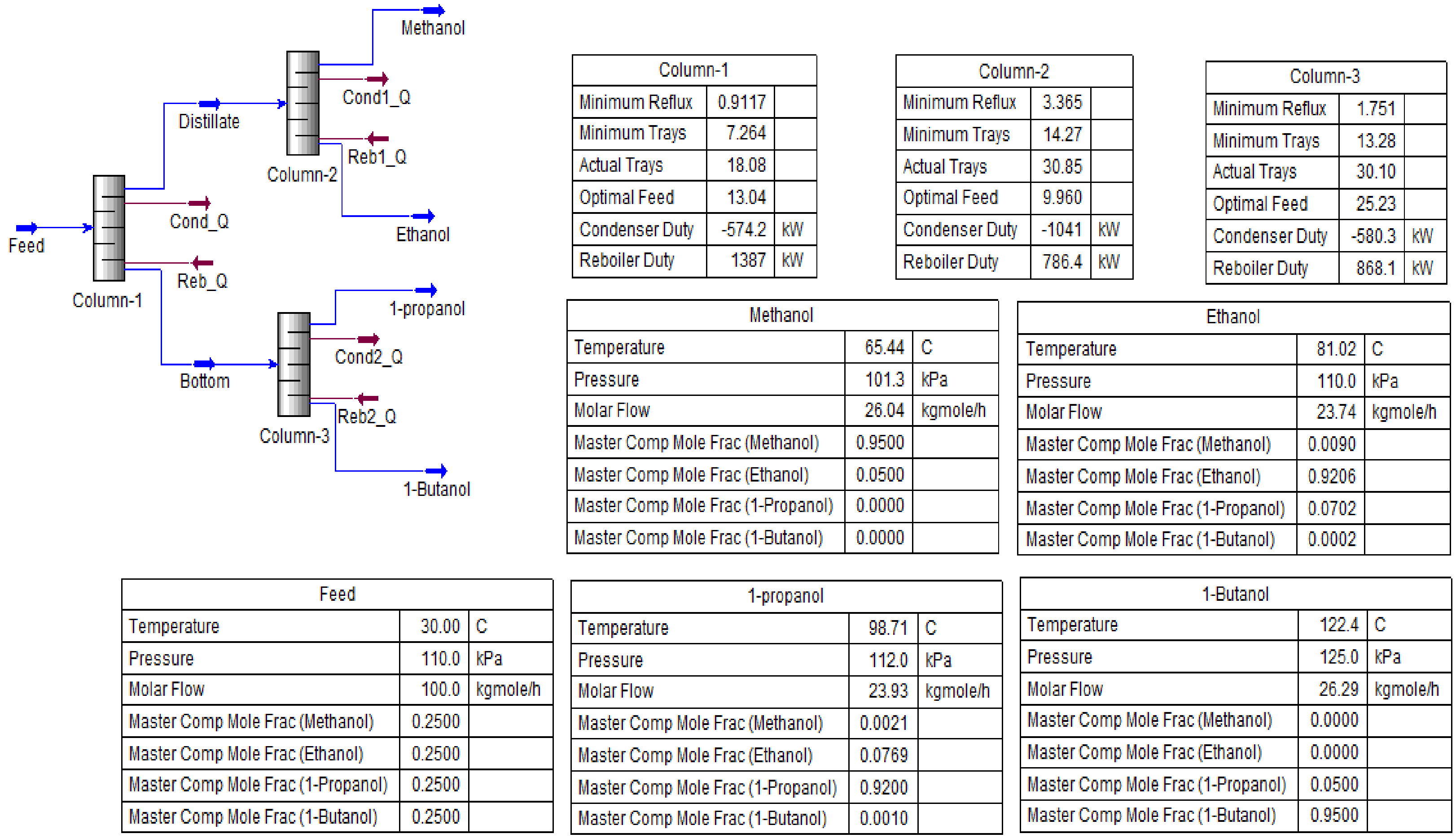
Ethanol		
Temperature	86.43	C
Pressure	130.0	kPa
Molar Flow	27.45	kgmole/h
Master Comp Mole Frac (Methanol)	0.0001	
Master Comp Mole Frac (Ethanol)	0.8628	
Master Comp Mole Frac (1-Propanol)	0.1371	
Master Comp Mole Frac (1-Butanol)	0.0000	

Feed		
Temperature	30.00	C
Pressure	110.0	kPa
Molar Flow	100.0	kgmole/h
Master Comp Mole Frac (Methanol)	0.2500	
Master Comp Mole Frac (Ethanol)	0.2500	
Master Comp Mole Frac (1-Propanol)	0.2500	
Master Comp Mole Frac (1-Butanol)	0.2500	

1-Propanol		
Temperature	102.2	C
Pressure	120.0	kPa
Molar Flow	20.99	kgmole/h
Master Comp Mole Frac (Methanol)	0.0000	
Master Comp Mole Frac (Ethanol)	0.0001	
Master Comp Mole Frac (1-Propanol)	0.9643	
Master Comp Mole Frac (1-Butanol)	0.0356	

1-Butanol		
Temperature	120.3	C
Pressure	115.0	kPa
Molar Flow	25.26	kgmole/h
Master Comp Mole Frac (Methanol)	0.0000	
Master Comp Mole Frac (Ethanol)	0.0001	
Master Comp Mole Frac (1-Propanol)	0.0396	
Master Comp Mole Frac (1-Butanol)	0.9603	

Figure 16: Indirect Sequence for Distillation Columns



Column-1		
Minimum Reflux	0.9117	
Minimum Trays	7.264	
Actual Trays	18.08	
Optimal Feed	13.04	
Condenser Duty	-574.2	kW
Reboiler Duty	1387	kW

Column-2		
Minimum Reflux	3.365	
Minimum Trays	14.27	
Actual Trays	30.85	
Optimal Feed	9.960	
Condenser Duty	-1041	kW
Reboiler Duty	786.4	kW

Column-3		
Minimum Reflux	1.751	
Minimum Trays	13.28	
Actual Trays	30.10	
Optimal Feed	25.23	
Condenser Duty	-580.3	kW
Reboiler Duty	868.1	kW

Methanol		
Temperature	65.44	C
Pressure	101.3	kPa
Molar Flow	26.04	kgmole/h
Master Comp Mole Frac (Methanol)	0.9500	
Master Comp Mole Frac (Ethanol)	0.0500	
Master Comp Mole Frac (1-Propanol)	0.0000	
Master Comp Mole Frac (1-Butanol)	0.0000	

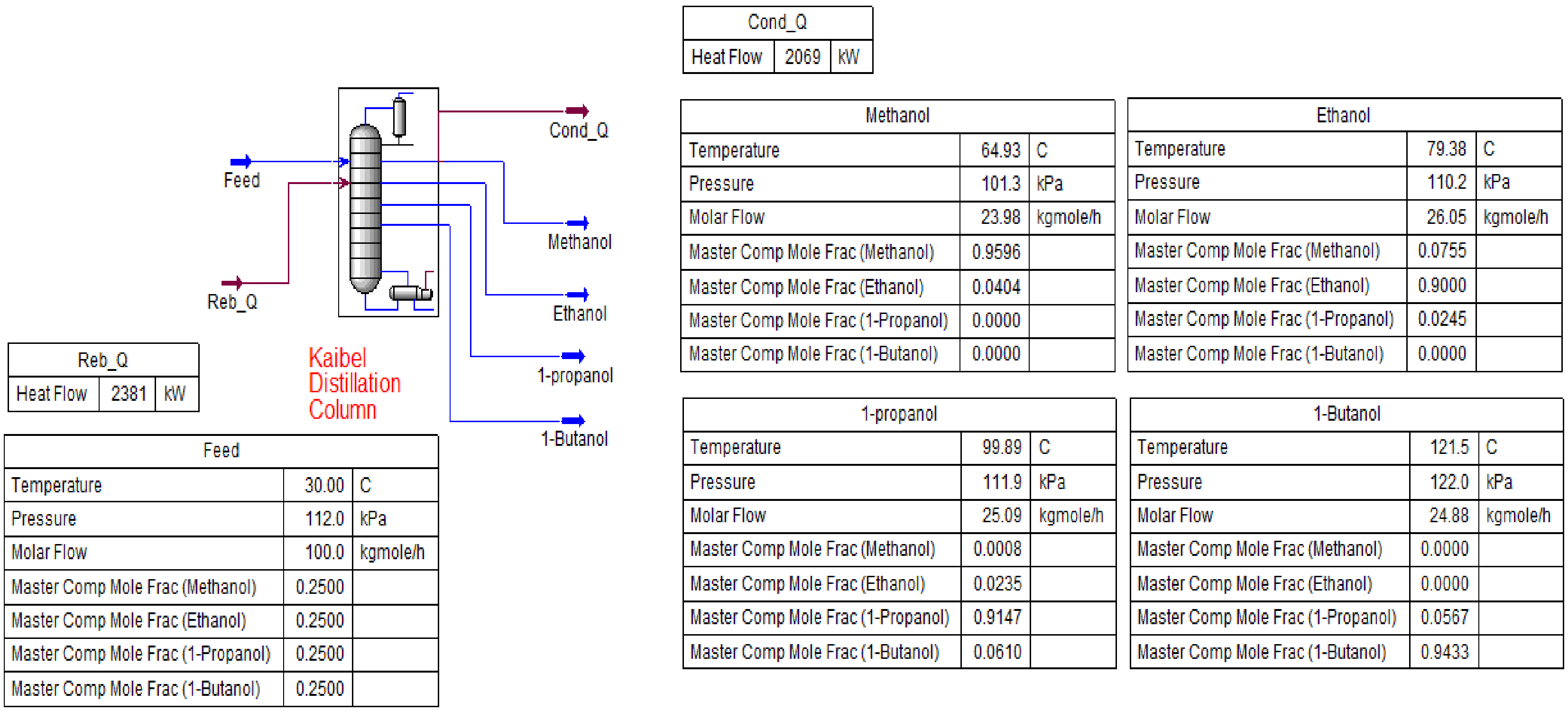
Ethanol		
Temperature	81.02	C
Pressure	110.0	kPa
Molar Flow	23.74	kgmole/h
Master Comp Mole Frac (Methanol)	0.0090	
Master Comp Mole Frac (Ethanol)	0.9206	
Master Comp Mole Frac (1-Propanol)	0.0702	
Master Comp Mole Frac (1-Butanol)	0.0002	

Feed		
Temperature	30.00	C
Pressure	110.0	kPa
Molar Flow	100.0	kgmole/h
Master Comp Mole Frac (Methanol)	0.2500	
Master Comp Mole Frac (Ethanol)	0.2500	
Master Comp Mole Frac (1-Propanol)	0.2500	
Master Comp Mole Frac (1-Butanol)	0.2500	

1-propanol		
Temperature	98.71	C
Pressure	112.0	kPa
Molar Flow	23.93	kgmole/h
Master Comp Mole Frac (Methanol)	0.0021	
Master Comp Mole Frac (Ethanol)	0.0769	
Master Comp Mole Frac (1-Propanol)	0.9200	
Master Comp Mole Frac (1-Butanol)	0.0010	

1-Butanol		
Temperature	122.4	C
Pressure	125.0	kPa
Molar Flow	26.29	kgmole/h
Master Comp Mole Frac (Methanol)	0.0000	
Master Comp Mole Frac (Ethanol)	0.0000	
Master Comp Mole Frac (1-Propanol)	0.0500	
Master Comp Mole Frac (1-Butanol)	0.9500	

Figure 17: Distributed Sequence for Distillation Columns



Reb_Q		
Heat Flow	2381	kW

Feed		
Temperature	30.00	C
Pressure	112.0	kPa
Molar Flow	100.0	kgmole/h
Master Comp Mole Frac (Methanol)	0.2500	
Master Comp Mole Frac (Ethanol)	0.2500	
Master Comp Mole Frac (1-Propanol)	0.2500	
Master Comp Mole Frac (1-Butanol)	0.2500	

Cond_Q		
Heat Flow	2069	kW

Methanol		
Temperature	64.93	C
Pressure	101.3	kPa
Molar Flow	23.98	kgmole/h
Master Comp Mole Frac (Methanol)	0.9596	
Master Comp Mole Frac (Ethanol)	0.0404	
Master Comp Mole Frac (1-Propanol)	0.0000	
Master Comp Mole Frac (1-Butanol)	0.0000	

Ethanol		
Temperature	79.38	C
Pressure	110.2	kPa
Molar Flow	26.05	kgmole/h
Master Comp Mole Frac (Methanol)	0.0755	
Master Comp Mole Frac (Ethanol)	0.9000	
Master Comp Mole Frac (1-Propanol)	0.0245	
Master Comp Mole Frac (1-Butanol)	0.0000	

1-propanol		
Temperature	99.89	C
Pressure	111.9	kPa
Molar Flow	25.09	kgmole/h
Master Comp Mole Frac (Methanol)	0.0008	
Master Comp Mole Frac (Ethanol)	0.0235	
Master Comp Mole Frac (1-Propanol)	0.9147	
Master Comp Mole Frac (1-Butanol)	0.0610	

1-Butanol		
Temperature	121.5	C
Pressure	122.0	kPa
Molar Flow	24.88	kgmole/h
Master Comp Mole Frac (Methanol)	0.0000	
Master Comp Mole Frac (Ethanol)	0.0000	
Master Comp Mole Frac (1-Propanol)	0.0567	
Master Comp Mole Frac (1-Butanol)	0.9433	

Figure 18: Four Product Dividing-wall distillation (Kaibel) Column

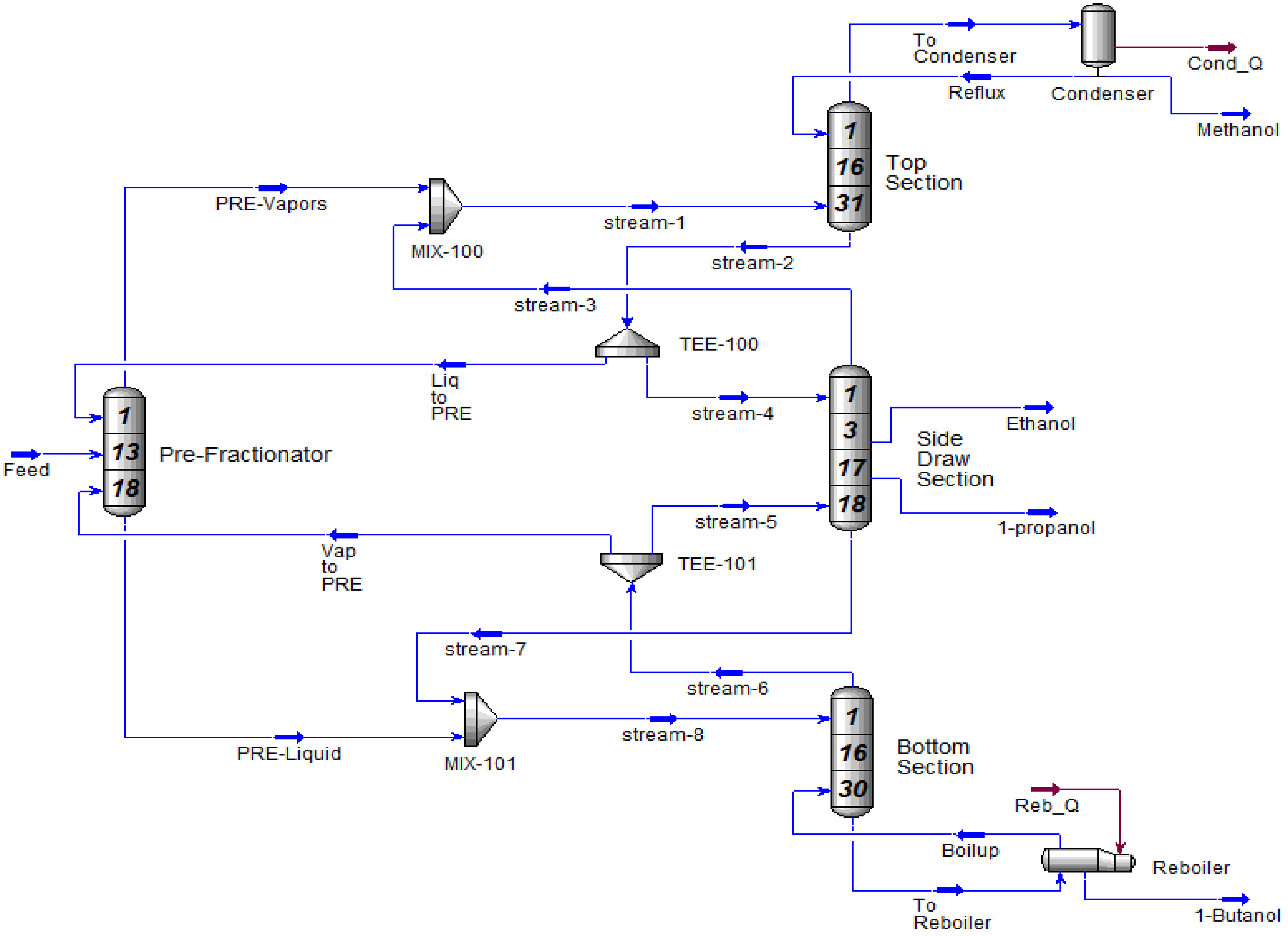


Figure 19: Sub flow sheet Kaibel distillation column in Aspen HYSYS

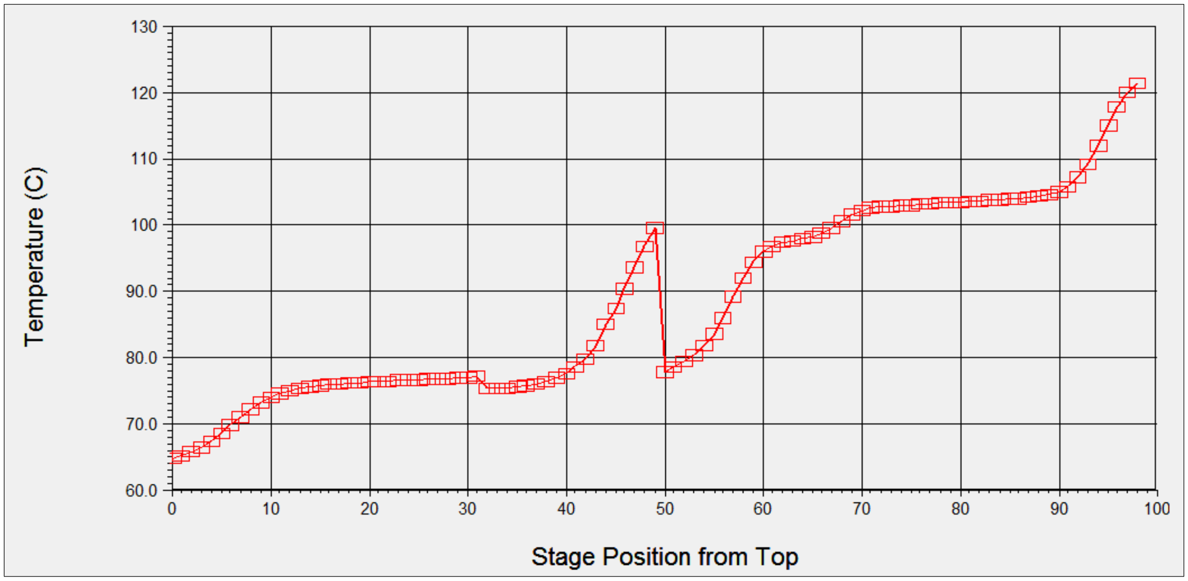


Figure 20: Temperature Profile of Kaibel distillation column

The above Figure 20 is showing the temperature profile across the distillation column. It is clear from the graph that temperature at the top of the column is about 65.5 ^{o}C and 121.5 ^{o}C is at the bottom of the distillation column. Similarly, the below Figure 22 is showing the composition profile of each component throughout the distillation column. Here, we can observe that methanol concentration is maximum at the top section of column and 1-Butanol is maximum at the bottom. While the maximum concentration i.e. 0.92 mole % of ethanol can be obtained from about 52th tray and 1-propanol is showing its maximum concentration from 61th tray to 64th tray.

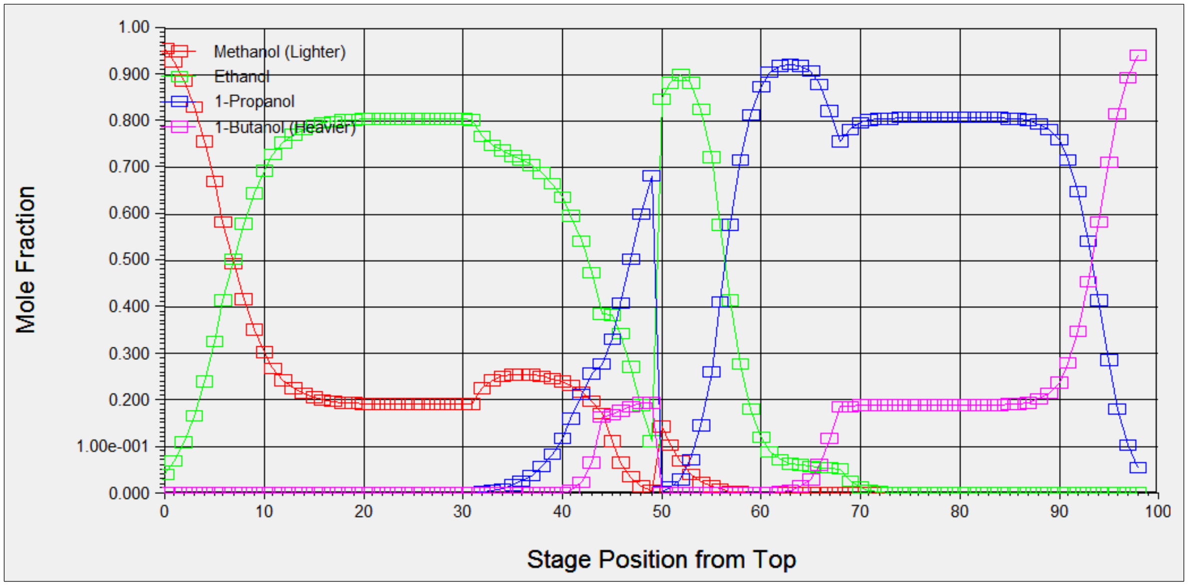
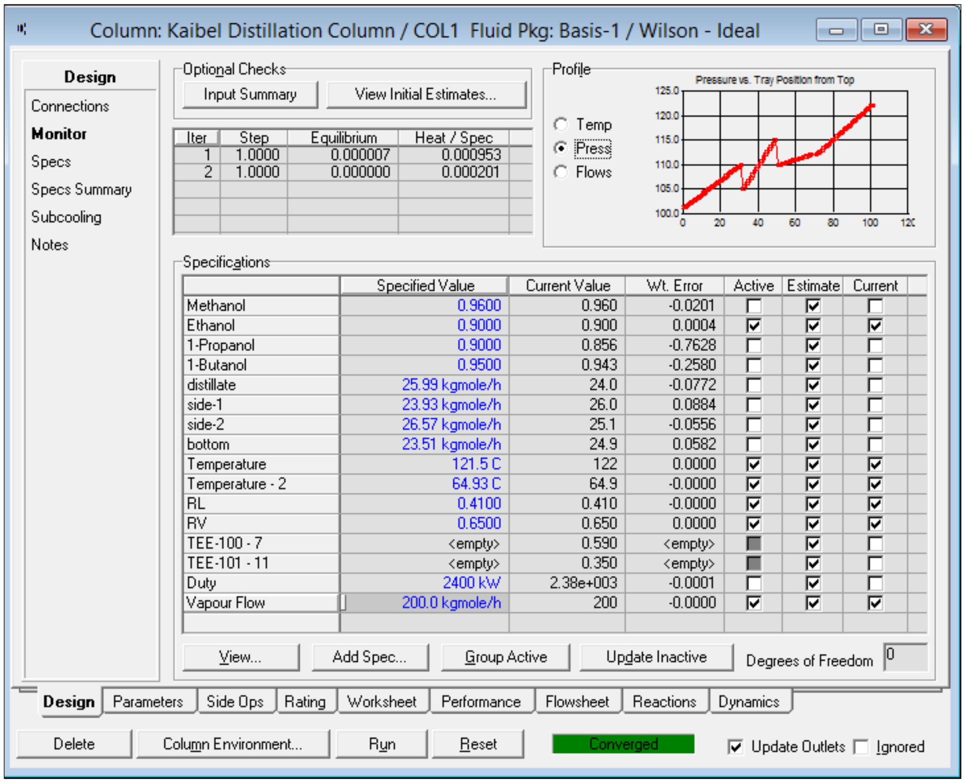


Figure 21: Composition profile throughout the distillation column

The Figure 21 is showing the composition profile for each component throughout the distillation column. The stage numbering is increasing from top to bottom of distillation column. At the top of distillation column, the most concentrated component is methanol i.e. about 0.95 %. While in the bottom of distillation column, 1-butanol is the most concentrated component. While the other two components i.e. ethanol and 1-propanol have its maximum concentration from stages 50 to 65.



Iter	Step	Equilibrium	Heat / Spec
1	1.0000	0.000007	0.000953
2	1.0000	0.000000	0.000201

Specifications

	Specified Value	Current Value	Wt. Error	Active	Estimate	Current
Methanol	0.9600	0.960	-0.0201	☐	☑	☐
Ethanol	0.9000	0.900	0.0004	☑	☑	☑
1-Propanol	0.9000	0.856	-0.7628	☐	☑	☐
1-Butanol	0.9500	0.943	-0.2580	☐	☑	☐
distillate	25.99 kgmole/h	24.0	-0.0772	☐	☑	☐
side-1	23.93 kgmole/h	26.0	0.0884	☐	☑	☐
side-2	26.57 kgmole/h	25.1	-0.0556	☐	☑	☐
bottom	23.51 kgmole/h	24.9	0.0582	☐	☑	☐
Temperature	121.5 C	122	0.0000	☑	☑	☑
Temperature - 2	64.93 C	64.9	-0.0000	☑	☑	☑
RL	0.4100	0.410	-0.0000	☑	☑	☑
RV	0.6500	0.650	0.0000	☑	☑	☑
TEE-100 - 7	<empty>	0.590	<empty>	▨	☑	☐
TEE-101 - 11	<empty>	0.350	<empty>	▨	☑	☐
Duty	2400 kW	2.38e+003	-0.0001	☐	☑	☐
Vapour Flow	200.0 kgmole/h	200	-0.0000	☑	☑	☑

Degrees of Freedom: 0

Figure 22: Final result window of Aspen HYSYS for Alcohol case

The above Figure 22 is the parameters monitor window of Aspen HYSYS obtained after completing the simulation. It is showing that on which parameters, the simulation case got converged. In this case, we have to define any six operational degree of freedom in order to completely specify the system. We provide the values of column vapor flow rate, liquid and vapor split ratios, outlet molar concentration of ethanol, the top temperature and bottom temperature of distillation column. The system can be converged by defining others parameter in order to achieve required results. In the top left corner of figure, the pressure profile of distillation column is also shown. From the pressure profile, it is clear that almost atmospheric pressure is there at the top of the column. The comparison of all above simulation results can be seen in the table below. This simulation represents the first mode of distillation column operation as described above.

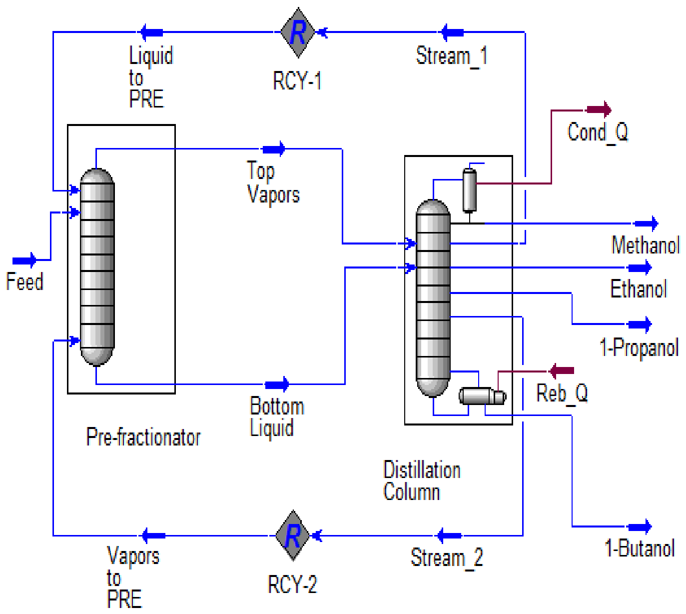
Similarly, if all the product compositions, liquid and vapor split ratios are kept active as degree of freedom then the minimum vapor flowrate should be provided to the distillation column is also 200 kgmole/hr. This is representing the second mode of divided wall distillation column operation.

Table 1: General comparison of results for all distillation column configurations

Column Arrangements	Methanol	Ethanol	1-Propanol	1-Butanol	Heat Energy (kW)
Direct Sequence	0.95	0.82	0.96	0.95	3055.2
Indirect Sequence	0.95	0.86	0.96	0.96	3095.5
Distributed Sequence	0.95	0.92	0.92	0.95	3041.5
Divided Wall Column	0.96	0.90	0.92	0.95	2381

In the above table, all the results obtained from above simulation are shown. It is clear from above table that about 22% of energy can be saved by using dividing wall distillation column as compared to distributed sequence. While the product purities obtained are also acceptable and almost same to other configurations.

The case study-01 is again simulated with almost same feed conditions in a different way as shown in Figure 23. Here, the thermal coupling between pre-fractionator and main distillation column is simulated in the main window of Aspen HYSYS. The streams “Top Vapors” and “Bottom Liquid” are going to be introduce in the main distillation column. While, the streams “stream_1” and “stream_2” are exiting from the main column and going back to pre-fractionator. This flow sheet made is itself depicting the structure of dividing wall column in HYSYS. Where it was assumed that prefractionator is acting as a partition wall inside the main distillation column.



Feed		
Temperature	82.27	C
Pressure	112.0	kPa
Molar Flow	100.0	kgmole/h
Master Comp Mole Frac (Methanol)	0.2500	
Master Comp Mole Frac (Ethanol)	0.2500	
Master Comp Mole Frac (1-Propanol)	0.2500	
Master Comp Mole Frac (1-Butanol)	0.2500	

Reb_Q		
Heat Flow	9059	kW

Cond_Q		
Heat Flow	8989	kW

Methanol		
Temperature	65.14	C
Pressure	101.3	kPa
Molar Flow	25.00	kgmole/h
Master Comp Mole Frac (Methanol)	0.9414	
Master Comp Mole Frac (Ethanol)	0.0586	
Master Comp Mole Frac (1-Propanol)	0.0000	
Master Comp Mole Frac (1-Butanol)	0.0000	

Ethanol		
Temperature	80.59	C
Pressure	111.3	kPa
Molar Flow	23.75	kgmole/h
Master Comp Mole Frac (Methanol)	0.0426	
Master Comp Mole Frac (Ethanol)	0.9000	
Master Comp Mole Frac (1-Propanol)	0.0574	
Master Comp Mole Frac (1-Butanol)	0.0000	

1-Propanol		
Temperature	97.84	C
Pressure	117.7	kPa
Molar Flow	26.25	kgmole/h
Master Comp Mole Frac (Methanol)	0.0169	
Master Comp Mole Frac (Ethanol)	0.0829	
Master Comp Mole Frac (1-Propanol)	0.9001	
Master Comp Mole Frac (1-Butanol)	0.0001	

1-Butanol		
Temperature	123.9	C
Pressure	125.0	kPa
Molar Flow	25.00	kgmole/h
Master Comp Mole Frac (Methanol)	0.0000	
Master Comp Mole Frac (Ethanol)	0.0000	
Master Comp Mole Frac (1-Propanol)	0.0009	
Master Comp Mole Frac (1-Butanol)	0.9991	

Figure 23: Four product Kaibel Distillation Column in Aspen HYSYS

The temperature and composition profiles for the main distillation column converged in the Figure 23 are shown in the below Figures 24 and 25. Here, we get the increased products composition as compared to the previous sequence of Kaibel distillation column.

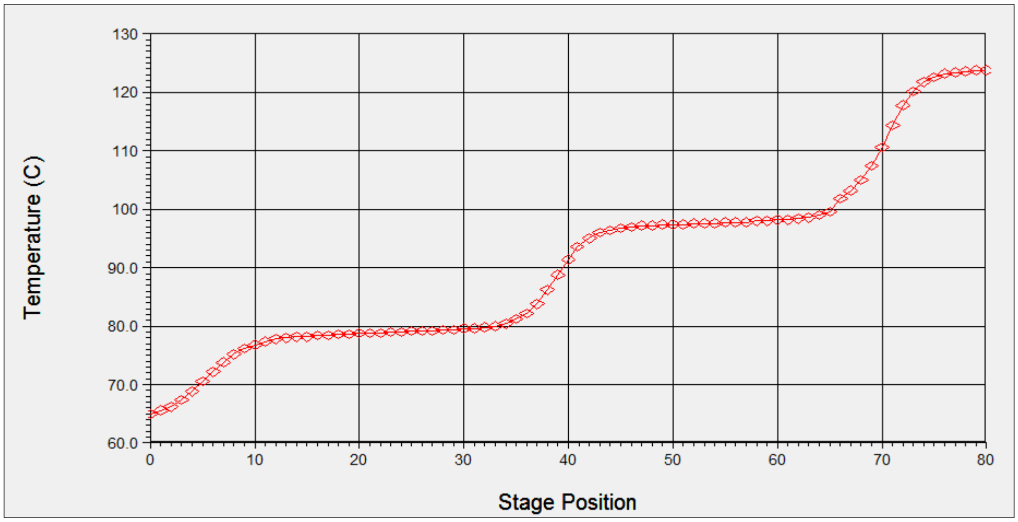


Figure 24: Temperature profile throughout the main distillation column

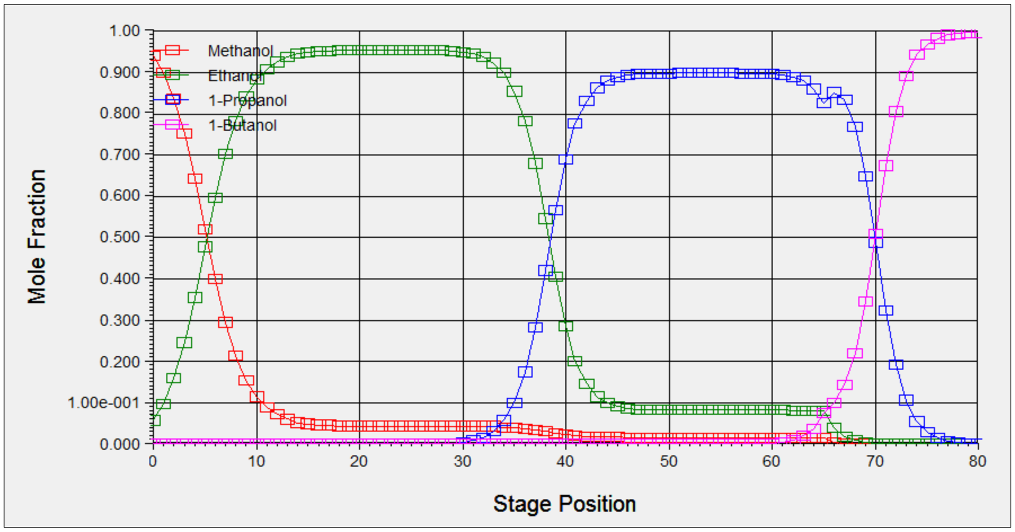
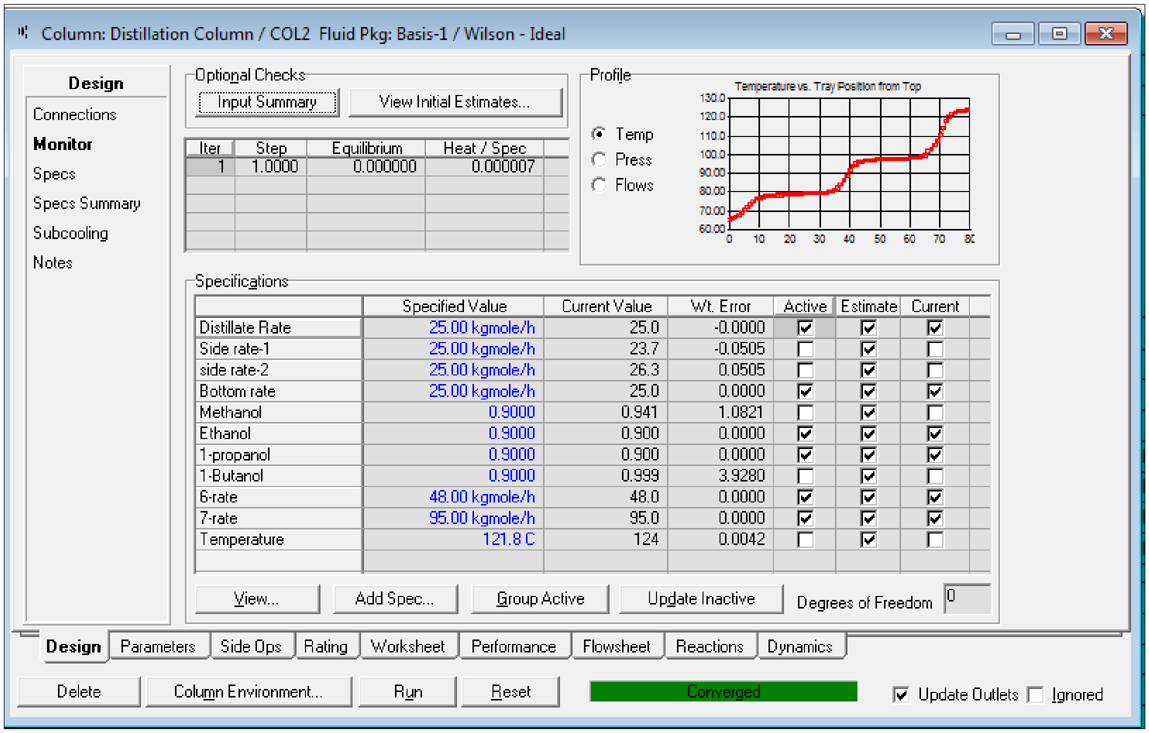


Figure 25: Composition profile throughout the main distillation column



Column: Distillation Column / COL2 Fluid Pkg: Basis-1 / Wilson - Ideal

Iter	Step	Equilibrium	Heat / Spec
1	1.0000	0.000000	0.000007

● Temp
○ Press
○ Flows

	Specified Value	Current Value	Wt. Error	Active	Estimate	Current
Distillate Rate	25.00 kgmole/h	25.0	-0.0000	☑	☑	☑
Side rate-1	25.00 kgmole/h	23.7	-0.0505	☐	☑	☐
side rate-2	25.00 kgmole/h	26.3	0.0505	☐	☑	☐
Bottom rate	25.00 kgmole/h	25.0	0.0000	☑	☑	☑
Methanol	0.9000	0.941	1.0821	☐	☑	☐
Ethanol	0.9000	0.900	0.0000	☑	☑	☑
1-propanol	0.9000	0.900	0.0000	☑	☑	☑
1-Butanol	0.9000	0.999	3.9280	☐	☑	☐
6-rate	48.00 kgmole/h	48.0	0.0000	☑	☑	☑
7-rate	95.00 kgmole/h	95.0	0.0000	☑	☑	☑
Temperature	121.8 C	124	0.0042	☐	☑	☐

Degrees of Freedom 0

Converged

☑ Update Outlets ☐ Ignored

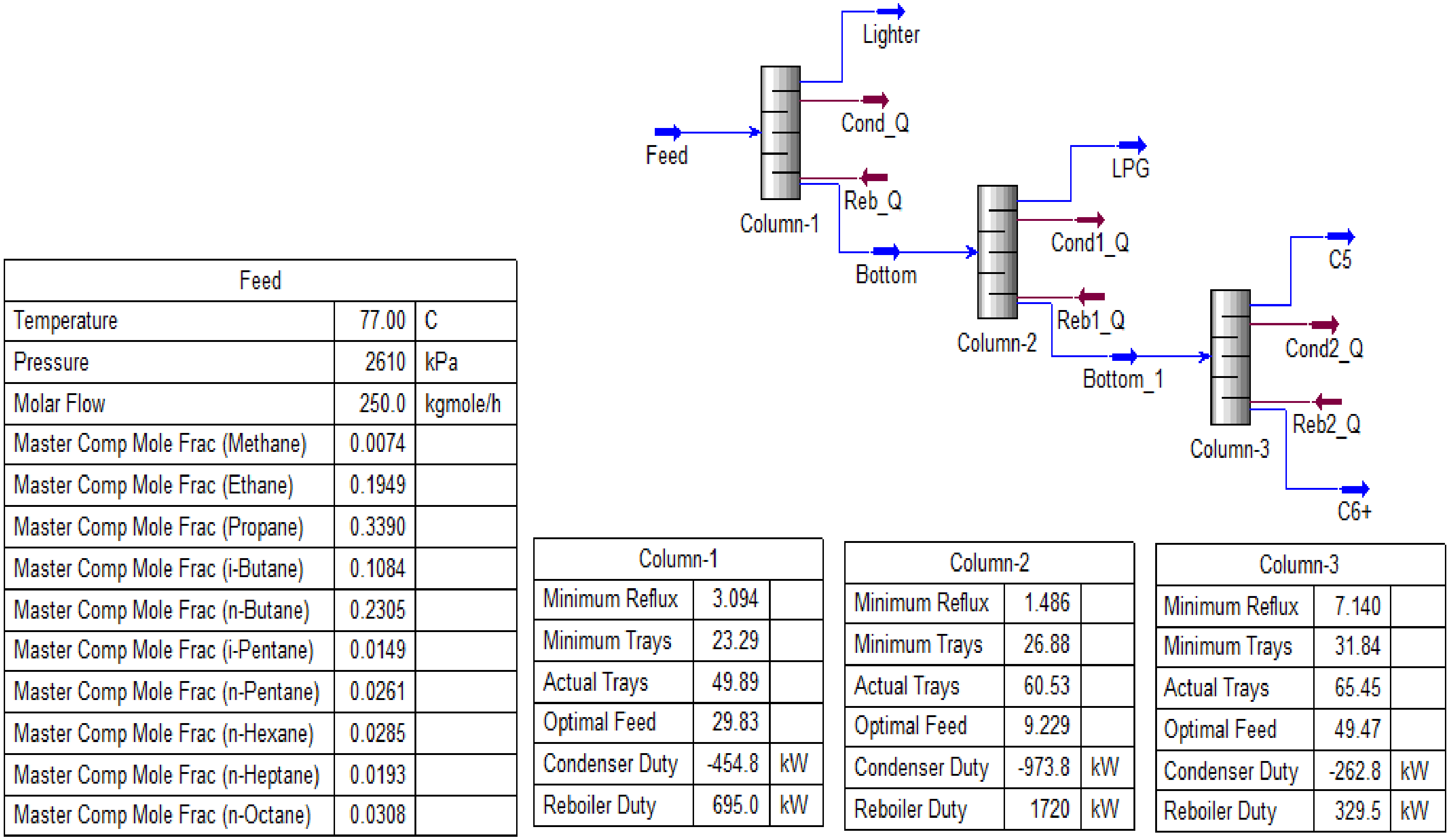
Figure 26: Design window of Aspen HYSYS showing the convergence parameters

Figures 26 is showing the convergence parameters for the simulation case. As the above figure is showing that simulation gets converged when the distillate flow rate, bottom flow rate, mole fraction of both side draw products and flow rates of recycle streams to pre-fractionator become active. While in the previous simulation, it gets converged on giving bottom vapor flow rate, liquid and vapor split ratio, top and bottom temperature of column and mole fraction of ethanol. But this does not matter that which parameters are getting active, it all depends upon that we are getting our required results or not.

5.2 Hydrocarbon stream as Feed

In the second case study, the feed mixture consists of hydrocarbon components from methane to octane (C_1-C_8) [38]. The hydrocarbon stream can be obtained from an oil refinery or crude oil exploration facilities. As number of valuable products like LPG, NGL etc. can be produced from this hydrocarbon stream and these products can be sold out as domestic fuel or any other. In industries, there are some process plants installed to process such exit streams to convert them into valuable products. Here, commercial simulation software (Aspen HYSYS) is utilized to simulate the whole process. The hydrocarbon rich stream of the below given composition is charged to dividing-wall distillation column. Then four different products are obtained i.e. ethane rich stream, LPG, pentane rich and the heaviest (C_6^+) one from the bottom of the distillation column. The thermodynamic model used to do flash calculations in Aspen HYSYS is Peng Robinson.

In this section, the system is observed by simulating the process through different arrangements of distillation columns. For example, the distillation columns are first converged as direct sequence, indirect and then distributed sequence. In the last, the complex arrangement of distillation column i.e. divided wall distillation column (DWC) is also simulated as shown in Figure 30. The advantage of using the complex configuration is to reduce the energy consumption to a great extent. Hence, it has been tabulated in the Table 4 that about 25 % of energy can be saved using dividing-wall distillation column.



Feed		
Temperature	77.00	C
Pressure	2610	kPa
Molar Flow	250.0	kgmole/h
Master Comp Mole Frac (Methane)	0.0074	
Master Comp Mole Frac (Ethane)	0.1949	
Master Comp Mole Frac (Propane)	0.3390	
Master Comp Mole Frac (i-Butane)	0.1084	
Master Comp Mole Frac (n-Butane)	0.2305	
Master Comp Mole Frac (i-Pentane)	0.0149	
Master Comp Mole Frac (n-Pentane)	0.0261	
Master Comp Mole Frac (n-Hexane)	0.0285	
Master Comp Mole Frac (n-Heptane)	0.0193	
Master Comp Mole Frac (n-Octane)	0.0308	

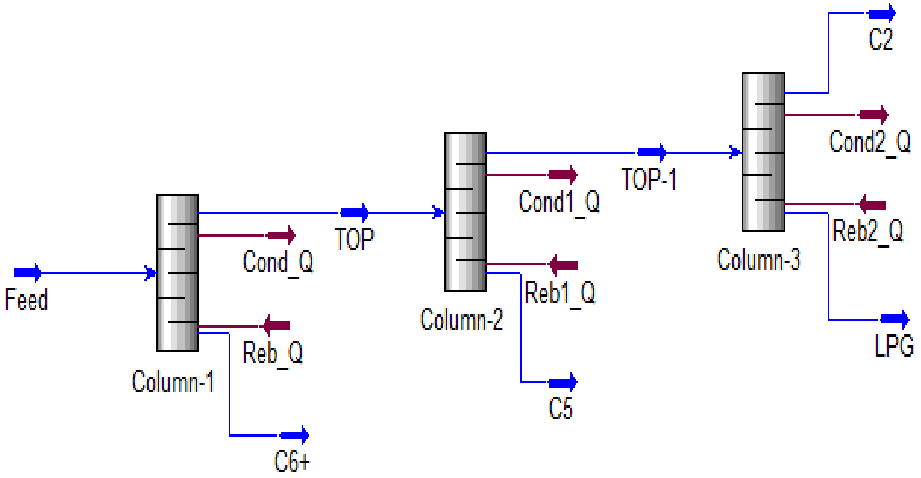
Column-1		
Minimum Reflux	3.094	
Minimum Trays	23.29	
Actual Trays	49.89	
Optimal Feed	29.83	
Condenser Duty	-454.8	kW
Reboiler Duty	695.0	kW

Column-2		
Minimum Reflux	1.486	
Minimum Trays	26.88	
Actual Trays	60.53	
Optimal Feed	9.229	
Condenser Duty	-973.8	kW
Reboiler Duty	1720	kW

Column-3		
Minimum Reflux	7.140	
Minimum Trays	31.84	
Actual Trays	65.45	
Optimal Feed	49.47	
Condenser Duty	-262.8	kW
Reboiler Duty	329.5	kW

Figure 27: Direct Sequences for Distillation Columns

Feed		
Temperature	77.00	C
Pressure	2610	kPa
Molar Flow	250.0	kgmole/h
Master Comp Mole Frac (Methane)	0.0074	
Master Comp Mole Frac (Ethane)	0.1949	
Master Comp Mole Frac (Propane)	0.3390	
Master Comp Mole Frac (i-Butane)	0.1084	
Master Comp Mole Frac (n-Butane)	0.2305	
Master Comp Mole Frac (i-Pentane)	0.0149	
Master Comp Mole Frac (n-Pentane)	0.0261	
Master Comp Mole Frac (n-Hexane)	0.0285	
Master Comp Mole Frac (n-Heptane)	0.0193	
Master Comp Mole Frac (n-Octane)	0.0308	



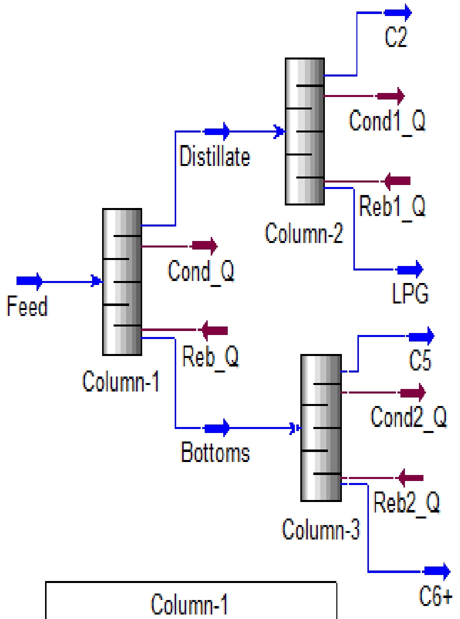
Column-1		
Minimum Reflux	0.4923	
Minimum Trays	26.24	
Actual Trays	66.18	
Optimal Feed	40.56	
Condenser Duty	-524.7	kW
Reboiler Duty	1596	kW

Column-2		
Minimum Reflux	0.9061	
Minimum Trays	33.48	
Actual Trays	78.70	
Optimal Feed	51.69	
Condenser Duty	-862.0	kW
Reboiler Duty	825.0	kW

Column-3		
Minimum Reflux	6.128	
Minimum Trays	14.97	
Actual Trays	31.48	
Optimal Feed	11.24	
Condenser Duty	-925.0	kW
Reboiler Duty	386.5	kW

Figure 28: Indirect Sequence for Distillation Columns

Feed		
Temperature	77.00	C
Pressure	2610	kPa
Molar Flow	250.0	kgmole/h
Master Comp Mole Frac (Methane)	0.0074	
Master Comp Mole Frac (Ethane)	0.1949	
Master Comp Mole Frac (Propane)	0.3390	
Master Comp Mole Frac (i-Butane)	0.1084	
Master Comp Mole Frac (n-Butane)	0.2305	
Master Comp Mole Frac (i-Pentane)	0.0149	
Master Comp Mole Frac (n-Pentane)	0.0261	
Master Comp Mole Frac (n-Hexane)	0.0285	
Master Comp Mole Frac (n-Heptane)	0.0193	
Master Comp Mole Frac (n-Octane)	0.0308	

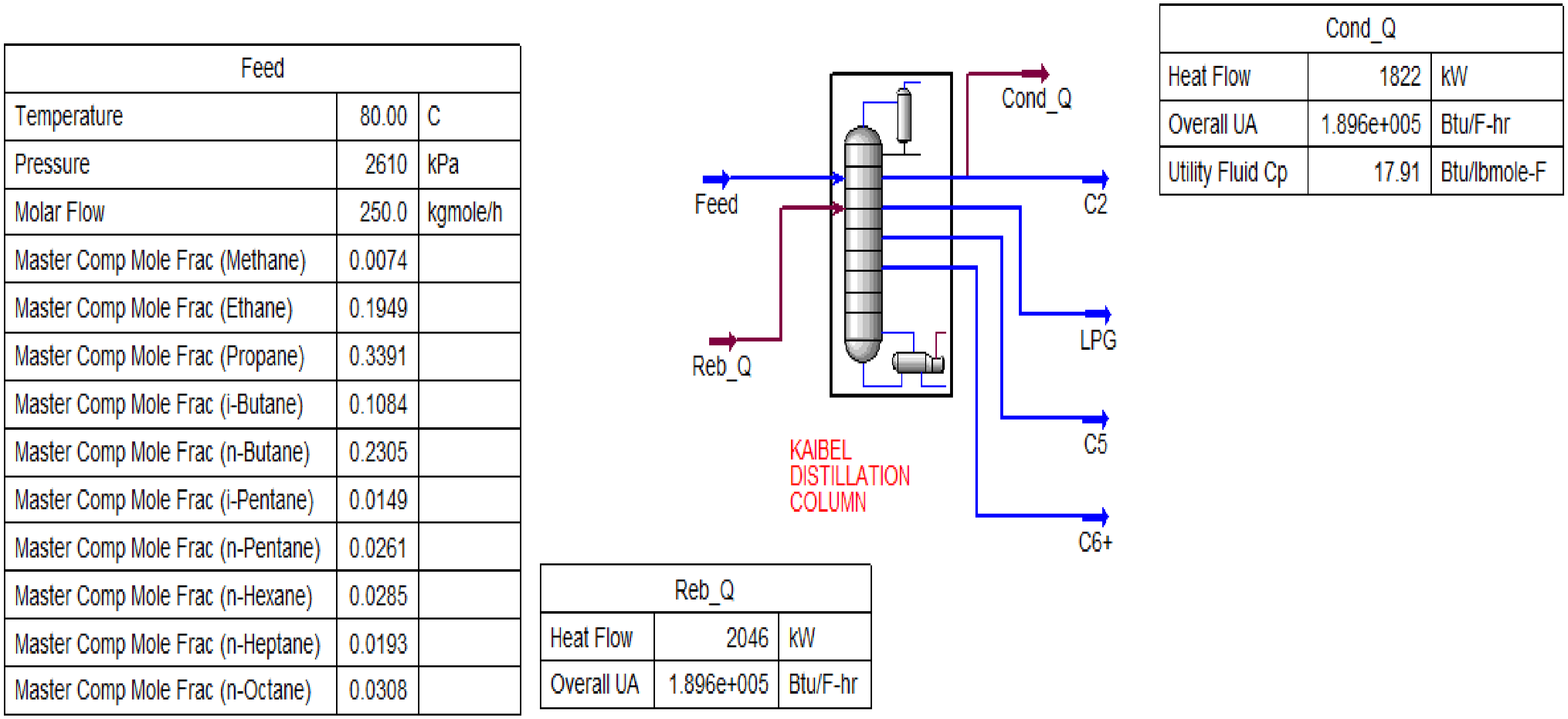


Column-1		
Minimum Reflux	0.3426	
Minimum Trays	7.627	
Actual Trays	21.11	
Optimal Feed	17.98	
Condenser Duty	-319.2	kW
Reboiler Duty	1260	kW

Column-2		
Minimum Reflux	5.189	
Minimum Trays	14.84	
Actual Trays	31.40	
Optimal Feed	22.08	
Condenser Duty	-1012	kW
Reboiler Duty	501.4	kW

Column-3		
Minimum Reflux	2.747	
Minimum Trays	21.40	
Actual Trays	46.27	
Optimal Feed	11.65	
Condenser Duty	-273.0	kW
Reboiler Duty	425.9	kW

Figure 29: Distributed Sequence for Distillation Columns



Feed		
Temperature	80.00	C
Pressure	2610	kPa
Molar Flow	250.0	kgmole/h
Master Comp Mole Frac (Methane)	0.0074	
Master Comp Mole Frac (Ethane)	0.1949	
Master Comp Mole Frac (Propane)	0.3391	
Master Comp Mole Frac (i-Butane)	0.1084	
Master Comp Mole Frac (n-Butane)	0.2305	
Master Comp Mole Frac (i-Pentane)	0.0149	
Master Comp Mole Frac (n-Pentane)	0.0261	
Master Comp Mole Frac (n-Hexane)	0.0285	
Master Comp Mole Frac (n-Heptane)	0.0193	
Master Comp Mole Frac (n-Octane)	0.0308	

Reb_Q		
Heat Flow	2046	kW
Overall UA	1.896e+005	Btu/F-hr

Cond_Q		
Heat Flow	1822	kW
Overall UA	1.896e+005	Btu/F-hr
Utility Fluid Cp	17.91	Btu/lbmole-F

Figure 30: Four Product Kaibel Distillation (DWC) Column

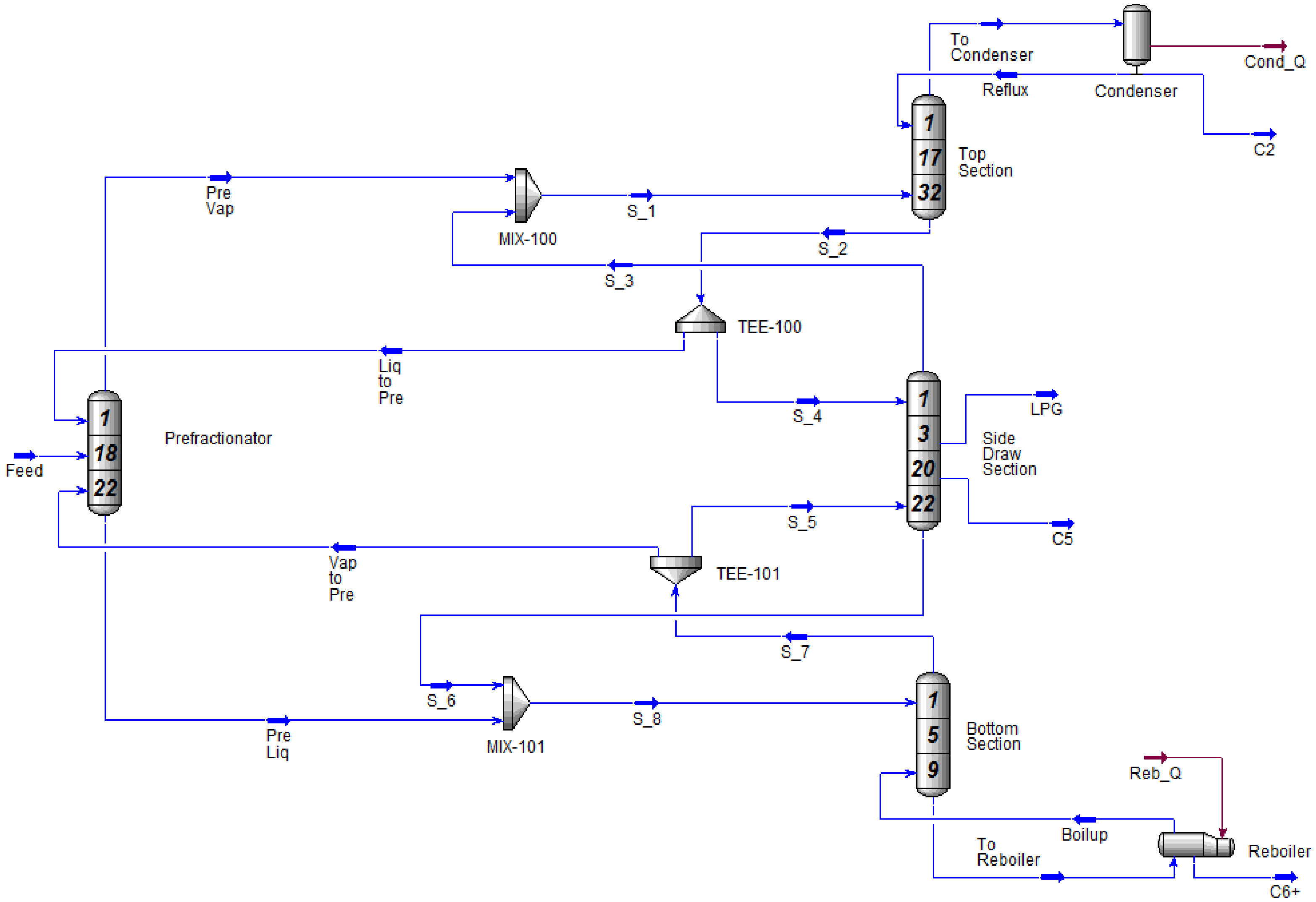


Figure 31: Flow sheet made under column environment of Kaibel distillation column

The product outlet condition and composition obtained from the simulations (direct sequence and indirect sequence for distillation column arrangements) converged in Figures 27 and 28 are shown in the table 02 below. While the simulation results obtained for distributed sequence and divided wall distillation column are shown in table 03 below. The units of temperature, pressure and molar flow are **^{o}C**, **kPa** and **kgmole/hr** respectively.

Table 2: Simulations results for Direct and Indirect Sequences

	DIRECT SEQUENCE				**INDIRECT SEQUENCE**			
	C_2	LPG	C_5	C_6^+	C_2	LPG	C_5	C_6^+
Temperature	1.191	100.2	179.7	264.4	2.801	95.02	176.2	263.2
Pressure	2590	2550	2615	2640	2615	2640	2600	2630
Molar Flow	50.58	169.6	10.74	19.1	50.94	169.2	10.22	19.65
Master component mole fraction								
Methane	0.0368	0.00	0.00	0.00	0.0366	0.00	0.00	0.00
Ethane	0.9630	0.0001	0.00	0.00	0.9534	0.001	0.00	0.00
Propane	0.0001	0.4998	0.00	0.00	0.01	0.4979	0.00	0.00
i-Butane	0.00	0.1559	0.0003	0.00	0.00	0.1602	0.00	0.00
n-Butane	0.00	0.3390	0.0122	0.00	0.00	0.3405	0.001	0.00
i-Pentane	0.00	0.0010	0.3293	0.001	0.00	0.0003	0.3596	0.00
n-Pentane	0.00	0.0002	0.5962	0.0052	0.00	0.00	0.6372	0.001
n-Hexane	0.00	0.00	0.0619	0.3382	0.00	0.00	0.0023	0.3615
n-Heptane	0.00	0.00	0.0001	0.2521	0.00	0.00	0.00	0.2452
n-Octane	0.00	0.00	0.00	0.4035	0.00	0.00	0.00	0.3923

Table 3: Simulation results for Distributed and Divided wall Distillation Column

	DISTRIBUTED SEQUENCE				DIVIDED WALL COLUMN			
	C_2	LPG	C_5	C_6^+	C_2	LPG	C_5	C_6^+
Temperature	12.14	94.32	177.8	280.4	10	97.91	147.1	255.6
Pressure	2550	2600	2615	2640	2570	2594	2626	2640
Molar Flow	56.41	157	22.84	13.71	67.19	157	4.919	20.89
Master component mole fraction								
Methane	0.0330	0.00	0.00	0.00	0.0275	0.00	0.00	0.00
Ethane	0.8637	0.0001	0.0001	0.00	0.8558	0.0126	0.0018	0.00
Propane	0.1033	0.5015	0.0076	0.00	0.1167	0.4196	0.0584	0.0002
i-Butane	0.00	0.1649	0.0528	0.00	0.00	0.1690	0.1067	0.002
n-Butane	0.00	0.3226	0.002	0.00	0.00	0.3538	0.1237	0.0119
i-Pentane	0.00	0.0056	0.1243	0.0002	0.00	0.0185	0.0987	0.0160
n-Pentane	0.00	0.0051	0.5526	0.001	0.00	0.0264	0.5007	0.0553
n-Hexane	0.00	0.0001	0.2499	0.1019	0.00	0.0001	0.1013	0.3169
n-Heptane	0.00	0.00	0.01	0.3348	0.00	0.00	0.0067	0.2294
n-Octane	0.00	0.00	0.0002	0.5621	0.00	0.00	0.002	0.3682

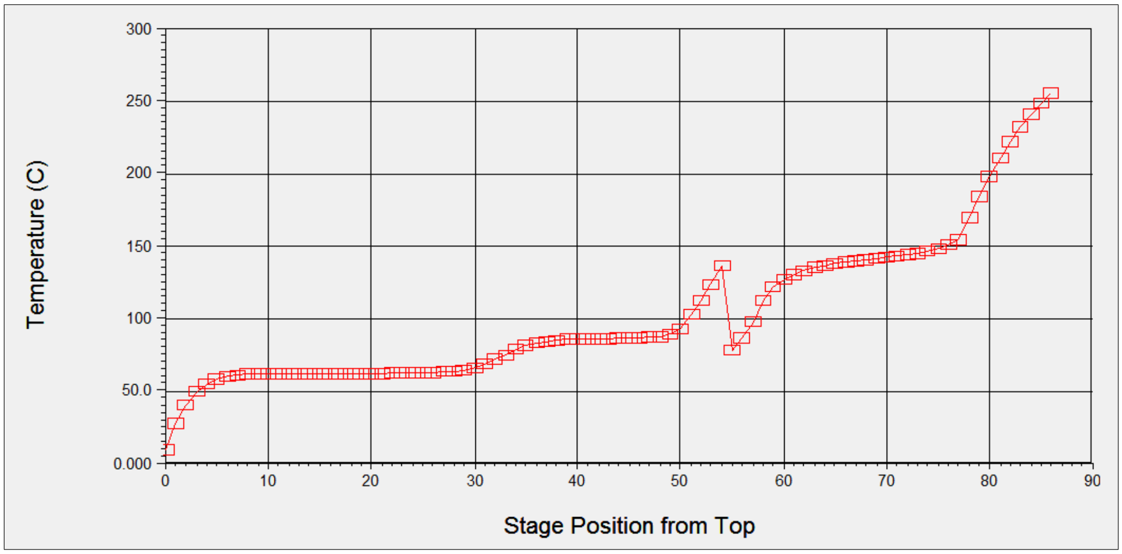


Figure 32: Temperature profile throughout the distillation column

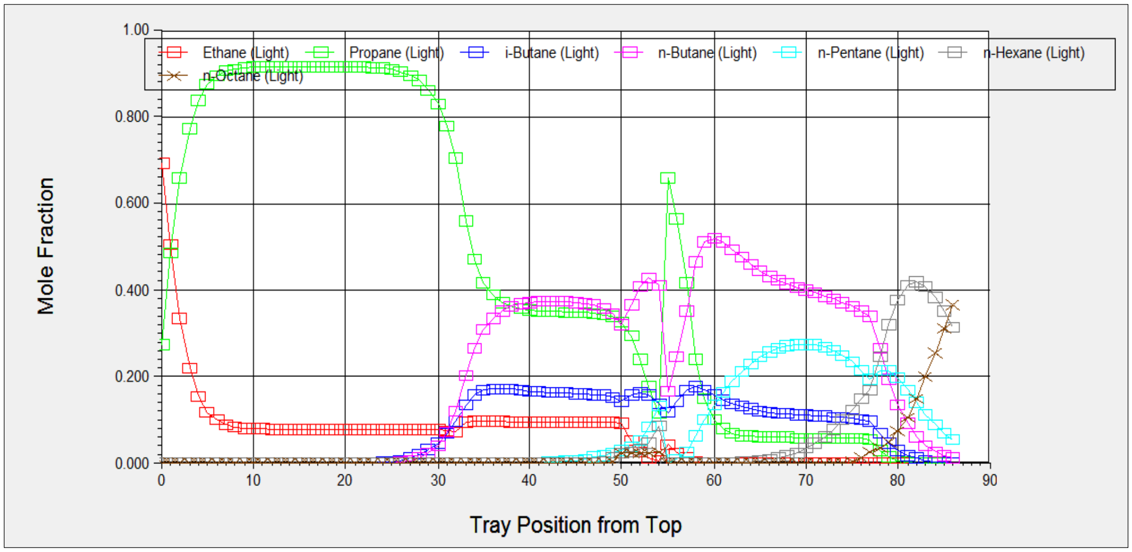
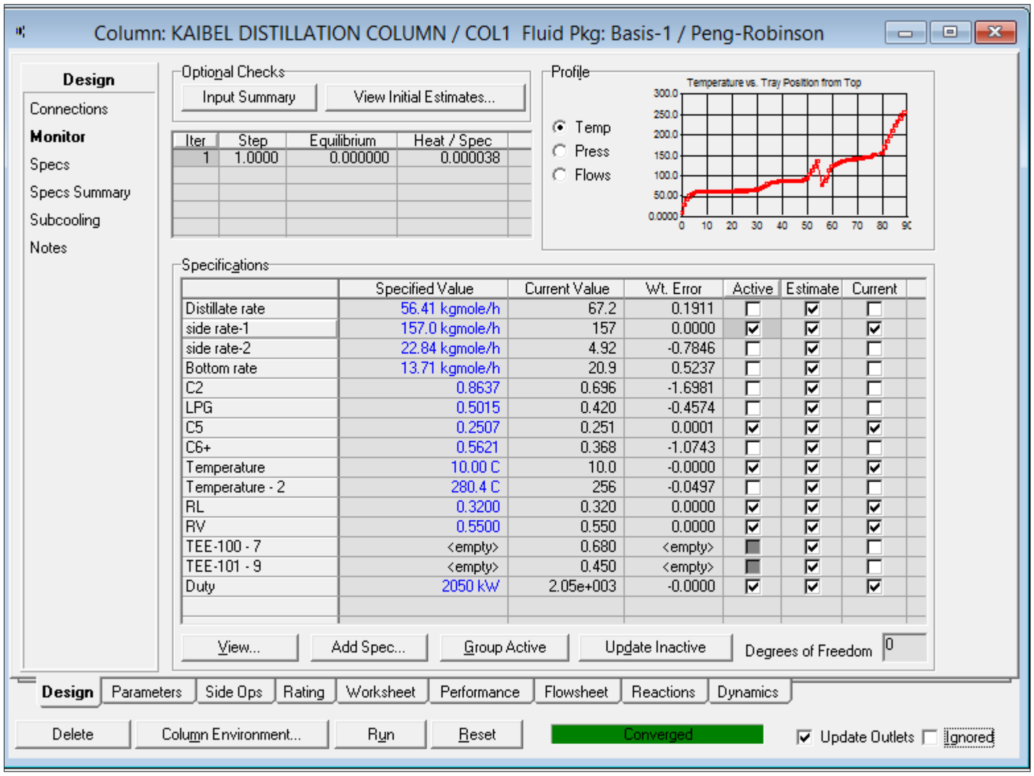


Figure 33: Composition profile throughout the distillation column



Iter	Step	Equilibrium	Heat / Spec
1	1.0000	0.000000	0.000038

	Specified Value	Current Value	Wt. Error	Active	Estimate	Current
Distillate rate	56.41 kgmole/h	67.2	0.1911	☐	☑	☐
side rate-1	157.0 kgmole/h	157	0.0000	☑	☑	☑
side rate-2	22.84 kgmole/h	4.92	-0.7846	☐	☑	☐
Bottom rate	13.71 kgmole/h	20.9	0.5237	☐	☑	☐
C2	0.8637	0.696	-1.6981	☐	☑	☐
LPG	0.5015	0.420	-0.4574	☐	☑	☐
C5	0.2507	0.251	0.0001	☑	☑	☑
C6+	0.5621	0.368	-1.0743	☐	☑	☐
Temperature	10.00 C	10.0	-0.0000	☑	☑	☑
Temperature - 2	280.4 C	256	-0.0497	☐	☑	☐
RL	0.3200	0.320	0.0000	☑	☑	☑
RV	0.5500	0.550	0.0000	☑	☑	☑
TEE-100 - 7	<empty>	0.680	<empty>	■	☑	☐
TEE-101 - 9	<empty>	0.450	<empty>	■	☑	☐
Duty	2050 kW	2.05e+003	-0.0000	☑	☑	☑

Degrees of Freedom 0

Figure 34: Convergence result for Hydrocarbon case in Aspen HYSYS

The hydrocarbon stream obtained from an exploration facility was charged to Kaibel distillation column in order to obtained almost pure ethane gas, LPG and heavier hydrocarbons. Distillation column is simulated in the Aspen HYSYS and two product compositions, one product flow rate, liquid & vapor splits ratios and duty of the distillation column was specified as shown in the above Figure 34.

The main composition of key component in all the products and the heat energy required to achieve the required results are shown in the below Table 04. According the results, about 07 % of heat energy can be saved by using divided wall distillation column as compared to distributed sequence of distillation columns. Although the product composition obtained are almost the same as the others.

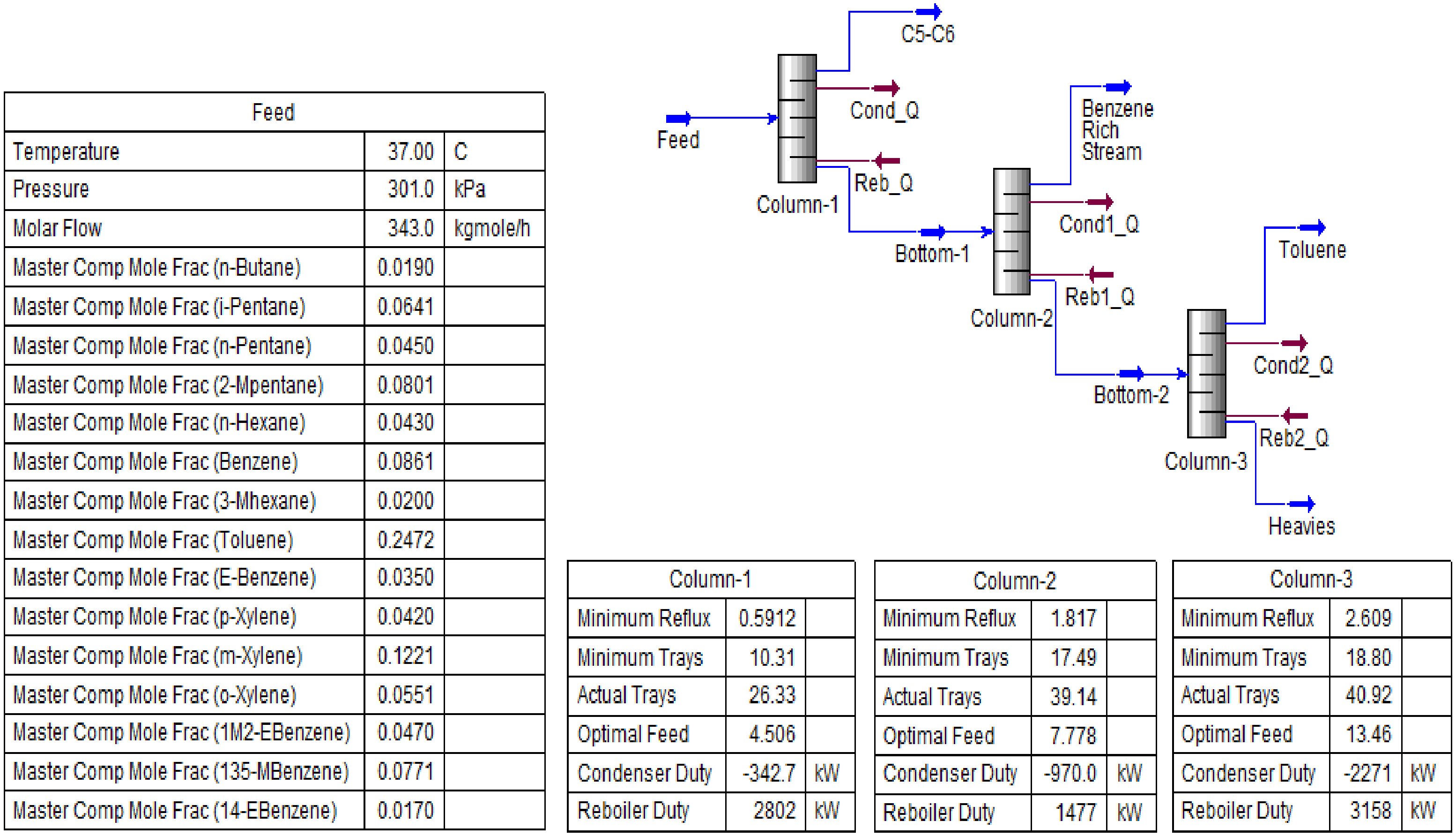
Table 4: Overall results obtained from all the possible distillation column sequences

Column Arrangements	C_2 (Ethane)	LPG (Propane / n-butane)	C_5 (n-pentane)	C_6^+ (n-octane)	Heat Energy (kW)
Direct Sequence	0.96	0.4998 / 0.3390	0.5962	0.4035	2744.5
Indirect Sequence	0.9534	0.4979 / 0.3405	0.6372	0.3923	2806.5
Distributed Sequence	0.8637	0.5015 / 0.3226	0.5526	0.5621	2187.3
Dividing Wall Column	0.8558	0.4196 / 0.3538	0.5007	0.3682	2046

5.3 Aromatic Mixture as Feed

The third case study is related to an oil refinery plant effluent stream which contains number of aromatics components [39]. Actually in an oil refinery, crude distillation unit (CDU) is the one of the key unit of the facility which separates the all valuable products from crude oil. But some of the products (naphtha, kerosene, furnace oil etc.) obtained from CDU need more processing to be used as consumer required product. This is why, all these products are sent to other processing refinery units (Platformer unit, Merox, Vacuum distillation unit etc.) to obtain the final useable product like gasoline, kerosene, diesel, light diesel oil and furnace oil. In this case study, an effluent stream obtained platforming unit is studied. This refinery unit increase the octane number of straight run naphtha and also removes sulfur contents from in it. As this aromatic rich stream can give us many valuable components like benzene etc. to be used in many petrochemical industries.

The distillation operation of the given feed is studied in both simple / conventional and complex configuration also. In the last, a short comparison have been done regarding the consumption of heat energy.



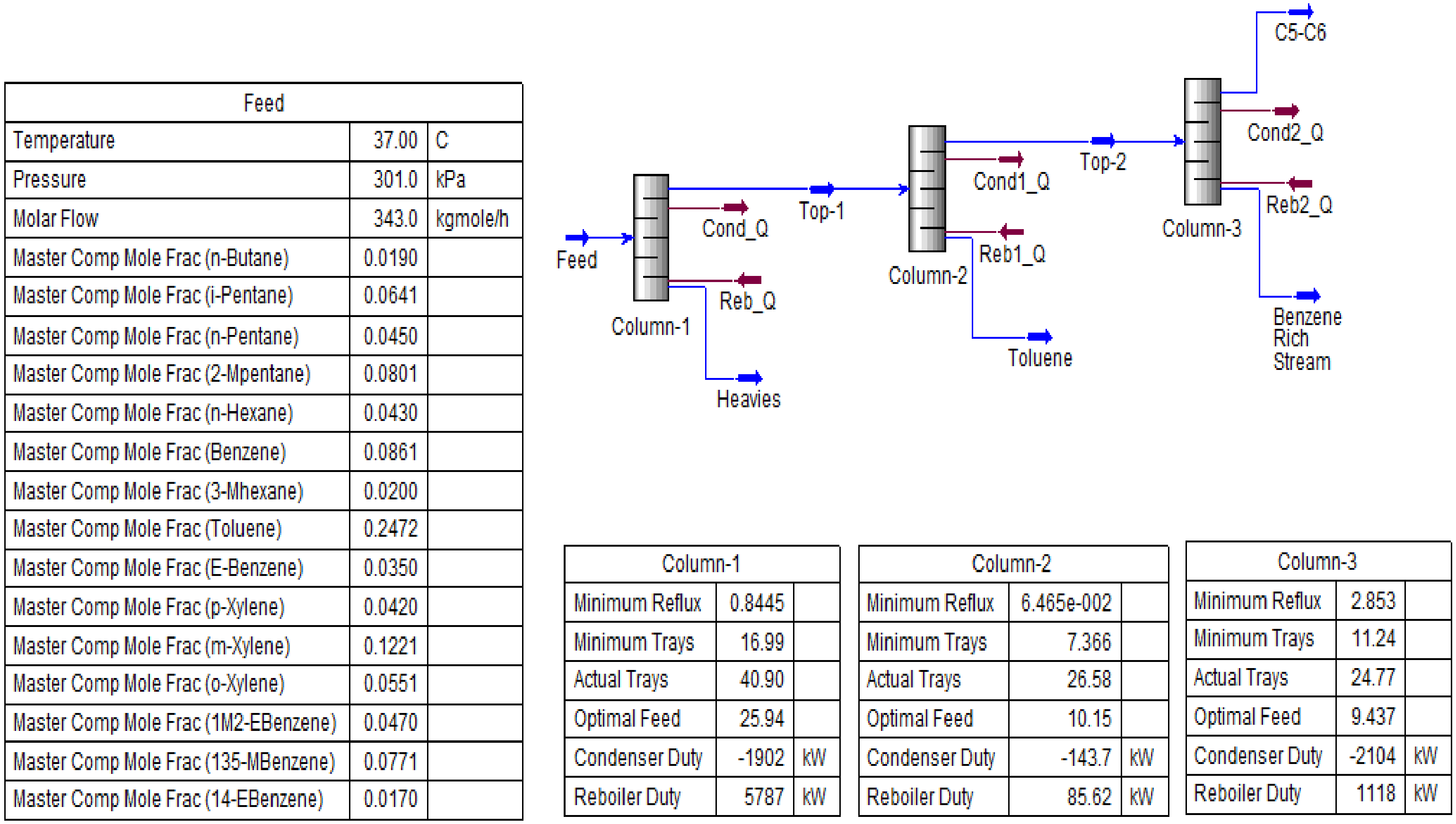
Feed		
Temperature	37.00	C
Pressure	301.0	kPa
Molar Flow	343.0	kgmole/h
Master Comp Mole Frac (n-Butane)	0.0190	
Master Comp Mole Frac (i-Pentane)	0.0641	
Master Comp Mole Frac (n-Pentane)	0.0450	
Master Comp Mole Frac (2-Mpentane)	0.0801	
Master Comp Mole Frac (n-Hexane)	0.0430	
Master Comp Mole Frac (Benzene)	0.0861	
Master Comp Mole Frac (3-Mhexane)	0.0200	
Master Comp Mole Frac (Toluene)	0.2472	
Master Comp Mole Frac (E-Benzene)	0.0350	
Master Comp Mole Frac (p-Xylene)	0.0420	
Master Comp Mole Frac (m-Xylene)	0.1221	
Master Comp Mole Frac (o-Xylene)	0.0551	
Master Comp Mole Frac (1M2-EBenzene)	0.0470	
Master Comp Mole Frac (135-MBenzene)	0.0771	
Master Comp Mole Frac (14-EBenzene)	0.0170	

Column-1		
Minimum Reflux	0.5912	
Minimum Trays	10.31	
Actual Trays	26.33	
Optimal Feed	4.506	
Condenser Duty	-342.7	kW
Reboiler Duty	2802	kW

Column-2		
Minimum Reflux	1.817	
Minimum Trays	17.49	
Actual Trays	39.14	
Optimal Feed	7.778	
Condenser Duty	-970.0	kW
Reboiler Duty	1477	kW

Column-3		
Minimum Reflux	2.609	
Minimum Trays	18.80	
Actual Trays	40.92	
Optimal Feed	13.46	
Condenser Duty	-2271	kW
Reboiler Duty	3158	kW

Figure 35: Direct Sequence for Distillation Columns



Feed		
Temperature	37.00	C
Pressure	301.0	kPa
Molar Flow	343.0	kgmole/h
Master Comp Mole Frac (n-Butane)	0.0190	
Master Comp Mole Frac (i-Pentane)	0.0641	
Master Comp Mole Frac (n-Pentane)	0.0450	
Master Comp Mole Frac (2-Mpentane)	0.0801	
Master Comp Mole Frac (n-Hexane)	0.0430	
Master Comp Mole Frac (Benzene)	0.0861	
Master Comp Mole Frac (3-Mhexane)	0.0200	
Master Comp Mole Frac (Toluene)	0.2472	
Master Comp Mole Frac (E-Benzene)	0.0350	
Master Comp Mole Frac (p-Xylene)	0.0420	
Master Comp Mole Frac (m-Xylene)	0.1221	
Master Comp Mole Frac (o-Xylene)	0.0551	
Master Comp Mole Frac (1M2-EBenzene)	0.0470	
Master Comp Mole Frac (135-MBenzene)	0.0771	
Master Comp Mole Frac (14-EBenzene)	0.0170	

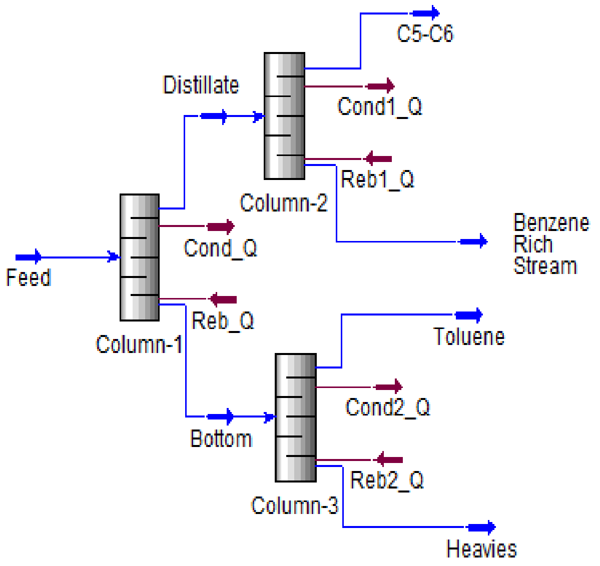
Column-1		
Minimum Reflux	0.8445	
Minimum Trays	16.99	
Actual Trays	40.90	
Optimal Feed	25.94	
Condenser Duty	-1902	kW
Reboiler Duty	5787	kW

Column-2		
Minimum Reflux	6.465e-002	
Minimum Trays	7.366	
Actual Trays	26.58	
Optimal Feed	10.15	
Condenser Duty	-143.7	kW
Reboiler Duty	85.62	kW

Column-3		
Minimum Reflux	2.853	
Minimum Trays	11.24	
Actual Trays	24.77	
Optimal Feed	9.437	
Condenser Duty	-2104	kW
Reboiler Duty	1118	kW

Figure 36: Indirect Sequence for Distillation Columns

Feed		
Temperature	37.00	C
Pressure	301.0	kPa
Molar Flow	343.0	kgmole/h
Master Comp Mole Frac (n-Butane)	0.0190	
Master Comp Mole Frac (i-Pentane)	0.0641	
Master Comp Mole Frac (n-Pentane)	0.0450	
Master Comp Mole Frac (2-Mpentane)	0.0801	
Master Comp Mole Frac (n-Hexane)	0.0430	
Master Comp Mole Frac (Benzene)	0.0861	
Master Comp Mole Frac (3-Mhexane)	0.0200	
Master Comp Mole Frac (Toluene)	0.2472	
Master Comp Mole Frac (E-Benzene)	0.0350	
Master Comp Mole Frac (p-Xylene)	0.0420	
Master Comp Mole Frac (m-Xylene)	0.1221	
Master Comp Mole Frac (o-Xylene)	0.0551	
Master Comp Mole Frac (1M2-EBenzene)	0.0470	
Master Comp Mole Frac (135-MBenzene)	0.0771	
Master Comp Mole Frac (14-EBenzene)	0.0170	

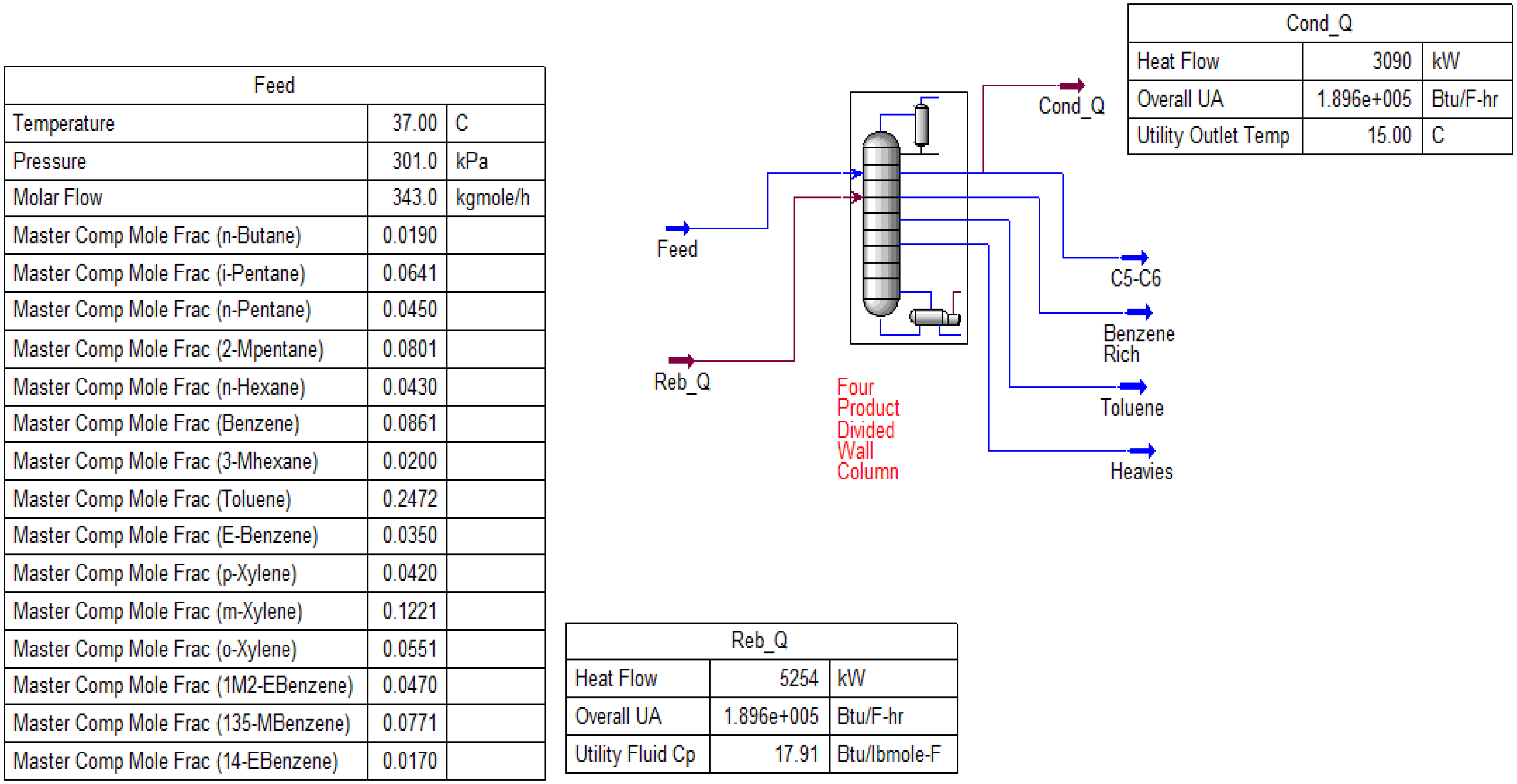


Column-1		
Minimum Reflux	0.2785	
Minimum Trays	6.999	
Actual Trays	20.03	
Optimal Feed	15.70	
Condenser Duty	-331.2	kW
Reboiler Duty	3355	kW

Column-3		
Minimum Reflux	2.516	
Minimum Trays	19.10	
Actual Trays	41.65	
Optimal Feed	14.60	
Condenser Duty	-2243	kW
Reboiler Duty	3098	kW

Column-2		
Minimum Reflux	2.065	
Minimum Trays	18.14	
Actual Trays	40.15	
Optimal Feed	17.49	
Condenser Duty	-1488	kW
Reboiler Duty	1157	kW

Figure 37: Distributed Sequence for Distillation Columns



Feed		
Temperature	37.00	C
Pressure	301.0	kPa
Molar Flow	343.0	kgmole/h
Master Comp Mole Frac (n-Butane)	0.0190	
Master Comp Mole Frac (i-Pentane)	0.0641	
Master Comp Mole Frac (n-Pentane)	0.0450	
Master Comp Mole Frac (2-Mpentane)	0.0801	
Master Comp Mole Frac (n-Hexane)	0.0430	
Master Comp Mole Frac (Benzene)	0.0861	
Master Comp Mole Frac (3-Mhexane)	0.0200	
Master Comp Mole Frac (Toluene)	0.2472	
Master Comp Mole Frac (E-Benzene)	0.0350	
Master Comp Mole Frac (p-Xylene)	0.0420	
Master Comp Mole Frac (m-Xylene)	0.1221	
Master Comp Mole Frac (o-Xylene)	0.0551	
Master Comp Mole Frac (1M2-EBenzene)	0.0470	
Master Comp Mole Frac (135-MBenzene)	0.0771	
Master Comp Mole Frac (14-EBenzene)	0.0170	

Cond_Q		
Heat Flow	3090	kW
Overall UA	1.896e+005	Btu/F-hr
Utility Outlet Temp	15.00	C

Reb_Q		
Heat Flow	5254	kW
Overall UA	1.896e+005	Btu/F-hr
Utility Fluid Cp	17.91	Btu/lbmole-F

Figure 38: Four Product Divided Wall Distillation (Kaibel) Column

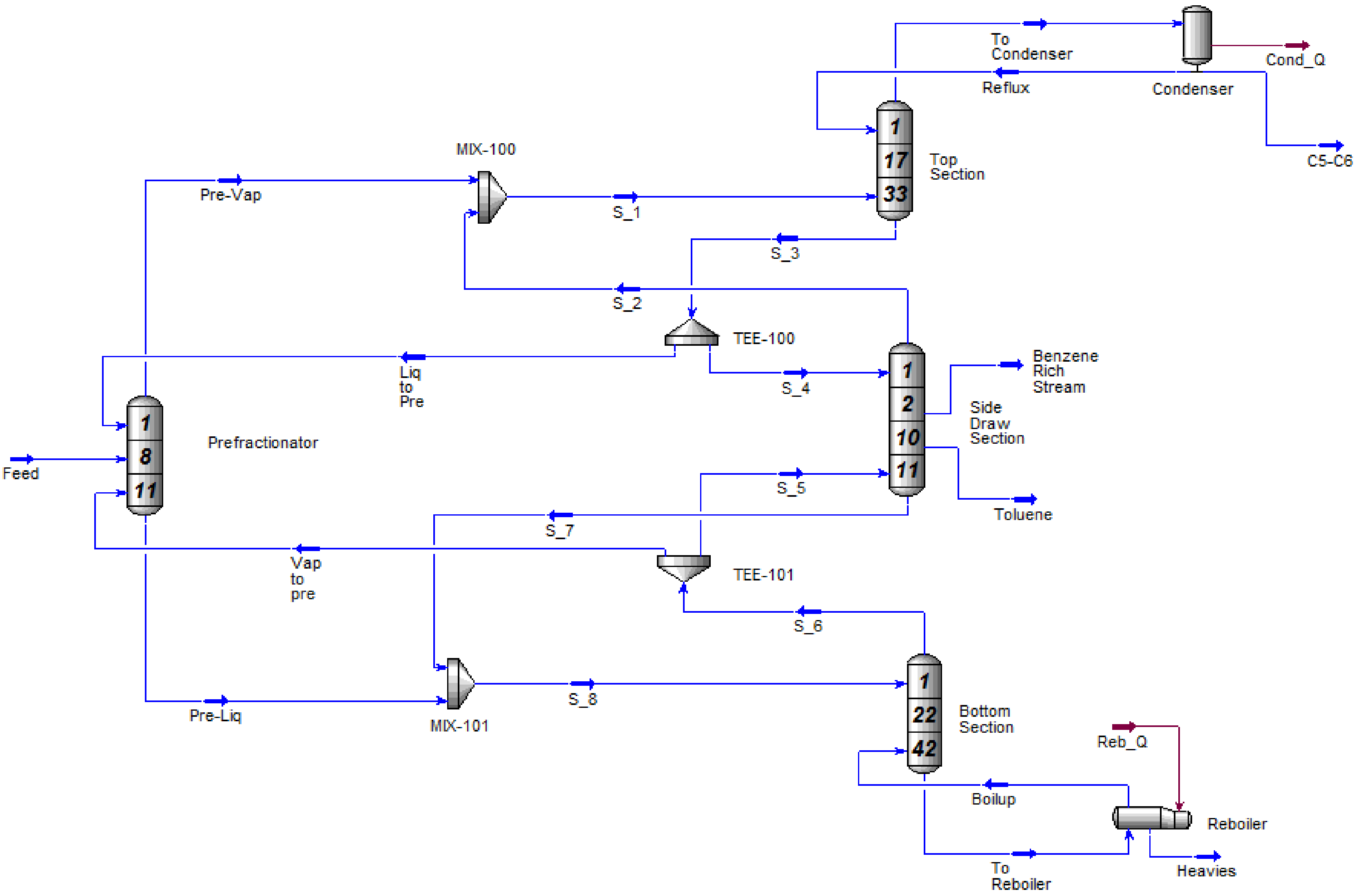


Figure 39: Sub Flow Sheet made under column environment of Kaibel Distillation Column

The product outlet condition and composition obtained from the simulations (direct sequence and indirect sequence for distillation column arrangements) converged in Figures 35 and 36 are shown in the table 05 below. While the simulation results obtained for distributed sequence and divided wall distillation column are shown in table 06 below. The units of temperature, pressure and molar flow are **ºC**, **kPa** and **kgmole/hr** respectively.

Table 5: Simulations results obtained from Direct and Indirect Sequences

	DIRECT SEQUENCE				INDIRECT SEQUENCE			
	C_5-C_6	BRC	Toluene	Heavies	C_5-C_6	BRC	Toluene	Heavies
Temperature	78	110.3	157.10	204.8	89.45	148.2	158.5	201.2
Pressure	280	270	320	370	320	370	317	345
Molar Flow	66.3	56.66	85.27	134.8	84.08	118.5	5.295	135.20
Master component mole fraction								
n-Butane	0.098	0.00	0.00	0.00	0.0776	0.00	0.00	0.00
i-Pentane	0.331	0.0001	0.00	0.00	0.2614	0.00	0.00	0.00
n-Pentane	0.233	0.0005	0.00	0.00	0.1837	0.00	0.00	0.00
2-MPentane	0.278	0.159	0.00	0.00	0.3126	0.01	0.00	0.00
n-Hexane	0.046	0.2066	0.00	0.00	0.1243	0.0364	0.00	0.00
Benzene	0.013	0.5055	0.0003	0.00	0.04	0.2208	0.0016	0.00
3-Mhexane	0.0001	0.1182	0.0019	0.00	0.0004	0.0576	0.0010	0.00
Toluene	0.00	0.010	0.9864	0.001	0.00	0.6746	0.8952	0.001
E-Benzene	0.00	0.00	0.0042	0.0865	0.00	0.0003	0.0407	0.0871
p-Xylene	0.00	0.00	0.0019	0.1058	0.00	0.0001	0.0156	0.1060
m-Xylene	0.00	0.00	0.005	0.3076	0.00	0.0002	0.0420	0.3081
o-Xylene	0.00	0.00	0.0004	0.1399	0.00	0.00	0.0038	0.1396
1M2-Ebenzene	0.00	0.00	0.00	0.1197	0.00	0.00	0.00	0.1194
135-Mbenzene	0.00	0.00	0.00	0.1962	0.00	0.00	0.00	0.1956
14-Ebenzene	0.00	0.00	0.00	0.0433	0.00	0.00	0.0	0.0432

Table 6: Simulation results obtained from Distributed and Dividing-Wall Distillation Column

	DISTRIBUTED SEQUENCE				**DIVIDED WALL COLUMN**			
	C_5-C_6	BRC	Toluene	Heavies	C_5-C_6	BRC	Toluene	Heavies
Temperature	81.8	121.3	155.5	204.8	70.48	117.2	148.4	200
Pressure	270	317	320	370	270	284.6	335.7	370
Molar Flow	81.14	39.64	87.29	134.9	79.54	22.31	106.2	134.9
Master component mole fraction								
n-Butane	0.0804	0.00	0.00	0.00	0.0819	0.0001	0.00	0.00
i-Pentane	0.2708	0.00	0.00	0.00	0.2730	0.0017	0.00	0.00
n-Pentane	0.1904	0.00	0.00	0.00	0.19	0.0013	0.00	0.00
2-MPentane	0.3322	0.01	0.0013	0.00	0.2856	0.0654	0.0016	0.00
n-Hexane	0.1132	0.1351	0.0025	0.00	0.1318	0.0415	0.0014	0.00
Benzene	0.00	0.6481	0.0318	0.00	0.0376	0.6922	0.0312	0.00
3-Mhexane	0.00	0.1053	0.0308	0.00	0.00	0.1030	0.3110	0.00
Toluene	0.00	0.1008	0.9242	0.001	0.00	0.0948	0.9412	0.0958
E-Benzene	0.00	0.0002	0.0035	0.0868	0.00	0.00	0.0015	0.0747
p-Xylene	0.00	0.0001	0.0015	0.1759	0.00	0.00	0.0011	0.0719
m-Xylene	0.00	0.0003	0.0040	0.2378	0.00	0.00	0.0012	0.2874
o-Xylene	0.00	0.0001	0.0003	0.1398	0.00	0.00	0.0019	0.1243
1M2-Ebenzene	0.00	0.00	0.00	0.1196	0.00	0.00	0.00	0.1146
135-Mbenzene	0.00	0.00	0.00	0.1959	0.00	0.00	0.00	0.1885
14-Ebenzene	0.00	0.00	0.00	0.0433	0.00	0.00	0.00	0.0427

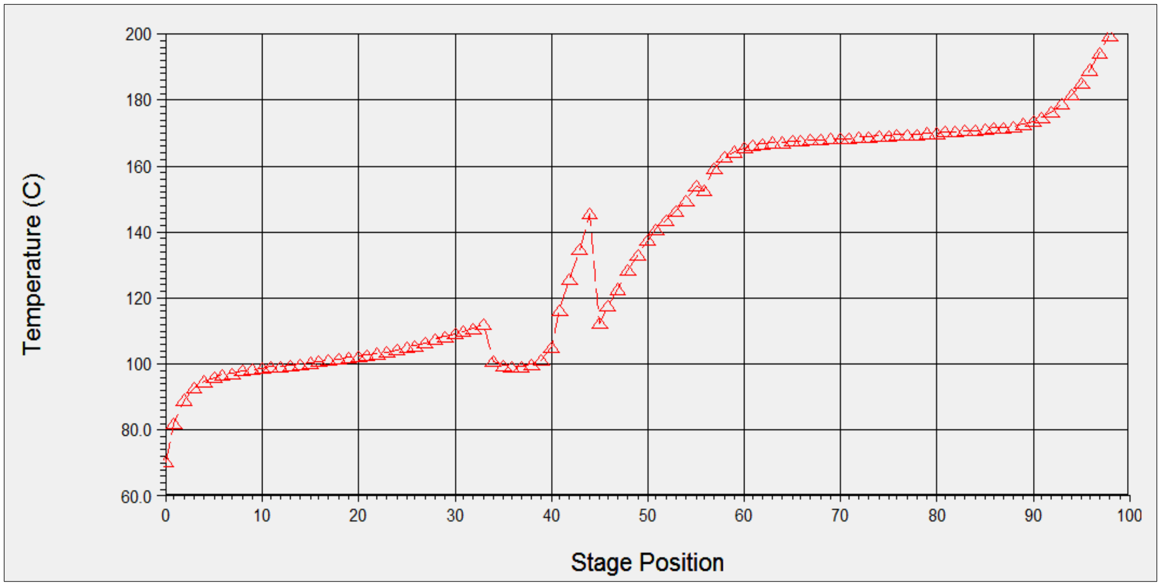


Figure 40: Temperature profile throughout the distillation column

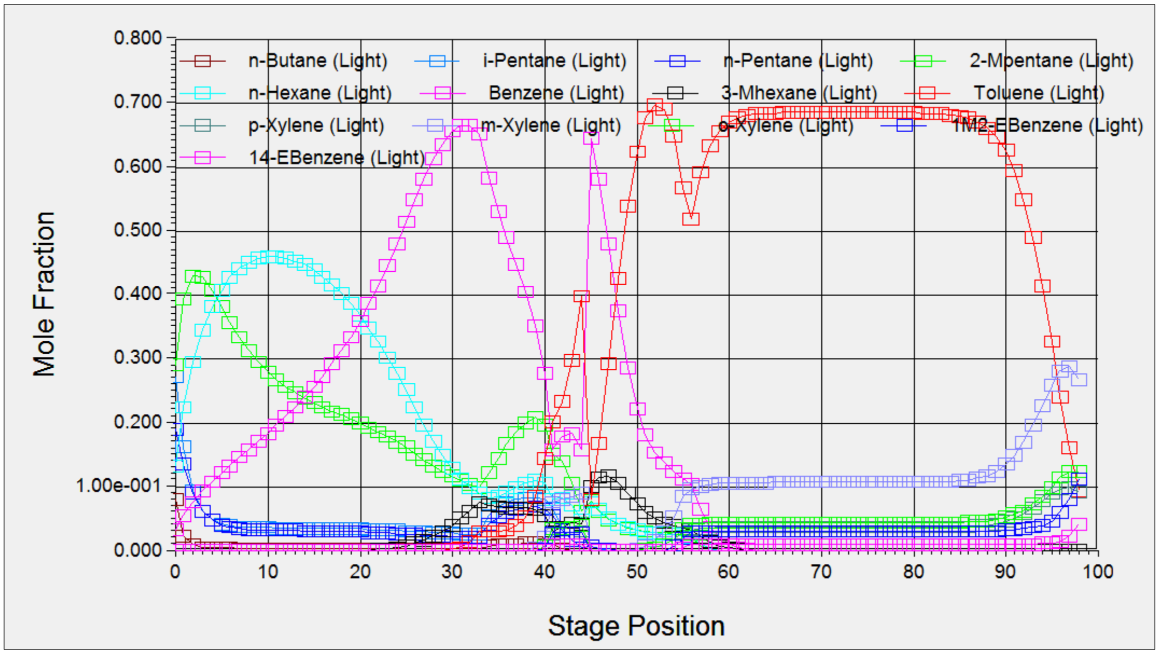
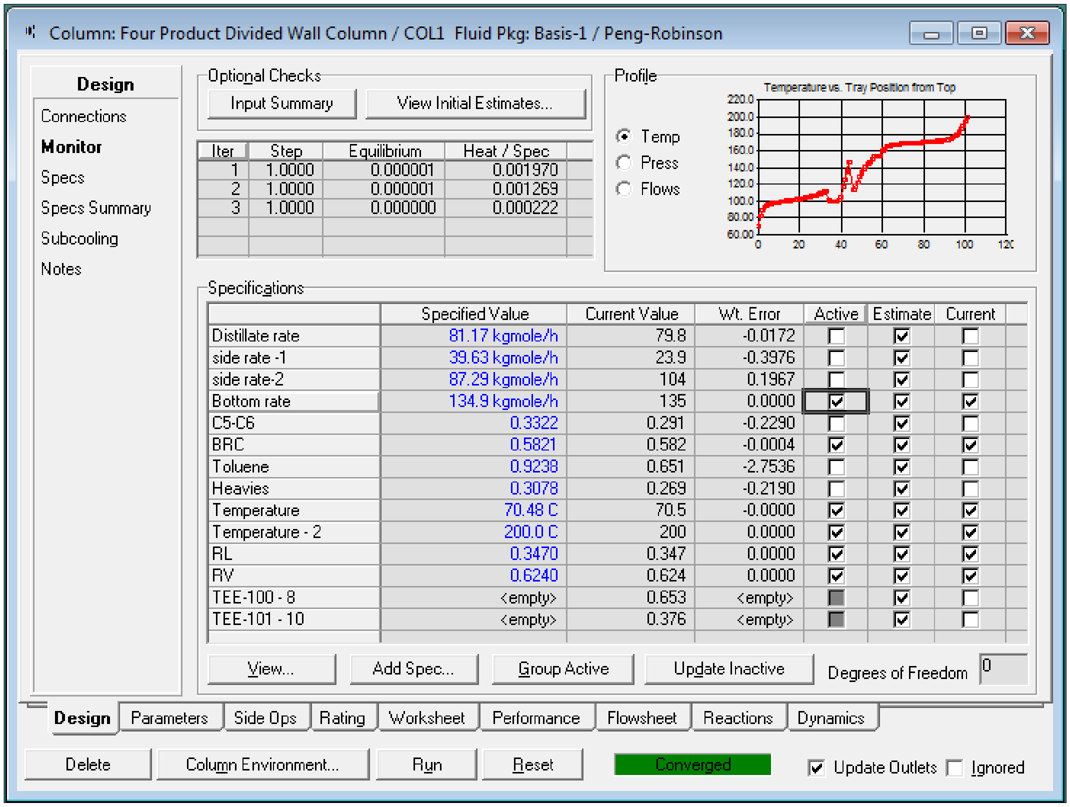


Figure 41: Composition profile of the distillation column



Column: Four Product Divided Wall Column / COL1 Fluid Pkg: Basis-1 / Peng-Robinson

Iter	Step	Equilibrium	Heat / Spec
1	1.0000	0.000001	0.001970
2	1.0000	0.000001	0.001269
3	1.0000	0.000000	0.000222

● Temp
○ Press
○ Flows

	Specified Value	Current Value	Wt. Error	Active	Estimate	Current
Distillate rate	81.17 kgmole/h	79.8	-0.0172	☐	☑	☐
side rate -1	39.63 kgmole/h	23.9	-0.3976	☐	☑	☐
side rate-2	87.29 kgmole/h	104	0.1967	☐	☑	☐
Bottom rate	134.9 kgmole/h	135	0.0000	☑	☑	☑
C5-C6	0.3322	0.291	-0.2290	☐	☑	☐
BRC	0.5821	0.582	-0.0004	☑	☑	☑
Toluene	0.9238	0.651	-2.7536	☐	☑	☐
Heavies	0.3078	0.269	-0.2190	☐	☑	☐
Temperature	70.48 C	70.5	-0.0000	☑	☑	☑
Temperature - 2	200.0 C	200	0.0000	☑	☑	☑
RL	0.3470	0.347	0.0000	☑	☑	☑
RV	0.6240	0.624	0.0000	☑	☑	☑
TEE-100 - 8	<empty>	0.653	<empty>	■	☑	☐
TEE-101 - 10	<empty>	0.376	<empty>	■	☑	☐

Degrees of Freedom 0

Converged

☑ Update Outlets ☐ Ignored

Figure 42: Convergence Window for Aromatic case obtained from Aspen HYSYS

An aromatic stream obtained from an oil refinery facility was charged to Kaibel distillation column in order to obtain some pure streams like Benzene, Toluene and other heavier components. Distillation column is simulated in the Aspen HYSYS and one product compositions, one product flow rate, liquid & vapor splits ratios and temperatures at the top & bottom of the distillation column was specified as shown in the above Figure 42.

The main composition of key component in all the products and the heat energy required to achieve the required results are shown in the below Table 07. According the results, about 31 % of heat energy can be saved by using divided wall distillation column as compared to distributed sequence of distillation columns. Although the product composition obtained are almost the same as the others.

Table 7: Overall simulation results obtained from all possible distillation columns arrangements

Column Arrangements	C_5-C_6 (C5 family)	BRC (Benzene)	Toluene	Heavies	Heat Energy (kW)
Direct Sequence	0.84	0.50	0.98	0.80	7437
Indirect Sequence	0.75	0.22	0.89	0.80	6990.62
Distributed Sequence	0.79	0.64	0.92	0.73	7610
Dividing Wall Column	0.75	0.69	0.94	0.75	5254

CHAPTER 6

CONTROL OF DIVIDED WALL COLUMN

In the past, it was very difficult to achieve the required performance of process plants. Because regulatory environmental conditions, variable economic conditions, market competition and safety regulations were the key factors which usually make difficult to target the required product specifications. Along this, another complication was that modern plants having highly integrated process and complex operation were also not easy to operate. For such process plants, it is not easy to eliminate the disturbance without interfering the other connected process units. To overcome such complications and unsafe plant operation, researchers and many scholars focused on “process control” and “process dynamics”. These two subjects lead the process plant operation to a safe and economic way.

6.1 Introduction to Process Control

The main concern of process control is to operate the process plant at the desired operating conditions, by following the safety and environmental standards. In order to achieve the plant safety and the required product specification, it is very important to implement the process control conditions. Because this subject knows that how to achieve the targets. At large scale of process plants like oil refineries, fertilizer plants and other petrochemical plants have thousands of process variables which should be controlled at the desired value. For example, composition of products, reactor temperature, vessel level, column pressure etc. are the some key variables which should be controlled at the given set point. Without the control of such variables, it is impossible to get the required product specifications. This is why, the subject of process control got a key importance in the field of chemical engineering.

On the other side, process dynamics deals with the unsteady state processes. Transient process (unsteady state) occurs during the start-up, shutdown of process plants and other unexpected process disturbances. With the passage of time, both these field get developed and ultimately engineers achieve the optimal operation and control. In this chapter, the process control and process dynamics is implemented on multi-products divided wall distillation column with the help of commercial simulation software (Aspen HYSYS). Before approaching towards the main process, it is very important to define some key terms, rules etc. of this field.

In the field of process control, three different types of process variables are there; controller variable, manipulated variable and disturbance variables. They can be defined as;

Controlled variable (CVs): The process variable that should be controlled in order to get the desired product specifications. The desired value of this variable is also known as "set point".

Manipulated variable (MVs): The process variables that are regulated or manipulated in order to keep the controlled variables at it set point value or very near to it. In most cases, the manipulated variables are flow rates.

Disturbance variables (DVs): These are process variables which disturb the controlled variables and cannot regulated or adjust. They are generally occur with the change of environmental conditions, change in feed composition etc. some disturbances can be measured and avoided before charging to plant, but some cannot be measured.

In the design and analysis of control system, the process variables are usually classified as either "output variables" or "input variables". The output variables are known as dependent variables, which usually depends upon the process conditions of the system like product composition, vessel level, temperature and flowrate etc. these variables are also associated with the outlet streams. In order to achieve perfect control, some of the output variables should be controlled and these variables are known as controlled variables, as described above. On the other hand, the variables which directly affect the one or more output variables are known as input variables and these input variables can be put in the category of manipulated variables or disturbance variables. Actually, manipulated variables are very important because they are manipulated to adjust the product flow rates, vessel temperature, pressure and level etc.

6.2 Classification of Process Control Strategies

It is very important to discuss the different process control strategies and their relative advantages and disadvantages. The operation of any process plant can be controlled with number of control strategy such as feedback control, feedforward control, or combination of both feedback and feedforward strategies can also be used and many others. The interesting feature of feedback control system is that it measures the controlled variable and compares the value with the set point. This will tell us the error or idea that how much difference is there between our controlled variable and the given set point. After comparing the values, it takes action to adjust the manipulated variable in order to achieve the set point value. This control scheme do not measure the disturbance variable. But the corrective action of feedback control did not account the source of disturbance. Another scheme is known as feedforward control strategy. In this scheme, disturbance variable is measured and controller takes corrective action before the deviation of controlled variable from the set point. This control system do not measure the controlled variable. The key disadvantages of feedforward scheme are 1) the disturbance variable should be measured accurately with precise measuring devices 2) no corrective action will be taken for an unknown or unmeasured disturbance occurred in the process system 3) a process model should be available.

The Figure 43 shown below is the block diagram of feedback control system. Which are showing the basic and important elements of any process control loop. For example, in any control loop there will be a controller, final control element and process measuring device. If we start the explanation of the below block diagram from the set point then it will be easy to understand the basic working principle of all the feedback control loops. Actually before a controller, there is a comparator which compares the given set point value with the measured process value from a measuring device (e.g. temperature, pressure, level measuring devices etc.). There will be three possibilities here that the set point value may be equal, greater or smaller than the measured process value. According to the result, controller gives signal to final control element in order to reach the set point. According the process, we can install proportional (P), Proportional Integral (PI) or Proportional Integral Derivative (PID) controller. The final control element is usually a control vale in most of the cases. Which either opens or close its stem opening as per the instruction given by controller signal. So that a controlled stream can be introduced in the system or process.

But there are some disturbances which may occur from any source like, weather condition, varying feed conditions etc. This is why, it is necessary to measure continuously the output variable in order to operate and control the system at satisfactory level.

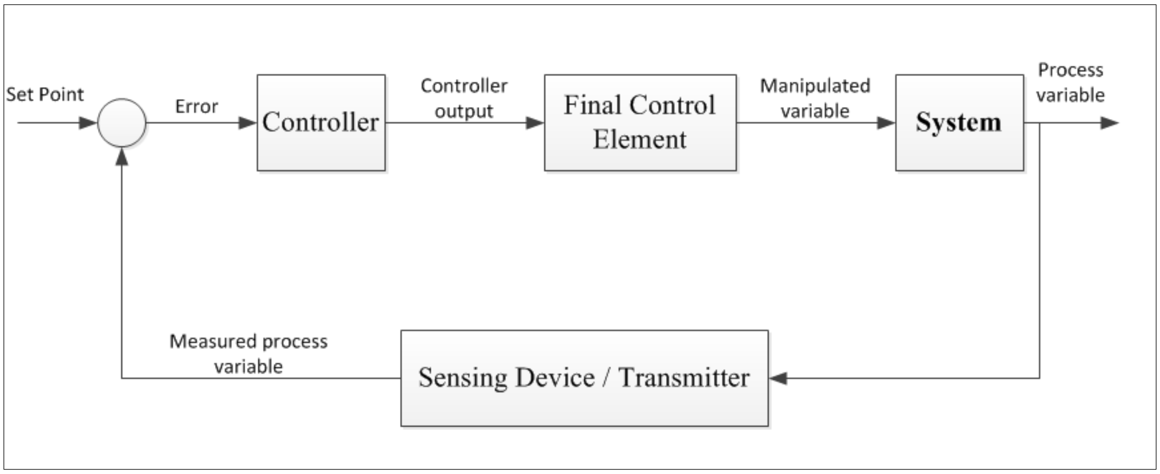


Figure 43: Block diagram for a feedback control system

Although all the elements are very important to make the system stable. But controller tuning or setting is very important for the stability of closed loop. There are number of techniques available for PID controller tuning, some of them are listed below;

i. Direct Synthesis (DS) method
ii. Internal Model Control (IMC) method
iii. Controller tuning relations
iv. Frequency response techniques
v. Computer simulation
vi. On-line tuning after the control system is installed

As the controller tuning is a huge concept in the field of process control, this is why it is not going to be discuss any more. The first two tuning methods are based on transfer functions models, while the third method are the correlations and analytical expressions for the PID controller tuning. The computer simulation method is best to see the actual dynamic behavior and performance of control system. This is why, we used here computer simulation method for the tuning of PID controller used in the case study discussed below.

6.3 Control of Dividing-Wall Distillation Column

The optimal control of four product dividing-wall (kaibel) distillation column is studied by using dynamic mode of Aspen HYSYS. Dynamic simulation are time dependent and transient nature of the distillation column can be studied. The feed consist of equimolar first four alcohol i.e. methanol, ethanol, 1-propanol and 1-butanol. It is required to achieve almost 95% pure product from each draw. For this purpose, different controllers are installed at different location of distillation column. The details of control scheme is shown in the table below. The general flow sheet diagram of four product dividing-wall distillation column is shown in Figure 44. In which, it is shown the manipulated variables used to adjust the controlled variables.

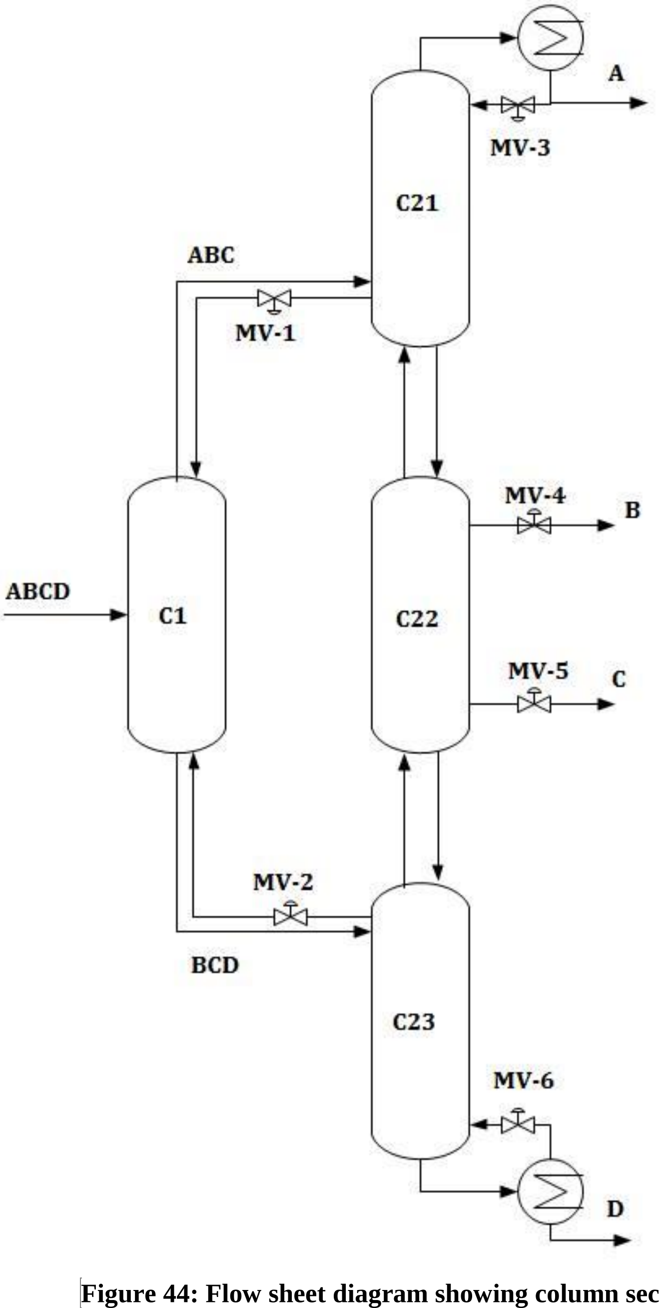


Figure 44: Flow sheet diagram showing column sections in Kaibel distillation column

Table 8: Controller used in the dynamic simulation and their objectives

Pressure Controller (PIC-100)	Controlling the top tower pressure at 101.3 kPa by manipulating the condenser duty
Reflux drum level Controller (LIC-101)	Controlling the level of reflux drum at 50% of its volume to ensure the smooth flow of distillate and reflux
Flowrate Controller (FIC-100)	Controlling the flowrate of side draw-1 at the given set point value
Flowrate Controller (FIC-101)	Controlling the flowrate of side draw-2 at the given set point value
Composition Controller (XIC-100)	Controlling the composition of side draw-1 at the given set point value by manipulating the reflux flow
Temperature Controller (TIC-100)	Controlling the bottom temperature of distillation column at a given set point value by manipulating the available heat energy
Level Controller (LIC-100)	Controlling the level of reboiler vessel to ensure the smooth flow of bottom product as well as the safety of vessel
Ratio Controller (RATIO-100)	Controlling the ratio specified of liquid split between pre-fractionator and main distillation column

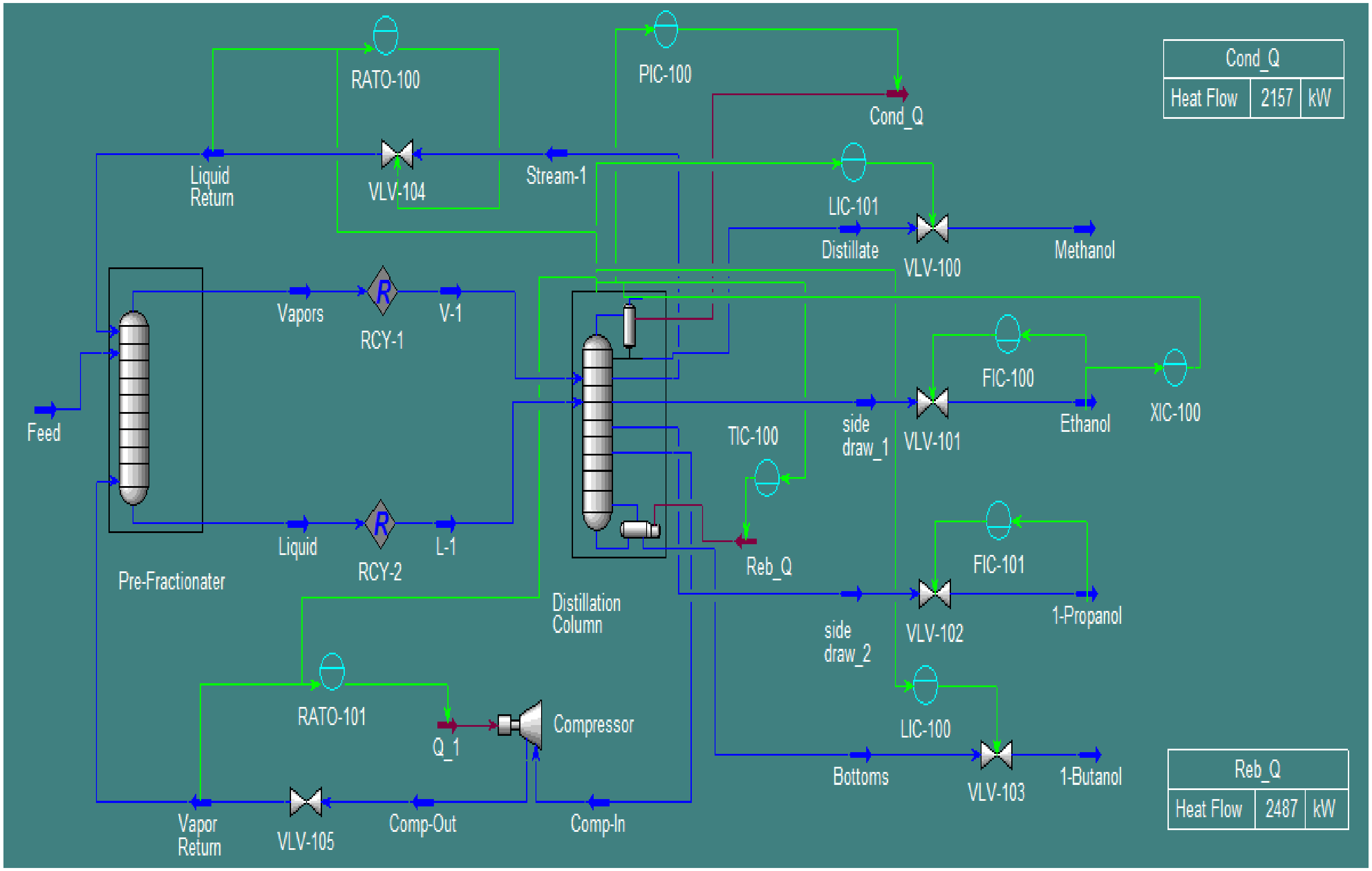


Figure 45: Dynamic simulation of Kaibel distillation column in Aspen HYSYS

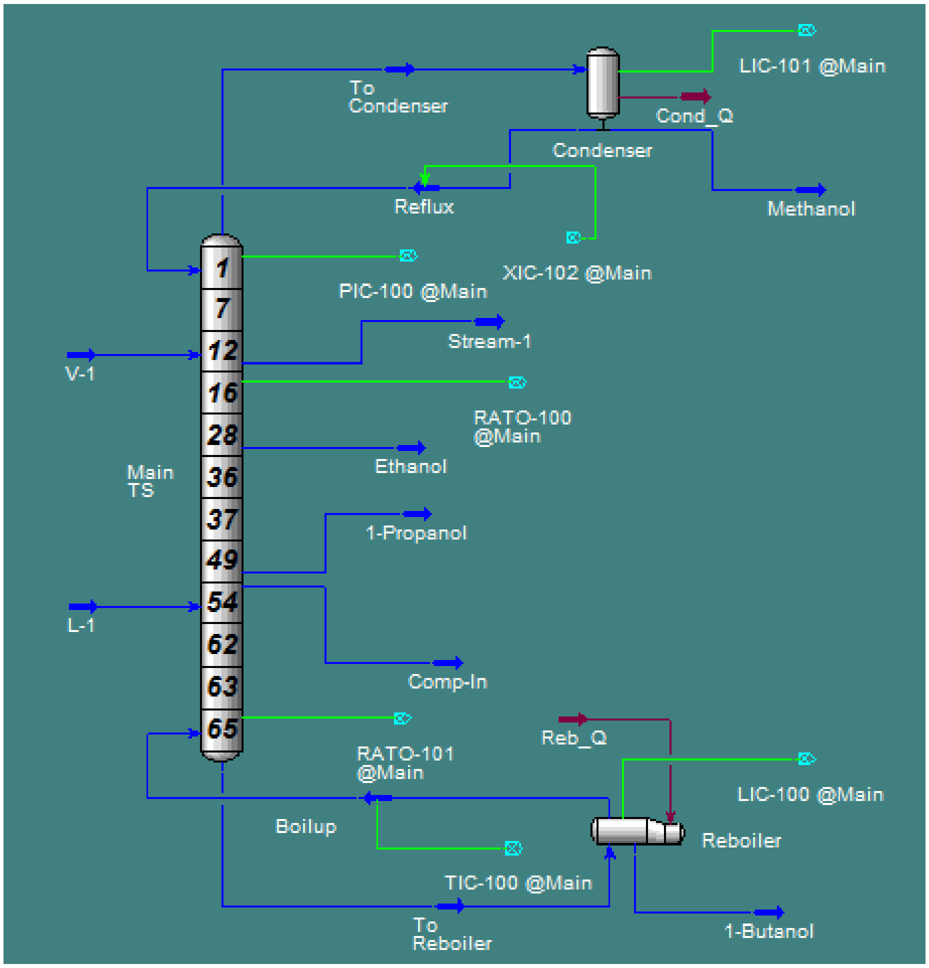
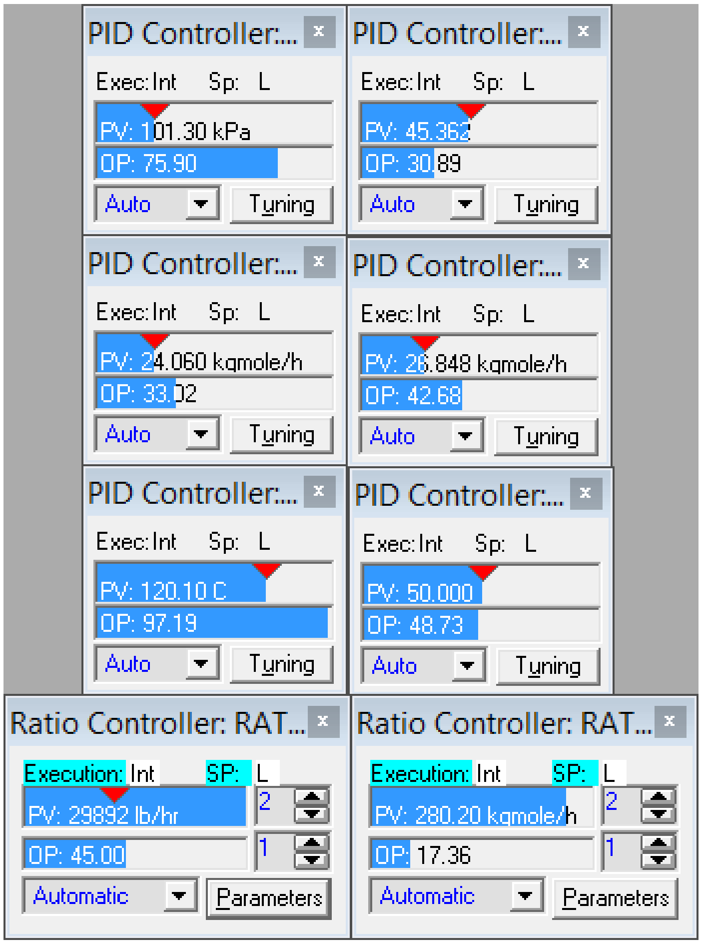


Figure 46: Column environment view of main distillation unit



PID Controller:...
Exec: Int Sp: L
PV: 101.30 kPa
OP: 75.90
Auto

PID Controller:...
Exec: Int Sp: L
PV: 45.362
OP: 30.89
Auto

PID Controller:...
Exec: Int Sp: L
PV: 24.060 kgmole/h
OP: 33.02
Auto

PID Controller:...
Exec: Int Sp: L
PV: 26.848 kgmole/h
OP: 42.68
Auto

PID Controller:...
Exec: Int Sp: L
PV: 120.10 C
OP: 97.19
Auto

PID Controller:...
Exec: Int Sp: L
PV: 50.000
OP: 48.73
Auto

Ratio Controller: RAT...
Execution: Int SP: L
PV: 29892 lb/hr 2
OP: 45.00 1
Automatic

Ratio Controller: RAT...
Execution: Int SP: L
PV: 280.20 kgmole/h 2
OP: 17.36 1
Automatic

Figure 47: Face plates of the controller used in the dynamic simulation

After the application of complete control scheme on the dividing-wall distillation column, the system was tested by giving disturbance through the feed conditions. For example, change in product flowrates, compositions and energy consumption are examined with the increase and then decrease of feed flow rate. The below Figures 48 -53 are showing the response of control scheme. Usually the disturbance was introduced after 200 minutes of dynamic simulation. It has been also observed that the almost all controller tracks the set point value and rejects the effect of disturbance as shown in the graphs. To regain the original position shows that system has the disturbance rejection capability. Sometimes the process value (PV) of controller just fluctuates around its set point value, but this fluctuations can be ignored if the product specifications allows.

At last, it can be concluded that distillation column can be controlled at its optimum value if the control strategy works proper. All the controller tuning parameters are obtained very accurate at which it can track set point value very efficiently without a considerable time delay. The PID controller tuning was done using the “Auto tuning” mode available in the dynamic simulation of Aspen HYSYS. Along this, the control strategy used in the above case study also controls the distillation column operation very accurate with the utilization of minimum heat energy.

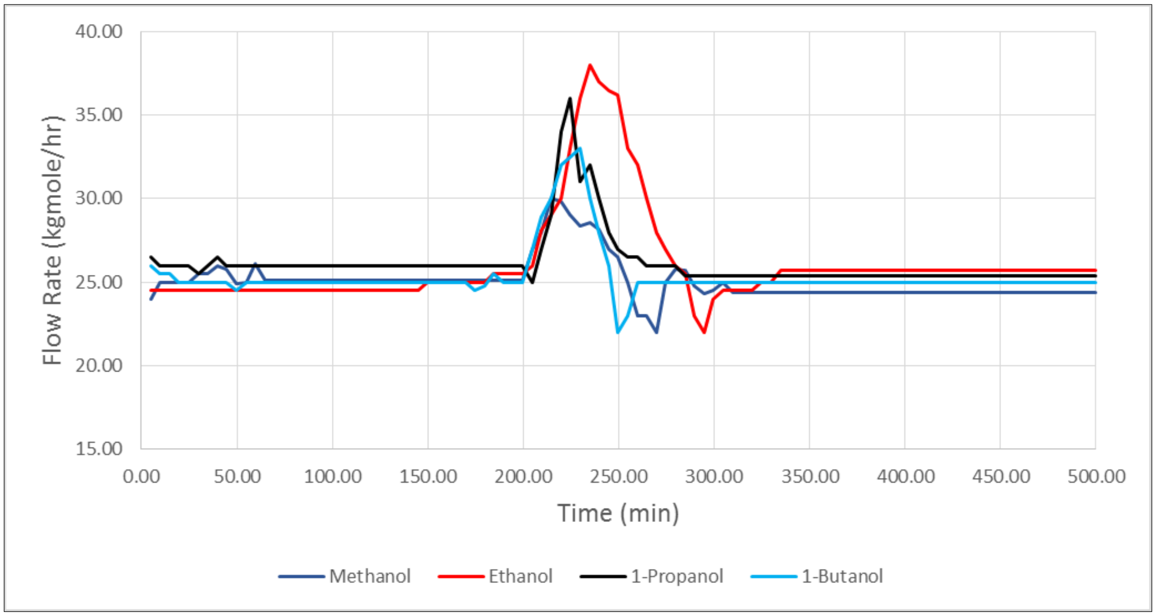


Figure 48: Response of product flowrate upon increasing feed flowrate by 20%

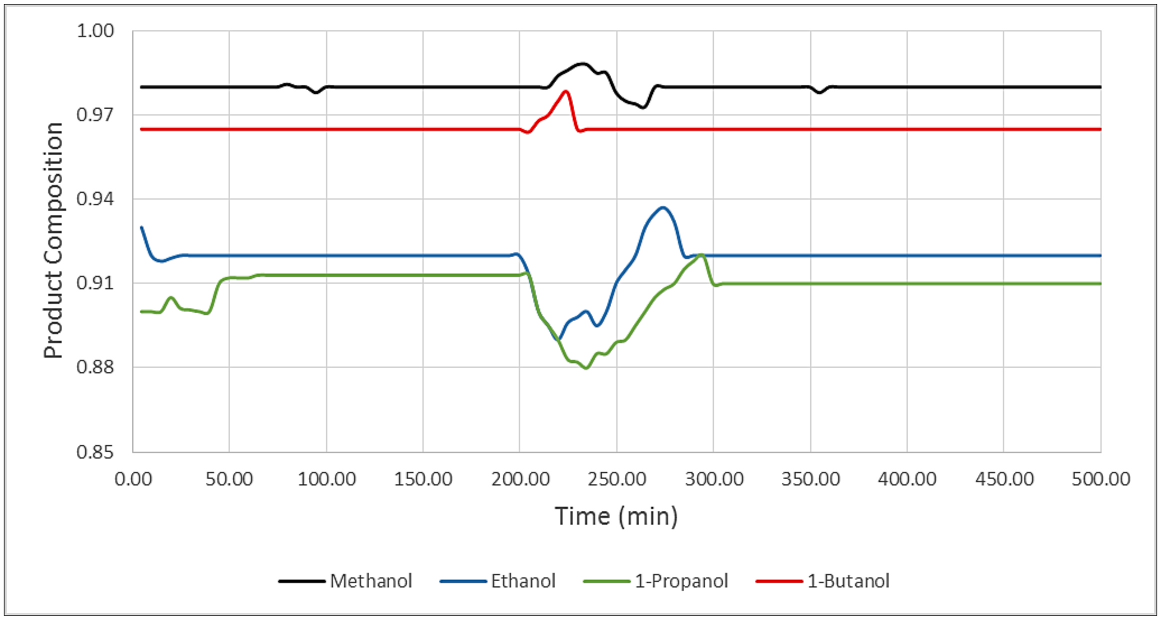


Figure 49: Response of product composition upon increasing the feed flowrate by 20%

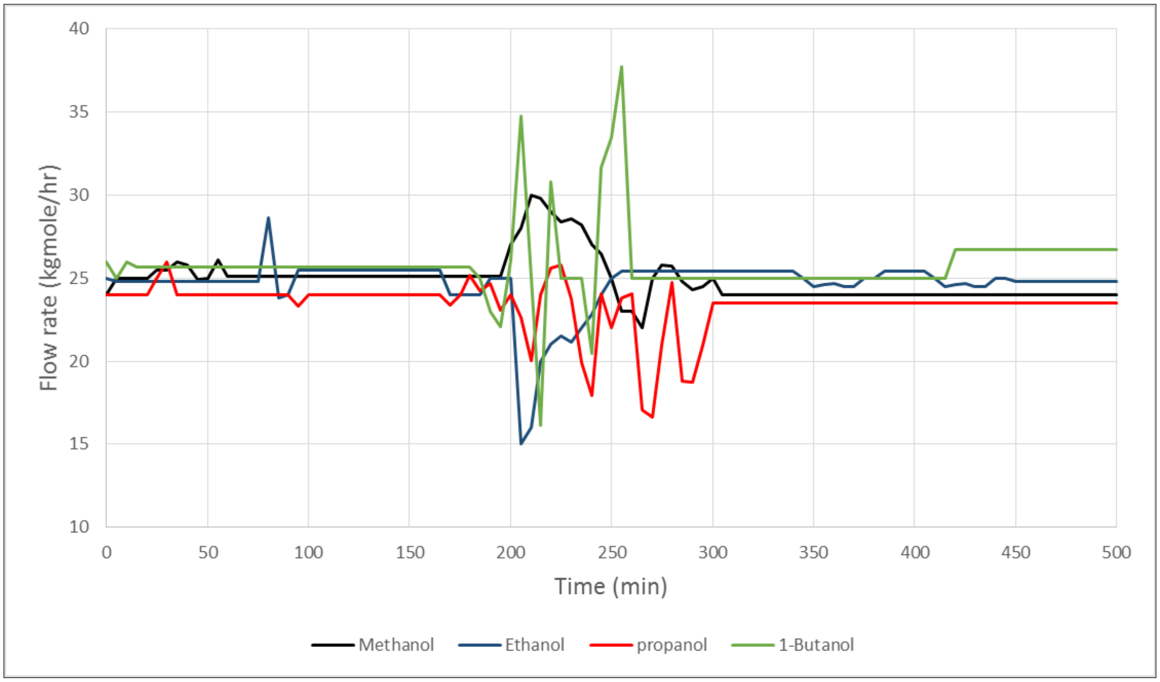


Figure 51: Response of product flowrate upon decreasing the feed flowrate by 20%

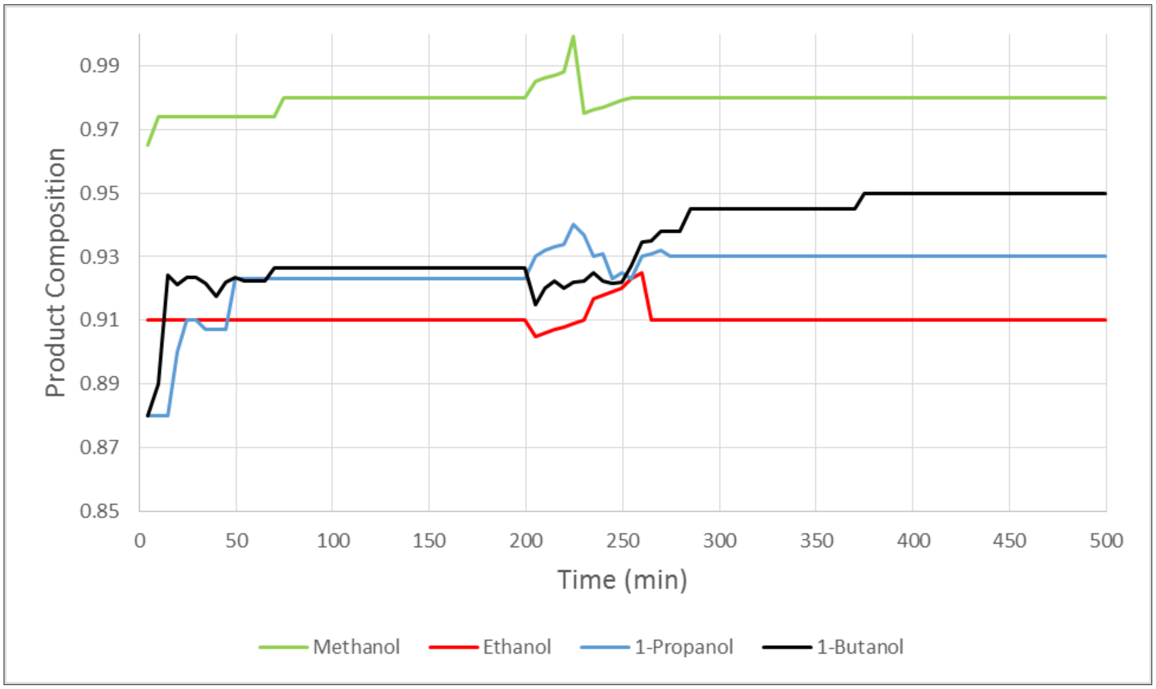


Figure 50: Response of product composition upon decreasing the feed flowrate by 20%

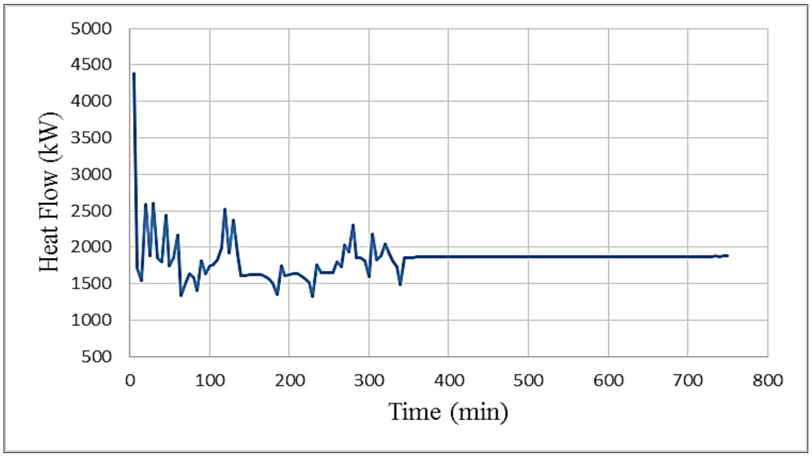


Figure 52: Response of heat energy upon increasing the feed flowrate

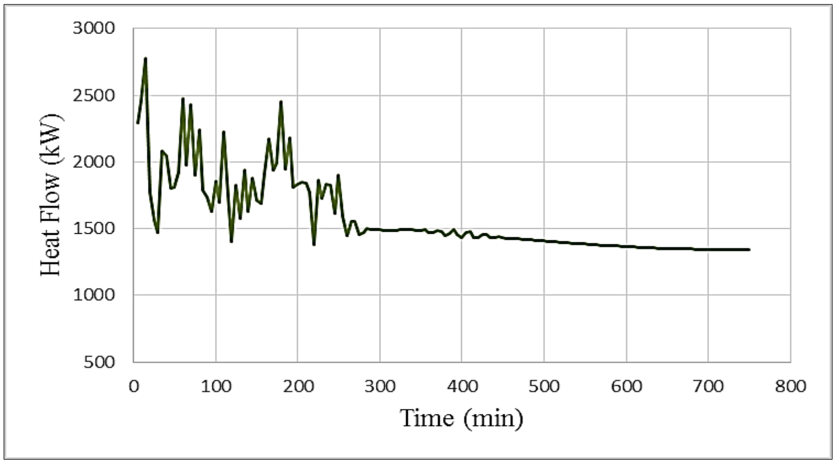


Figure 53: Response of heat energy upon decreasing the feed flowrate

The above shown Figures 52 and 53 are showing the behavior of heat energy upon increasing and then decreasing the flowrate of feed. At high feed flowrate, the system is achieving its product specification at the average value of 1900 kW. While the same results can be obtained, at less feed flowrate and low required heat energy i.e. 1450 kW.

CHAPTER 7

CONCLUSION AND RECOMMENDATION

7.1 Conclusions

In this research work, the potential advantages of using divided wall distillation column is studied and it has been concluded that divided wall distillation column is more energy efficient configuration as compared to conventional distillation column arrangements. Steady-state simulations results have shown that about 10 – 30% of energy consumption can be saved by using this typical complex configuration for distillation columns. Not only the energy consumption, considerable amount of operational and investment cost can be saved by using this complex configuration. The control of divided wall column is studied by converting the steady-state simulation to dynamic simulation in Aspen HYSYS. It has been concluded that the implemented control scheme on DWC have disturbance rejection and setpoint tracking capability.

7.2 Recommendation

In this research work, single partition wall divided wall distillation column was studied. But the efficiency towards energy saving of multi-partition wall divided wall distillation column needs to be studied. Although there is no industrial implementation of such distillation column, but it can be studied first at pilot plant and then at industrial scale. Because according to research, multi-partition wall dividing-wall distillation column is more energy efficient as compared to single partition wall distillation column.

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Vitae

Name : FARRUKH ILYAS ABID

Nationality : PAKISTANI

Date of Birth : 2/27/1991

Email : Ilyas.farukh@yahoo.com

Address : House no. A-72, Allama Iqbal Town, Lahore, Pakistan.

Academic Background : B.Sc. Chemical Engineering, University of the Punjab, Lahore, Pakistan
M.Sc. Chemical Engineering, King Fahd University of Petroleum & Minerals, KSA.

Publication : Abid, F.I., Al-Shammari, A., & Shamsuzzoha, M. “Dynamic Behavior of Kaibel Distillation Column”. Computers & Chemical Engineering (2015) (submitted).