SIMULATION STUDY OF DIVIDED WALL DISTILLATION COLUMN

A

Thesis Report

Submitted in partial fulfillment of the requirement for the award of the Degree of

Master of Technology

IN

CHEMICAL ENGINEERING

Submitted By

LOVEDEEP KAUR
Roll No. 600911006

Under the Guidance of:
Mr. V.K Sangal
Assistant Professor
Thapar University,
Patiala-147004

DEPARTMENT OF CHEMICAL ENGINEERING
THAPAR UNIVERSITY
PATIALA-147004, INDIA
JUNE 2011

DECLARATION

I hereby declare that the thesis entitled **"Simulation study of divided wall distillation column"** is an authentic record of my work carried out as per the requirements for the award of degree of **M.Tech. in Chemical Engineering** at **Thapar University, Patiala**, under the guidance of **Mr. V.K.Sangal**, **Assistant Professor, Department of Chemical Engineering**, Thapar University, Patiala during **July 2010 to June 2011**. The matter embodied in this thesis has not been submitted in part or full to any other university or institute for the award of any degree.

Dated: **(Lovedeep Kaur)**

This is to certify that above declaration made by the student concerned is correct to the best of our knowledge and belief.

Mr.V.K. Sangal
Assistant Professor
Department of Chemical Engineering
Thapar University
Patiala-147004

(Counter signed by)

Dr. D. Gangacharyulu
Professor and Head
Department of Chemical Engineering
Thapar University,
Patiala-147004

Dr. S.K. Mohapatra
Dean of Academic Affairs
Thapar University,
Patiala-147004

ACKNOWLEDGEMENT

Words are often less to revels one’s deep regards. With an understanding that work like this can never be the outcome of a single person, I take this opportunity to express my profound sense of gratitude and respect to all those who helped me through the duration of this work.

This work would not have been possible without the encouragement and able guidance of supervisor Mr. V.K Sangal. His enthusiasm and optimism made this experience both rewarding and enjoyable. Most of the novel ideas and solutions in this work are the result of our numerous stimulating discussions. His feedback and editorial comments were also invaluable for the writing of this thesis.

My heartfelt gratitude goes to Dr. D. Gangacharyulu, Head of department for providing all the facilities required for the completion of my work.

I am also very grateful to my all friends and colleague for accompanying me during the most outstanding year of my life and standing by me in every situation.

I would like to thank to all the faculty members and employees of Chemical Engineering Department, Thapar University, and Patiala for their everlasting support.

Last but not least, I would like to thank “ALMIGHTY” for his blessings and all HIS and kindness.

Lovedeep Kaur
Registration No: 600911006

ABSTRACT

Separations performed in distillation columns are responsible for largest fraction of immense amount of energy consumed in process industries. Application of non-standard complex column arrangements can lead to substantial savings in energy consumption. Among these alternatives, dividing-wall columns (DWCs) for separating mixtures of three or more components appear to be the most attractive as they provide substantial savings in both energy consumption as well as capital investment.

Dividing wall column (DWC) is a single shell, fully thermally coupled distillation column capable of separating mixtures of three or more components into high purity products. Compared to conventional columns-in-series and/or in-parallel configurations, a DWC requires much less energy, capital and space. This makes DWC to something that corresponds with the present day idea of sustainable process technology.

The simulation of a non-standard column like DWC is more complex than that of a conventional distillation as there are more degrees of freedom involved and more parameters to be manipulated. Simulation studies were done in ASPEN but it does not include a DWC in its library operations. Hence, DWC is simulated based on the configuration of fully thermally coupled column, called Petlyuk column. The MultiFrac model of ASPEN Plus™ has been used For rigorous simulation.

The purpose of this study was to investigate the effects of structural and operational variables on product purities, reboiler duty and pressure across the divided wall for C4, C5, and C6 ternary separation in a DWC.

The structural variables such as feed location, side location, number of stages in main column and in postfractionator and liquid and vapor split locations have no significant effect on reboiler duty, but the position of divided wall have a small effect on energy efficiency of DWC. The liquid and vapour split locations affects the side stream purities more as compared to top and bottom product purities. The pressure drop across the divided wall is greatly affected by varying liquid and vapor split locations towards the bottom of the column.

The operational variables liquid split ratio and vapour split ratio affects the side stream purity significantly as compared to distillate and bottom product purities. The operational variables, reflux ratio and vapour split shows a great effects on pressure drop across the divided wall as compare to liquid split ratio. The operational variables such as reflux ratio, liquid split and vapor split ratio have a great affect on the reboiler duties.

The thermodynamic efficiency of DWC is 28.3% more than the columns in direct sequence. The total annualized cost of DWC is 28% less than the column in direct sequence.

CONTENTS

Page Number

LIST OF FIGURES

LIST OF TABLES

ABBREVATIONS

DWC	Divided Wall Column
CPI	Chemical Process Industry
LK	Light Key
HK	Heavy Key
MK	Middle Key
C2C	Conventional two column
VLE	Vapor-Liquid Equilibria
PR	Peng-Robinson
CEPCI	Chemical Engineering Plant Cost Index

CHAPTER 1

INTRODUCTION

Efficient design of separation systems is the key to success in chemical process industry (CPI). Distillation is still the bullwork of the separation technology in CPI, even when important developments have taken places in new separation technologies in the last two decades. Distillation continues to be the most important separation method although it is the most energy intensive unit operation.

Distillation is defined as:

A process in which a liquid or vapor mixture of two or more components are separated into its component fractions of desired purity, by the application and removal of heat.

Separations performed in distillation columns are responsible for largest fraction of immense amount of energy consumed in process industries. Therefore distillation operations became a major concern within sustainability challenge, i.e. a primary target of energy saving efforts in industrially developed countries. Being by far the most widely used separation process in industrial practice, utilizing largest scale equipment, distillation is also one of most capital intensive process technologies. Driven by global industrial growth it tends to grow in both number and size of applications (Olujic et al., 2009). Hence the present day challenge is to design distillation systems that at the same time are sustainable and economically feasible, i.e. industrially viable.

When considering the workhorse of process industry, a distillation column with one feed and two, i.e. overhead and bottom products, a better overall performance can be achieved, if appropriate, by employing better operation and control, by using more advanced column internals. These options are particularly interesting because they allow capacity and/or efficiency increase (reduction of specific energy requirement) of existing columns at minimum investment. However substantial energy savings can be expected only from implementation of energy saving concepts in new designs.

A problem with new designs, i.e. implementation of highly efficient energy saving technologies is that these are generally capital intensive. Typical example is employment of heat pump assisted distillation, which, technically speaking solves the problem at its source, by avoiding use of external heat source in reboiler. However, due to high capital expenditures required to purchase fitting compressor, it appeared to be industrially viable only in case of large capacity, end of the train (practically binary) separations of close boiling mixtures which require minimum compressor/compression effort related costs. This appeared to be the case mainly with separation of rather light hydrocarbons, like C_2, C_3 and C_4 components, where adiabatic exponent of substances is large enough to enable a significant temperature rise by a relatively low compression effort. Costlier and more risk associated option in this respect is to implement theoretically and experimentally proven, but industrially not yet applied column configurations that offer potential for energy saving beyond that achievable with conventional heat pump assisted distillations. Typical example is so called internally heat integrated column, which, by combining direct vapour recompression with uniform distribution of heat duty along integrated part of the column allows minimization of energy requirement of a distillation column. However, being a heat pump assisted process requiring a heavy heat transfer infrastructure to enable a uniform distribution of required heat duty along the column, a heat integrated column represents a complex and capital highly intensive column configuration (Olujic et al., 2006).

In binary distillation, a feed mixture of two components is separated into two products, including and often limited to, an overhead distillate and a bottoms, whose compositions differ from that of feed. Most often, the feed is a liquid or vapor-liquid mixture. The bottom product is almost always a liquid, but the distillate may be liquid or a vapor or both.

Distillation is used for about 95% of liquid separations in chemical process industries, and the energy used for this accounts for an estimated 3% of world's energy consumption (Hewitt et al., 1999). For separation of a binary mixture, a single distillation column which consists of single reboiler and condenser is used. The Light key (LK) component is recovered from the top and Heavy key (HK) component is recovered from the bottom.

Distillation is well suited for the separation of high purity products from a liquid mixture since any degree of separation can be obtained by increasing the number of trays (equilibrium stages) in one column. For more than two components in the mixtures (or mixtures forming azeotropes) cascading of more than one distillation column is required. The column sequencing leads to increase the energy consumption because as number of columns increases, the energy consumption will also increase. So, the heat integrated column arrangements are used which saves 30-40% of energy. The thermal coupling of column will leads to energy reduction. The thermally coupled distillation column is thermodynamically equivalent to divided wall distillation column. The dividing-wall distillation column (DWC) offers an alternative to conventional distillation towers, with the possibility of savings in both energy and capital costs.

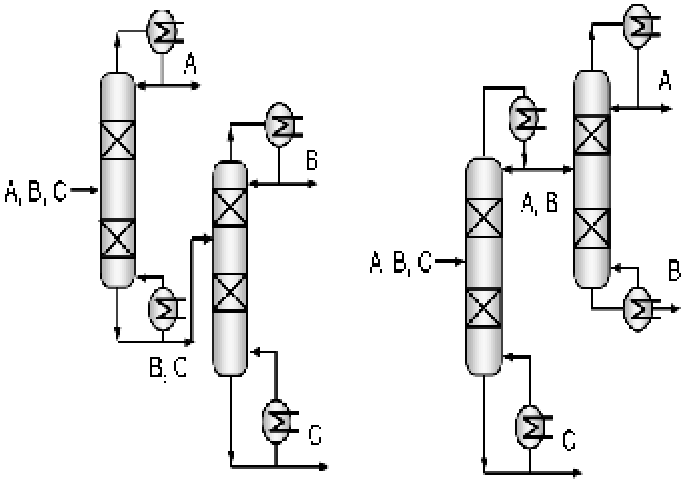
1.1 Multicomponent Distillation

A single distillation column is used in the separation of a binary mixture, but for more than two components we use the sequence of columns. For separation of more than two components or multicomponent, we use number of columns in sequence (for N components we use N-1 columns for separation).but it increases the energy consumption and cost of the process.

For N-1 columns, the N-1 reboilers and condensers are used which leads to increase in energy consumption and capital cost.

1.2 Direct and Indirect Sequence Columns

Normally, the separation of process stream into low-(A), intermediate-(B) and high boiling(C) fractions is accomplished in successive topping and tailing steps or direct sequence (Fig.1a): The light component(A) comes off the first distillation column, and the intermediate and high boiling components (B & C) are then separated in second column. This sequence is generally considered to be less energy-intensive than conducting the tailing step first or indirect sequence (Fig.1b), because in Fig.1a, the light component is only boiled off once.



(a) (b)

Figure 1.1: (a) Direct and (b) indirect sequence

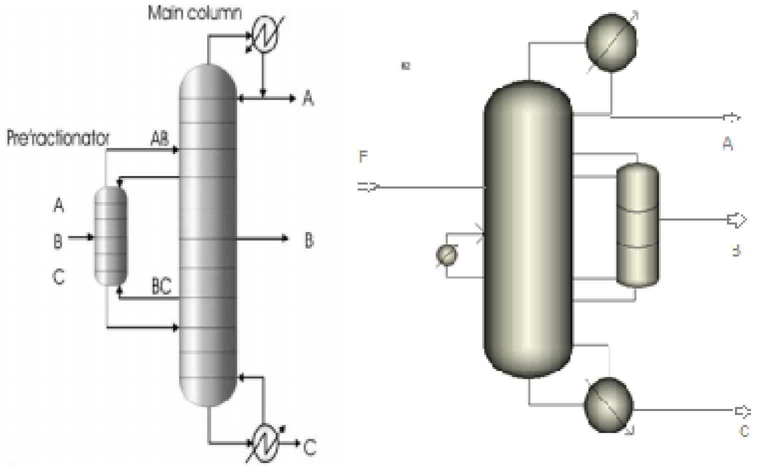
However, it is preferable to conduct the tailing step first under certain circumstances; for example, if the amount of high boiling material to be removed is relatively small.

For separation of N components, N-1 columns as well as reboilers and condensers should required, as the result, the energy consumption and capital cost will increase.

Engineer in chemical process industries are giving more attention to type of distillation column, called partitioned columns or divided wall columns (DWC) or petlyuk column, that contains vertical baffle in its middle section. Hence, from a single column, three essentially pure product streams can be withdrawn.

1.3 Thermally Coupled or Petlyuk Columns

In thermally coupled arrangement, one column (called as prefractionator or postfractionator) is thermally coupled with main column by connect streams as shown in figure 1.2.When post fractionator is attached to main column, the column is called as Petlyuk column. Prefractionator arrangement shown in figure 1.2(a) requires significantly less energy than conventional column configurations. The reason for this is the avoidance of remixing of internal streams, which in two columns in series arrangements exhibits concentration peaks of middle boiling components either above or below the feed. Additional gain in this respect comes from the fact that the prefractionator arrangement, which distributes the intermediate component between top and bottom, allows greater freedom to match the feed composition with a tray in the column to further reduce mixing losses at the feed tray. This mixing as well as remixing of streams with different compositions that occurs at feed point and along column, which is inevitably accompanied by entropy of mixing formation, is an intrinsic source of thermodynamic inefficiency of the separation process occurring in a multicomponent distillation column.



(a) (b)

Figure 1.2: Thermally coupled columns (a) with prefractionator (b) with post fractionator or Petlyuk column.

A further capital saving benefit can be arranged, where appropriate, by removing condenser and the reboiler of the prefractionator column. This leads to a configuration shown schematically in Figure 1.2(b) (Petlyuk et al., 1965) and is generally known as "Petlyuk column". In fact, omitted condenser and reboiler are effectively replaced by thermal (heat) coupling of prefractionator column with the main column, with the necessary condenser and reboiler being attached to the main column. Therefore this configuration is generally known as "fully thermally (heat) coupled column".

This is not limited only to three component mixtures (Christiansen et al., 1997) in general a Petlyuk column is: "A column arrangement, separating three or more components using a single reboiler and a single condenser, in which any degree of separation (purity) can be obtained by increasing the number of stages, provided the reflux is above a certain minimum value and the separation is thermodynamically feasible."

1.4 Divided Wall Distillation Column

Distillation is used for about 95% of liquid separations in chemical process industries, and the energy used for this accounts for an estimated 3% of world's energy consumption (Hewitt et al., 1999). Application of non-standard complex column arrangements can lead to substantial savings in energy consumption. Among these alternatives, dividing-wall columns (DWCs) for separating mixtures of three or more components appear to be the most attractive as they provide substantial savings in both energy consumption as well as capital investment (Agrawal and Fidkowski et al., 1999). As suggested by the name, DWC contains a vertical wall that divides the middle section of the column into two parts to accommodate the pre-fractionator in the same shell. This column configuration splits both the rectifying liquid coming from the column top and stripping vapor rising from the column bottom, to both sides of the wall.

DWC eliminates undesirable mixing near the feed stage in conventional columns, and thus reduces energy required for separation. When a multi-component feed is introduced to the pre-fractionator side of the DWC, the low- (LK) and high-boiling point components (HK) are separated in the pre-fractionator while the middle boiling component (MK) distributes to the top and the bottom of the wall along with LK and HK respectively. Further separation of LK and MK occurs in the upper section of the main column while the separation of HK and MK occurs in the lower section of the main column. As the composition of the MK at the top and the bottom of both sides of the dividing wall have to be matched, concentration of the MK reaches a peak value in the middle section on the other side of the wall. A high purity MK can then be withdrawn from the middle section of the main column, as a side draw. Sharp split between LK and HK achieved in the pre-fractionator effectively reduces the contamination of MK drawn at the other side of the wall. This is simply because neither the LK can pass to the bottom section of main column nor the HK can pass to the upper section of the main column provided there is no azeotrope present in the mixtures (Ennenbach et al., 2000). Hence, the MK can be withdrawn at its maximum concentration from the other side of the wall. Simultaneously, the problem of re-mixing in the conventional columns when feedstock contains more than two components is avoided (Triantafyllou and Smith, 1992). In addition, the distribution of MK between the top and the bottom of the pre-fractionator provides greater freedom for the selection of proper feed stage to ensure better matching between the feed stream composition and the composition of the tray. This leads to significant reduction in the mixing losses at the feed tray.

Separation efficiency of DWC is further improved by the additional thermal link between the pre-fractionator and the main column that provides heat integration. In fact, the least amount of rectifying liquid and stripping vapor is required by DWC among all the three-product distillation systems due to the improved vapor-liquid interaction in all sections of DWC (Fidkowsi and Krolikowski et al., 1987). Hence, energy saving up to 40% is achievable for a typical DWC design (Kolbe and Wenzel et al., 2004). Apart from energy savings, by housing pre-fractionator and main column in a single shell, savings in capital cost can also be achieved due to the elimination of an additional column, reboiler and condenser. In addition, construction of a DWC may bring other indirect benefits. For instance, elimination of a few major equipments will lead to a reduction in plot area required, shorter piping and electrical usage, as well as lower engineering cost.

To allow natural flow of vapor in between the sections in the column, the entire column has to be operated under the same pressure. As such, one of the split may not be taking place under optimum pressure, and hence increasing the overall reflux ratio required (Shah, 2002). However, DWC is very attractive if the required utility is readily available and if the energy cost is high compared to the capital cost. Industrial acceptance of DWC has been increasing due to the efforts put in by researchers to gain better understanding of design and control aspects of DWC, as well as increasing energy costs and environmental concerns. There are nearly 60 DWCs in industries in 2005, of which 42 are owned by BASF, the leader in this field (Parkinson, 2005). The recent study of Premkumar and Rangaiah, (2009) shows that operating cost can be reduced by more than 30% by using a DWC instead of a conventional 2-column (C2C) system in addition to some reduction in capital cost for new plants, and that retrofitting a C2C system to a DWC is attractive with payback period of less than 3 years for 5 of the 6 applications studied. Hence, there are better prospects of DWC in the near future and it might become a standard distillation configuration in chemical process industries (CPI) in the next 50 years (Schultz et al., 2002). The increasing energy cost and concern on global warming in the recent times have made DWC an attractive alternative to reduce the energy usage in CPI.

The divided wall column (DWC) to separate three components in a single distillation tower (as shown in Fig.1.3) is receiving interest in industrial applications due to the potentiality in energy and capital cost savings.

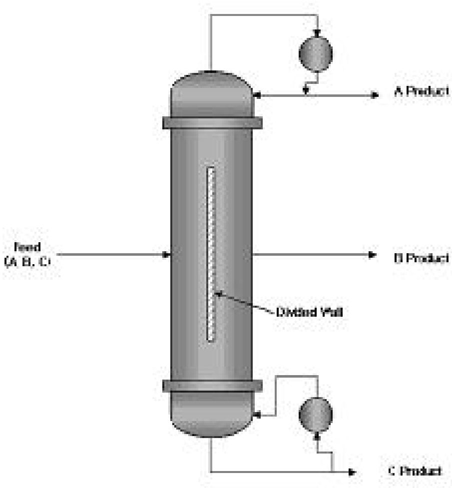


Figure 1.3: Dividing Wall Columns

Conventional distillation columns produce only two pure product streams one at the top and other at the bottom of the single column. Side products are contaminated by light or heavy components, depending on the location of the side stream in the rectifying or stripping section. This disadvantage is set aside by using a distillation column with a vertical partition.

The internal separation wall prevents lateral mixing of liquid and vapor in the central part of the column, forming their separate feed and outlet sections. In the presence of a vertical partition, three or four pure fractions can be obtained in a single distillation step. This is particularly advantageous when heat sensitive components are to be separated. On account of good thermodynamic properties, the energy consumption is 20 to 35% lower than that of other distillation arrangements.

Many studies indicate that separations consume 50% to 70% of the capital and energy of a traditional chemical process, so, seeking improvements in this area clearly should receive a high priority. One of the more effective methods of reducing both the capital and energy costs of separations units is installation of divided wall columns (DWC) where appropriate. While results, of course vary, a DWC typically can cut capital and energy costs by approximately 30% compared to a traditional two-column system.

The idea of the DWC is not new. For instance, in 2005 at the 7th World Congress of Chemical Engineering, BASF, a leader in DWC implementation, reported more than 40 DWC in commercial service. In a 2006 symposium, ExxonMobil announced the successful revamp of a 380-cm/430-cm-diameter tower that removes xylene from reformate. Dow has operated an experimental DWC facility in Midland, Mich., for about eight years. During the same time, numerical expertise for the modeling of DWC systems has been developed and bolstered and validated by the experimental units.

An important motivation for studying integrated distillation column arrangements (thermally coupled or divided wall column) is to reduce the energy consumption. On a global basis, distillation columns consume a large portion of the total industrial heat consumption.

1.5 To Sum up the Basics

The following four basic features to define this type of system for separating n component mixtures.

1. The total number of column sections is equal to one instead of *(n* - l), as used in conventional schemes.
2. It is sufficient to have only one condenser and one reboiler.
3. The key components in each column are the two components with extreme volatilities.
4. N products of given purities are obtained from the single divided wall column.

1.6 Advantages of DWC

The main advantages of divided wall columns include:

1. Two columns combined in one shell i.e. lowering of the overall capital cost.
2. Compact Design, lower space requirements.
3. Increased energy efficiency because only one reboiler and condenser is used.

1.7 Disadvantages of DWC

The main disadvantages of divided wall columns include:

1. Additional reflux divider is required to divide liquid split on both sides of wall.
2. Increased operational and maintenance complexity.
3. Pressure control is difficult.

1.8 Applications

We will give some general heuristics for when DWC installations should (and should not) be considered. However, different companies view capital, energy and risk differently and, thus, evaluate a project according to disparate sets of metrics:

1. Distillation columns with vertical partitions are capable of separating a feed mixture into 3 or 4 pure fractions.
2. This is advantageous especially for heat sensitive components. These can be separated from their higher and lower boiling impurities at a lower thermal stress.
3. Better product qualities are obtained.
4. DWC saves 30% energy and capital cost as compare to columns in sequence.

CHAPTER 2

LITERATURE REVIEW

Krolikowski and Fidkowski (1987) have compared several thermally coupled arrangements with conventional direct and indirect arrangements. They approximated energy requirements with the sum of vapor flow rates from all reboilers. This assumption can be used only if same type of cooling and heating medium is used in all condensers and reboilers. They found that when only energy consumption is compared, Petlyuk arrangement is the most favorable.

Agrawal and Fidkowski (1998 a, b, 1999) presented the basis for generating feasible alternatives for fully thermally coupled distillation systems in which all the heat is provided to the system by a single reboiler and all the heat is removed from the system by a single condenser. These basic rules were reviewed and systematized in the form of a minimum set of logic propositions by Caballero and Grossmann (2003, 2004) and translated into a set of linear equations for their use in a mathematical programming environment. Agrawal and Fidkowski (1999) and Agrawal (2000 a-c, 2001 and 2003) introduced possible modifications and improvements to the fully thermally coupled arrangements, including the possibility of decreasing the number of thermal links among columns, schemes for multieffect heat integration, and the basic rules for generating all the thermodynamically equivalent configurations for a given column configuration.

An optimal design of a DWC requires adequate models and computer-based simulations. However, commercial process simulators do not include particular subroutines for DWCs. The so-called decomposition method developed by Triantafyllou & Smith (1992) simplifies the design problem. The existing DWC configuration is replaced by a sequence of conventional distillation columns.

For the initial design of a DWC, the shortcut method suggested by Triantafyllou & Smith (1992) can be applied. This method is based on the equations introduced by Fenske, Underwood, Gilliland and Kirkbride. The calculations are relatively simple and can be used for mixtures of any number of components (Mueller, 2007). Another simple method for the conceptual design of DWCs is suggested by Halvorsen & Skogestad (2003). This method is based on a graphical treatment of the minimum energy represented by normalized vapor flow. Meanwhile, Aspen Plus suggests a routine for the design of Petlyuk configurations.

The latter are thermodynamically equivalent to a DWC if the heat transfer across the wall is neglected.

Rangaiah et al. (2009) developed a procedure for a quick design of DWCs using Hysis. This tool is based on the equilibrium stage model, which assumes that the streams leaving a column segment (stage) are in thermodynamic equilibrium.

The optimal design of thermally coupled distillation columns and divided wall column using mathematical optimization was considered by Dunnebier and Pantelides (1999). The Model assumed constant relative volatility, constant molar overflow and neglected heat transfer across the dividing wall. This model is able to simulate both conventional (direct sequence) and thermally coupled columns, which allowed the comparisons of different structural alternatives. Up to 30% possible saving in both operating and capital costs are illustrated using two case studies, one for the separation of close boiling C4's and the other for the separation of alkane mixtures. Design and optimization of fully thermally coupled distillation column was also studied by Amminudin et al. (2001) wherein the degree of freedom was optimized simultaneously and an optimized initial design was established for rigorous simulation. The procedure adopts the equilibrium stage composition concept to define a liquid composition by solving the mass balance rigorously on each equilibrium stage, while restricting the procedure to the assumption of constant molal overflow. Due to its semirigorous nature, there is no need to assume constant relative volatility. The procedure follows from the feasible product distribution, which must be estimated at minimum reflux conditions prior to the use of the concept for designing the fully thermally coupled column. While maintaining the use of a model based on three simple columns, the procedure begins with the use of a pre-fractionator arrangement to initialize and simplify the design of the dividing wall column. By transforming the design from the pre-fractionator to the fully thermally coupled column arrangement, the design can proceed to estimate the side-draw locations, composition, flow rates and the number of stages.

The implementation of the divided-wall column technology for processing petrochemical cuts (morphylane extractive distillation) was studied by Kolbe and Wenzel (2004).

Special proprietary simulation tools are developed for the design of the overall column configuration and an evolutionary algorithm was used to find the optimum column design based on the total annual costs. Uhde (Kolbe and Wenzel, 2004) designed and constructed commercial plants in parallel to the laboratory investigations. Practical operation was verified on a laboratory scale with a special set of divided-wall column elements designed as a variable unit construction kit. Using the process simulator, utility and investment costs was estimated. The data was taken from an industrial divided wall column for the processing of pyrolysis gasoline. Thermodynamic behavior was calculated using UNIFAC model and energy saving is 19.8% in the divided wall column as compared to conventional direct sequence columns.

Kim (2001 a, b) studied the structural design of fully thermally coupled distillation columns. A rigorous structural design procedure for fully thermally coupled distillation columns (FTCDC) was applied to the example system of butanol isomers in order to show the design performance. The procedure gives structural information of the column, and therefore iterative computation encountered in the design using conventional procedure and commercial packages could be eliminated. Using the outcome of the structural design, several features, such as thermodynamic efficiency, dividing wall column structure and the arrangement of interlinking streams, were investigated. A novel superstructure for designing sequence of distillation columns ranging from conventional to fully thermally coupled systems was given by Caballero and Grossmann (2004). They analyzed several alternative intermediate possibilities. The proposed method was based on a two stage decomposition procedure. In the first stage only the best sequence of separation tasks was obtained, in which each separation task is considered like a pseudo-column. Once the structure of separation tasks is established, the sequence of actual columns is extracted among all the thermodynamically equivalent alternatives. The model uses the Underwood–Fenske–Gilliland approximation and is formulated as a generalized disjunctive programming problem and solved as an MINLP. The model has proven to be very robust and reliable. This formulation also makes the model very flexible and allows the easy modification of the equations and even migration to other model types including rigorous tray-by-tray models. Rigorous simulations in HYSYS for the separation of a mixture of aromatics had shown good agreement with the shortcut model.

A structural design procedure for fully thermally coupled distillation columns was proposed by Kim (2005), using a semi-rigorous model and tested on three systems, butanol, BTX and hexane–heptane mixtures having different compositions of feed. The design procedure employed material balances and equilibrium calculated using

UNIQUAC activity model and the Peng–Robinson equation of state (EOS) for the computation of tray compositions. The structural information was utilized in HYSYS simulations to find the operating variables that would meet a given set of product specifications. The outcome of the proposed structural design procedure provides a good estimate for the rigorous simulation. The application result of the proposed design procedure to the example systems indicates its applicability to various systems having different equilibrium relations and feed compositions.

Kim (2006 a, b) also proposed a new system of a fully thermally coupled distillation column (FTCDC), and examined its performance on two industrial processes. The system had an extra column called postfractionator, attached to the main column of an original fully thermally coupled distillation column. Vapor liquid equilibrium (VLE) was calculated with Peng-Robinson EOS for both processes. The structure of fully thermally coupled distillation column system was implemented to the fractionation process of a naphtha reforming plant for BTX production and the gas concentration process to produce gas products from gas mixture drawn from crude distillation, naphtha reformation and naphtha-cracking processes in a refinery. The outcome of performance investigation using HYSIS indicated a 29% energy saving with fractionation process and a 7% saving with gas concentration process over the original fully thermally coupled distillation column. In addition, some considerations on the new column construction, such as arrangement of distillation column sections and divided wall construction, was also discussed.

Triantafyllou and Smith (1992), published a first design-oriented short-cut method for a 3-product DWC based on so called Fenske-Underwood-Gilliland-Kirkbride model (FUGK), a well known combination of individual models to establish the minimum number of equilibrium stages (Fenske), minimum reflux (Underwood), stage requirement at chosen operating reflux ratio (Gilliland), and the feed stage (Kirkbride) for a given separation. Basic assumptions of this model area are constant relative volatility and constant molar flows. Amminudin et al., (2001) pointed out that use of Kirkrbride equation, to find thermal coupling locations can lead to errors when transferred to rigorous simulation.

Sotudeh and Shahraki., (2007) proposed a method based on Underwood equations only, because they consider the use of Fenske equation for minimum number of stages inadequate for application in DWC design. This is due to the fact that Fenske equation is based on assumption of equal compositions of liquid and vapor streams at top and bottom of prefractionator, which, in case of DWC is clearly not the case. According to the case study presented in their paper, this method provided a more economical DWC design compared to the method of Muralikrishna et al. (2002)

Halvorsen and Skogestad (2003a-c) analyzed the minimum energy requirement for three and more than three products using Petlyuk arrangement. It was observed that the energy requirement was equal to the most difficult of the two separations (top/middle or middle/bottom product) in a conventional single column. They developed their model by assuming constant relative volatility and constant molar overflow for ternary feed and rigorously proved that fully thermally coupled systems always produce the lowest vapor flow rate (at least for systems with constant relative volatilities and constant molar flow in each column section) giving a simple explicit equation for this result. The graphical representation of the $V_{\min}$ versus distillate diagram is found to be a useful tool for obtaining conceptual insights about the process.

Rangaiah (2009) gave simulation and optimization results of DWC using HYSIS, they lead to useful guidelines for the design of DWCs. The three-column shortcut simulation is capable of providing reasonable estimates for the initialization of rigorous simulation and design of DWCs. Of these estimates, vapor and liquid splits in the column have significant impact on the energy requirement although their effect on condenser and reboiler duty is less pronounced within the optimum region.

The internal separation wall prevents lateral mixing of liquid and vapour in the central part of the column given by Kaibel (1987), forming their separate feed and outlet sections. In the presence of a vertical partition, 3 or 4 pure fractions can be obtained in a single distillation step. On account of good thermodynamic properties, the energy consumption is 20 to 35% lower than that of other distillation arrangements. The control behavior is similar or better than that of conventional distillation columns.

Hernandez-Gaona et al., 2005, employ exergy analysis approach to calculate efficiencies for several distillation sequences for separation of 3 and 4 components mixtures.

A controllability analysis of the diagonal feedback control using multiple input-multiple output (MIMO) linear analysis tools was done by Serra et al. (1999, 2000 and 2001) for the separation of different mixtures and for different operating conditions, including optimal operation. As a result, it was seen that a trade off appears between energy minimization and controllability. As an alternative, application of dynamic matrix control (DMC) to the divided wall column (DWC) was also evaluated. Through simulation, the ability of DMC for disturbance rejection and set point tracking was studied and compared with that of the feedback diagonal control. Serra et al. (2000) also studied the influence of design and operating conditions on the divided wall column controllability. Two designs for which the total distillation cost is minimized were compared and for each design, different optimal reflux to minimum reflux ratio was assumed. They compared three non- optimal designs with an optimal one. A 3 × 3 operation scheme, which has favorable indices of multivariable controllability, was examined by Kim (2002) to check the control performances of set-point tracking and regulation with a model predictive control.

The control properties of thermally coupled distillation sequences for different operating conditions were studied by Juan et al. (2006).

Plant wide design and control of acetic acid dehydration system via heterogeneous azeotropic distillation and divided wall distillation is studied by Wang et al. (2007). The control strategies using temperature loops are proposed for the acetic acid dehydration system. The effects of liquid split and vapor split ratios on the energy efficiency and controllability of a divided wall column system for separating ethanol, *n*-propanol, and *n*-butanol were investigated by Wang and Wong (2007).

The DWC configurations for the separation of a four components mixture with 5 different feed composition cases was introduced by Errico et al. (2009). The best SC (side column) configuration was chosen as the basis for the comparison with the new configurations obtained by introducing a Petlyuk/DWC structure. The most promising structure was first selected on the basis of the lowest energy consumption. From the calculations it was evidenced that the Petlyuk /DWC is not convenient when this configuration was utilized to replace two SCs with a high pressure difference. For all the simple configurations where there was a decreasing value of the pressure through the columns (i.e. direct, direct-indirect sequences) it was convenient to use first a SC and then to perform the last separation by using a Petlyuk/DWC arrangement. The most promising cases correspond to Petlyuk/DWC fed with equimolar of equal excess of lightest and middle component mixtures. With regard to the capital costs evaluation, a detailed evaluation was carried out considering separately the Petlyuk and the DWC configurations. The analysis was performed considering the total exchanger area together with the column internals and shell. The DWC diameter was estimated considering the prefractionator and the main column design of the corresponding Petlyuk structure. The DWC outperforms both the SC configuration and the Petlyuk structure. The main advantage of Petlyuk/DWC arrangements remains the potential in energy saving while a minor profit can be obtained for the capital costs.

When compared to the side draw column, the dividing wall column has a more complex nature, shown through degrees of freedom analysis as given by Mutalib and Smith (1998). This results from two additional manipulated variables, the liquid and vapor splits. However, it is impractical to manipulate the vapor split, which is fixed by the position of the dividing wall. On the other hand, the liquid split can be easily varied but has been found to have little benefit in comparison to the complication that will be added to the operation and control of the column. In the region of high liquid and vapor loading, varying the liquid split will also affect the vapor split considerably and this even affects the operation and control of the column further. The Column should be operated and controlled with a constant liquid split in addition to the fixed vapor split. The disadvantage of this proposal is that the impurities composition in the middle product cannot be controlled.

The optimum location for the liquid and vapor splits was found to be insensitive to the variation in the feed composition but this is not so for the variation in the product specification. The design for the liquid and the vapor split should be based on the highest product specification when the column is required to produce a range of product compositions.

Many authors analyzed the effect of minimizing the energy requirements on the controllability properties of the system, because an optimal design might give the highest energy savings, but lack good controllability (Segovia-Hernández et al., 2005; Tamayo-Galvan et al., 2008). Rong and Turunen (2006) reported a reliable synthesis method, whereas Gomez-Castro et al. (2008) proposed a robust method for the design of distillation sequences with dividing walls and recommended an analysis of both thermodynamic and controllability properties.

The alternative distillation systems present very similar values of energy demands in the reboilers and thermodynamic efficiencies. The energy savings of up to 50% predicted for the Petlyuk system can be obtained in practice through the industrial implementation of alternative distillation sequences with unidirectional flows, which are thermodynamically identical to the Petlyuk column but with better expected operational behavior.

The potential of energy savings that can accrue with the use of complex integrated columns has not been fully exploited by the industry so far. The industry is not confidence on the reliability of the design methods and on the operation and control of integrated columns. This hesitation stems from the maturity of the distillation technology over the last few decades. Therefore, a better understanding of the characteristics of these systems is required.

The above literature review shows that the reluctance in accepting this highly energy efficient technology is perhaps due to some gaps in our understanding of the divided wall distillation column. Certain deficiencies which need improvement are given below:

1. Several authors have studied the energy saving in optimal conditions; however, only limited information is available about the product quality and energy requirement when the operating condition deviates from the optimal condition.
2. Controllability of the divided wall distillation column is difficult due to only one energy source (reboiler) and two reflux ratios.

Objectives:

In view of the above, the following objectives are set for the proposed study:

- To study the effect of structural and process variables on product purity and energy efficiency of DWC.
- To estimate the thermodynamic efficiency of divided wall column.
- Sizing and costing of divided wall distillation column.

CHAPTER 3

SIMULATION OF DWC

The simulation of a non-standard column like DWC is more complex than that of a conventional distillation as there are more degrees of freedom involved and more parameters to be manipulated. All simulation studies are done in ASPEN but it does not include a DWC in its library operations. Hence, DWC is simulated based on the configuration of fully thermally coupled column, called Petlyuk column. Petlyuk column arrangement consists of main column and a postfractionator. Such representation is justifiable as these two column configurations are thermodynamically equivalent assuming that heat transfer across the dividing-wall is negligible (Schultz et al., 2002).

3.1 Simulation Model

Design, simulation and operation of a DWC require the simultaneous solution of the material, momentum and energy balance equations. For a simple distillation column, the momentum balance equations are important only at the design stage. The effect of pressure drop is usually ignored during simulation stage because of its insignificant impact on vapor-liquid equilibrium (Friday et al., 1964; Tomich, 1970; Napthali and Sandholm, 1971; Hess, 1977; Seader, 1989). For of a single distillation column, the overall column pressure (or constant pressure profile) predicts product yield and composition satisfactorily. In case of columns with connecting streams, such as Petlyuk column, connecting stream flow rate can be maintained between two columns at different pressures. Therefore, the prediction of pressure drop across each tray of a DWC is necessary.

A complete mathematical model of a distillation column is required to describe material, energy and momentum balance equations for each individual tray of the entire distillation column subject to thermodynamic constraints of VLE. Most of the existing models (Friday et al., 1964) ignore momentum balance equations and rely only upon material and energy balance equations with VLE. These model equations are commonly known as MESH equations (material balance, vapour-liquid equilibrium, summation, and enthalpy (H) balance equations). For a simple distillation column having N stages including condenser and reboiler with one feed and two products, Friday and Smith (1964) have given the component material balances, summation, and equilibrium and enthalpy balance equations.

Lockett (1986) has presented a detailed analysis of the relations between hydrostatic pressure head created in the down comer and the pressure drop across sieve trays. An abridged version of these correlations for sieve-tray column can be expressed as force balance equations:

$$(P_i - P_{i-1}) - \rho_L \, g \, ht_i = 0 \qquad (i=2 \ldots N\text{-}1) \qquad (1)$$

Where, $ht_i = (h_w + h_{ow} + h_d + h_r)_i$ (2)

and is defined as the liquid head equivalent to the pressure drop between i^{th} and $(i\text{-}1)^{th}$ trays and P_i is the absolute pressure of the gas phase in the vapour liquid disengagement space above i^{th} tray; and $h_{ow,}$ h_d and h_r are the heights of the liquid crest over the weir, pressure drop through the dry plate and residual head, respectively.

For the initialization of rigorous simulation, the structural variables as shown in Table 3.1, should be known. These variables are obtained from the shortcut simulation of DWC.

Table 3.1: Variables to be initialized for rigorous simulation

Structural variables
Number of trays in the Pre-fractionator or post fractionator
Feed stage
Number of trays in the Main Column
Side Draw stage

3.2 Shortcut Simulation of DWC

In this model, three shortcut DSTWU columns are used to represent the Prefractionator "SCPre", the top section of main column Main1, and the bottom section of main column Main2. The column pressure profile and an external reflux ratio must be specified in each shortcut column to obtain the number of trays, feed stage, and vapor and liquid traffic in rectifying and stripping sections. The reflux ratio is specified as 1.2 times the minimum reflux ratio. The middle product is represented by the addition of two material streams, namely "side1" and "side2".

"SCPre" represents the pre-fractionator; the effective binary pair in this column is the low-boiling point component and the high boiling point component. In addition, the overhead product in SCPre has to be in vapor phase to better represent the material stream that is thermally linked to the main column. For the other two shortcut columns, the overhead product should be in liquid phase to represent the respective product streams.

In Main1, separation between low-boiling point component and middle-boiling point component will take place. Likewise, separation between the middle-boiling point component and the high-boiling point component dominates in SCMain2.

To allow the addition of Side1 and Side2 to represent the middle product, compositions of these two streams have to be equal, especially for the middle key. Hence, the degree of separation between LK (light key) and HK (heavy key) in SCPre has to be altered to obtain equal compositions in Side1 and Side2. This can be done by adjusting mole fraction of the light key in the bottoms and heavy key in the distillate of SCPre, by trial and error. Upon equalization of compositions of Side1 and Side2, the shortcut simulation for the application is completed, and the estimated structural and operational parameters can be retrieved from ASPEN for initialization of the rigorous simulation. A case study of n-butane, n-pentane and n-hexane mixture has been taken . The feed and operating conditions are given in Table 2.

Initial estimate for the design variables can be obtain by decomposing the DWC into shortcut columns as used by Rangiah et al. (2006) and Amminudin et al., (2001). The initial design variables thus obtained are similar to that of Kim (2001) for BTX separation. For rigorous simulation, the MultiFrac model of ASPEN Plus™ has been used. 'Connecting Streams' have been used for interconnecting various columns. MultiFrac uses these connecting streams as internal variable streams.

Feed specifications are shown in Table 3.2. The other parameters required to be specified to operate the DWC under varying operating conditions are listed in Table 3.3. For easier convergence of the simulator, molar flow rates of the reflux and connect stream *r*, *l* and *v* were used as input parameters.

For calculating pressure drop, 'Tray Rating' feature of ASPEN Plus™ was used. For making hydrodynamic calculations using 'Tray Rating', additional column design specifications are required. These specifications are listed in Table 3.4.

Table 3.2: feed specifications

Components	Mole fraction	Conditions	Product specifications	Operating conditions	Fluid Package
n-butane	0.4	45kmol/hr	D=97mol%	Total condenser	PR
n-pentane	0.2	24.8 psi	S=99mol%	Pcond=21.08bar	
n-hexane	0.4	Saturated liquid	B=98mol%		

Table 3.3: Column, Feed, Product and Connect Stream Specifications

Main Column		*Section 2 of Main Column*	
No of stages (N)	28-45	No of stages ($N_{S2}-N_{S1}$)	10-33
Feed stage	5-35	Product draw stage (N_{S3})	2-16
Column pressure	21.08psi	Column pressure	21.08psi
Distillate rate	40.2 lbmol/hr		
Reflux ratio (r)	1.9-5.2		
Feed rate	45 kmol/hr	Product rate (S)	19 lbmol/hr
Feed condition	(24.8 psi, 100 F)	Product stream	Saturated liquid
Feed composition	Butane=0.4		
(mol fraction)	n-pentane=0.2	–	–
	n-hexane=0.4		
Connect Streams:	***From***	***To***	***Value***
l	Column 1, Stage (N_{S1})	Column 2, Stage 1	30-75 lbmol/hr
v	Column 1, Stage (N_{S2})	Column 2, Stage ($N_{S2}-N_{S1}$)	5-110 lbmol/hr
L_{NS1} (Internal Stream)	Column 2, Stage 1	Column 1, Stage (N_{S1})	–
V_{NS2} (Internal Stream)	Column 2, Stage ($N_{S2}-N_{S1}$)	Column 1, Stage (N_{S2})	–

Table 3.4: Tray Design Specifications

Tray diameter	1.80 m
Tray spacing	0.6096 m
Ratio of sieve hole area to tray active area	0.12
Weir height (h_w)	50 mm
Hole diameter	5 mm

The shortcut model is considered in ASPEN by taking three DSTWU models as shown in figure 3.1.

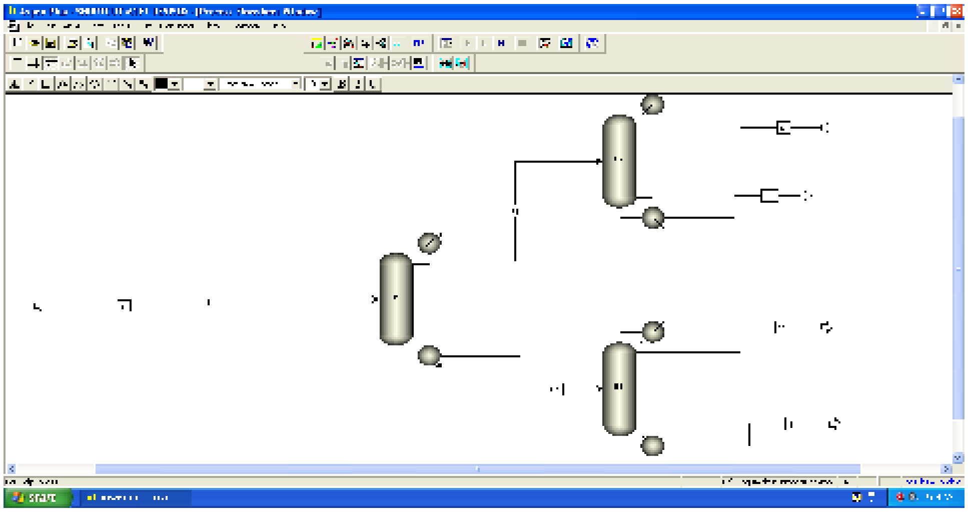


Figure 3.1: Shortcut simulation of DWC

S_1 and S_2 represents the middle product, compositions of these two streams have to be equal, especially for middle key (n-pentane). Hence, the degree of separation of between n-butane and n-hexane in prefractionator or in B1 has to be altered to obtain equal compositions in side1 and side 2. This can be done by adjusting mole fraction of the light key in bottoms and heavy key in distillate of prefractionator, by trial and error. Upon equalization of compositions of Side 1 and Side 2, the shortcut simulation for the application is completed, and the estimated structural and operational parameters can be retrieved from ASPEN flowsheet for initialization of rigorous simulation.

For above case study the following results were obtained from the shortcut simulation.

number of stages in prefractionator	17
Number of stages above the feed stage	16
Number of stages below the feed stage	19
feed stage	17
Side location	9

3.3 Rigorous Simulation of DWC

The results obtained from shortcut simulation are used for the initialization of rigorous simulation. Using the column "Multifrac" available in the equipment model library, developed the following process flow diagram in the flow sheet window by connecting the input and output streams as shown in figure 3.2. Here stream no.6, 5,7 and 4 was feed (F), distillate (D), side stream (S) and bottom product (B) respectively.

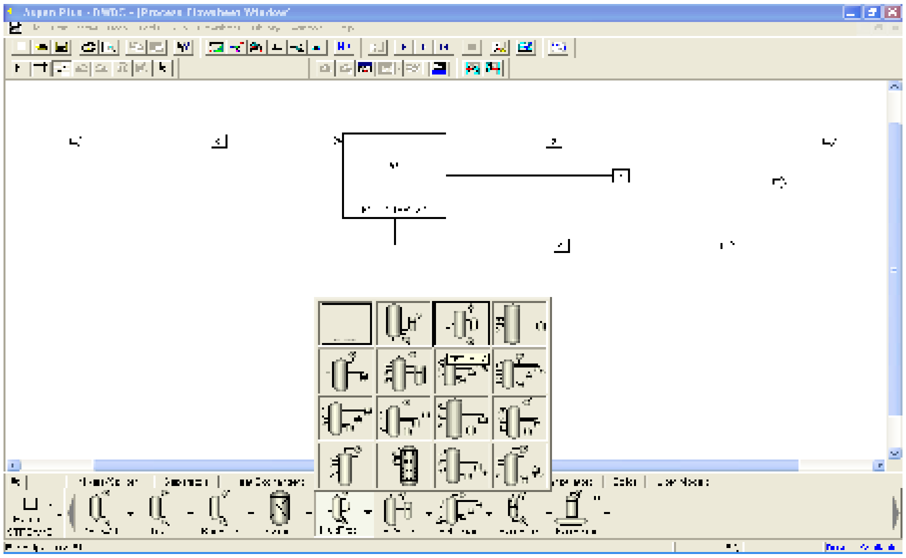


Figure 3.2: MULTIFRAC model in ASPEN flowsheet

From the data browser, choose setup/ specifications, give the title of the problem and fill up the *accounting information* as shown in figure 3.3.

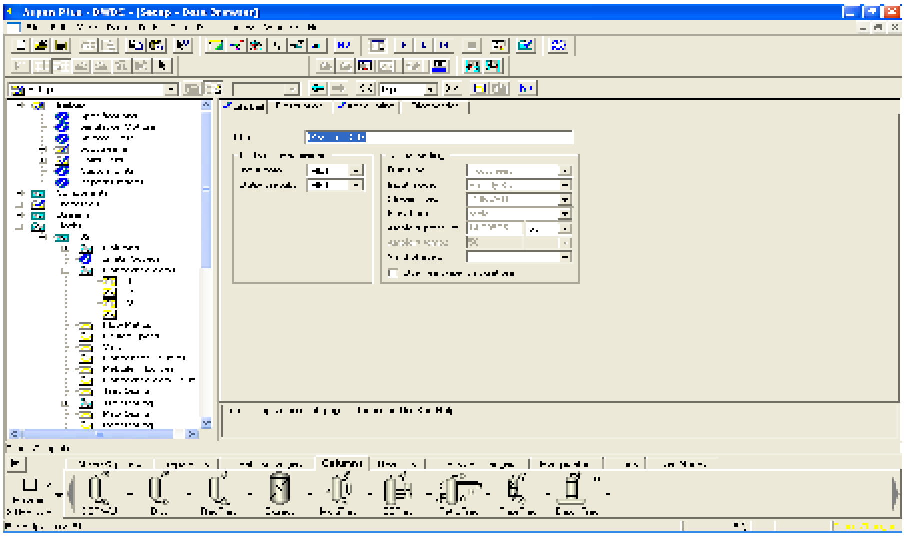


Figure 3.3: Account information in Aspen plus

Now choose the components in the list as shown in figure 3.4.

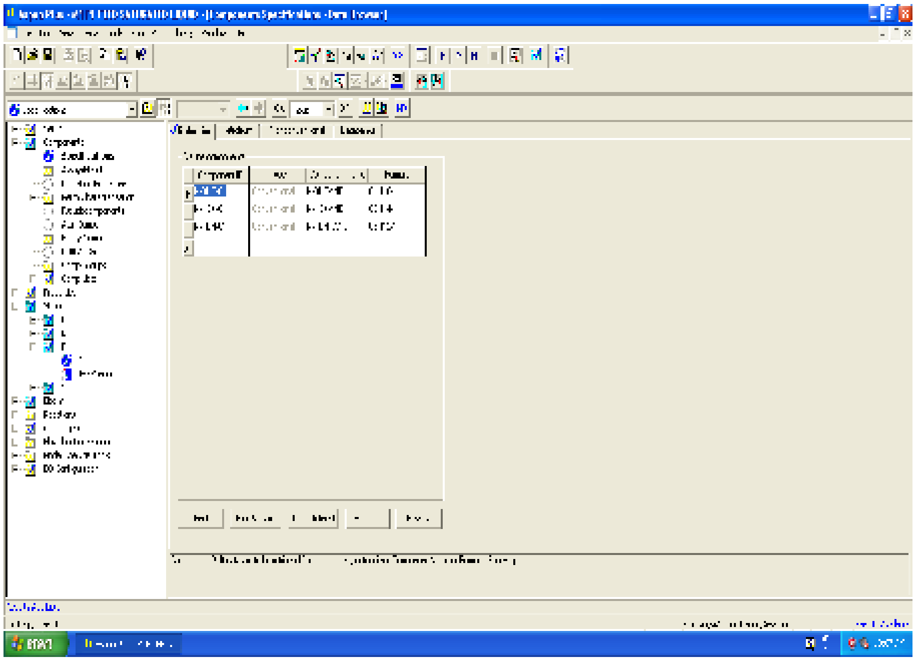


Figure 3.4: Selection of components

Select the property method “PENG-ROBINSON” as shown in figure 3.5.

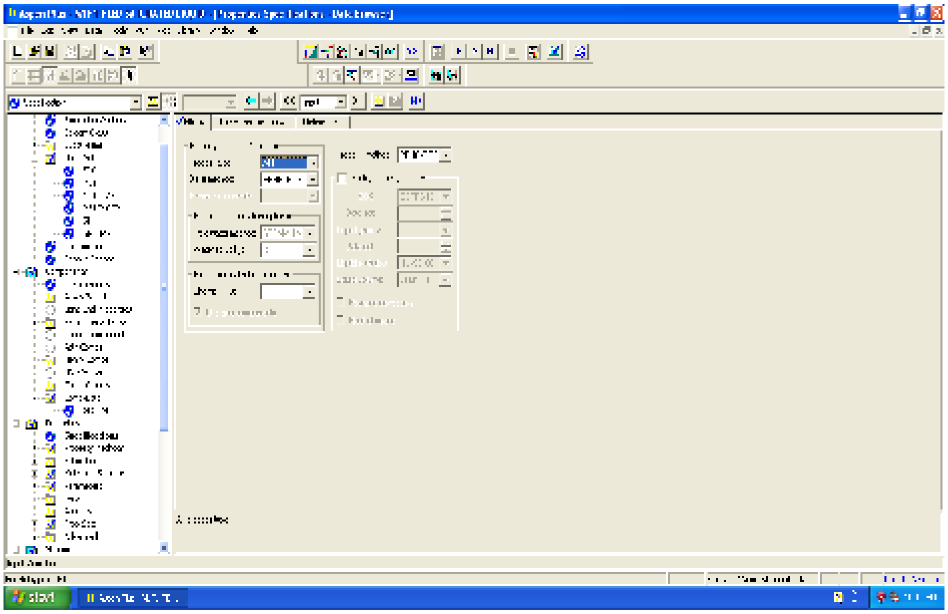


Figure 3.5: choose base method or property package

Specify the feed conditions as shown below in figure 3.6 by assuming that feed is completely specified .

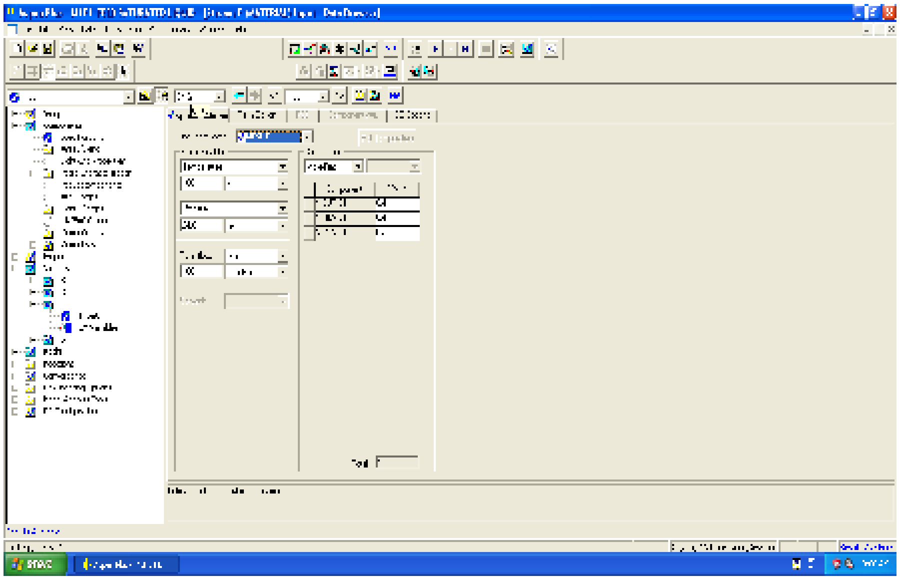


Figure 3.6: Feed specification

Now, add the new column 2, with in the main column as shown in figure 3.7.

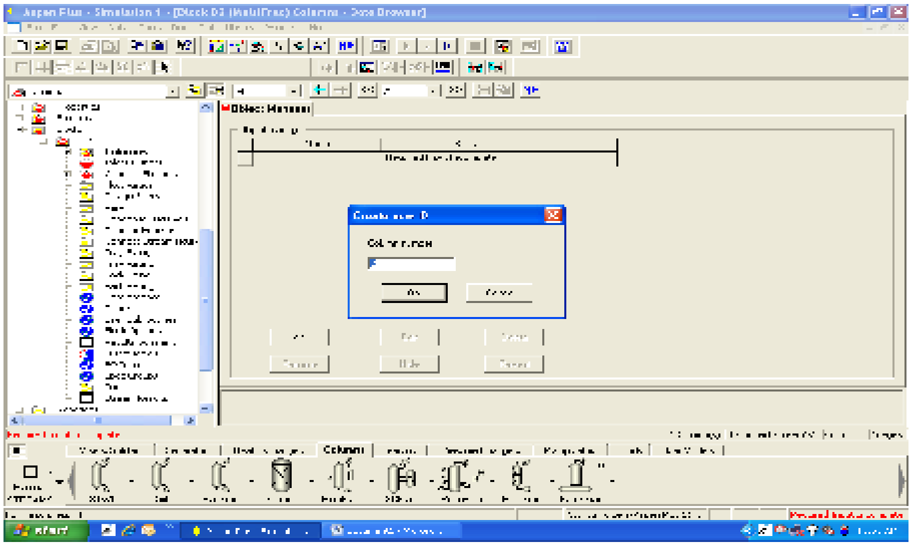


Figure 3.7: specify column 2.

Now for column 1 (main column), set the no. of stages, type of condenser and rebolier, along with the reflux and distillate rate as shown in figure 3.8.

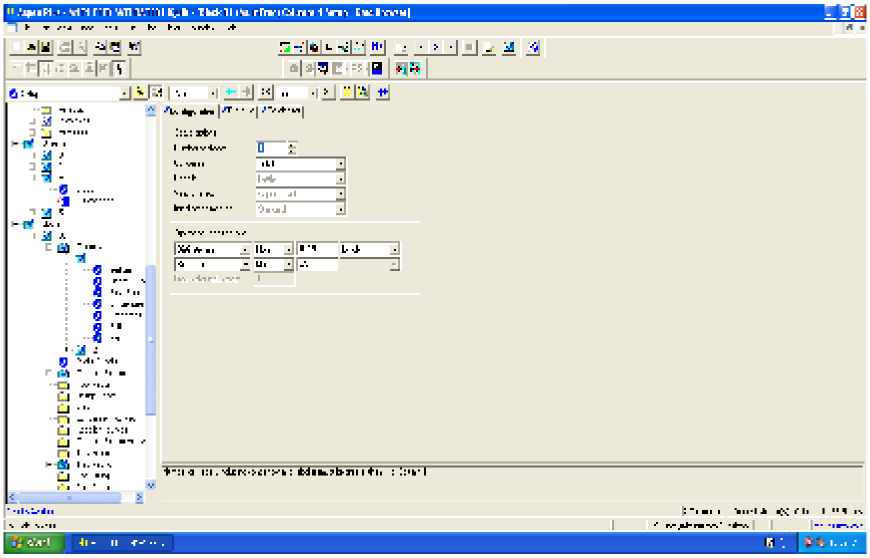


Figure 3.8: Specifications of column 1

Define the condenser pressure as shown in figure 3.9.

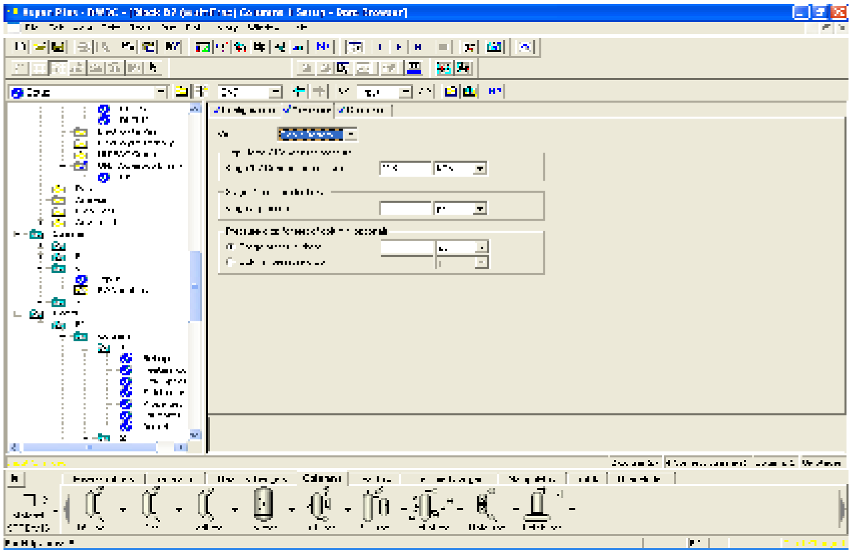


Figure 3.9: Specify condenser pressure

Give the temperature of top and bottom stage of the column as shown in figure 3.10

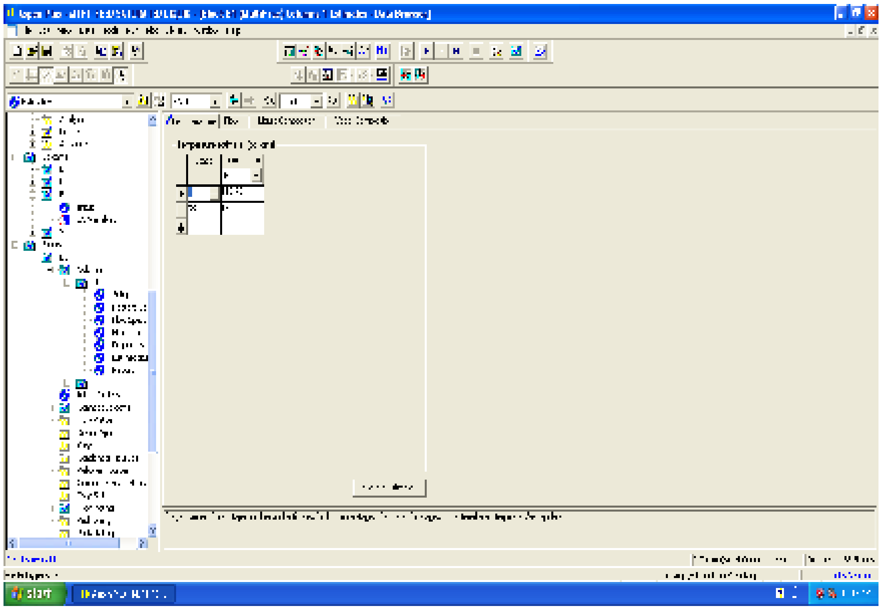


Figure 3.10: Define temperature of top and bottom stage

Now, for column 2 (section 2 of main column), set the no.of stages, condenser and rebolier type “None” as shown in figure 3.11.

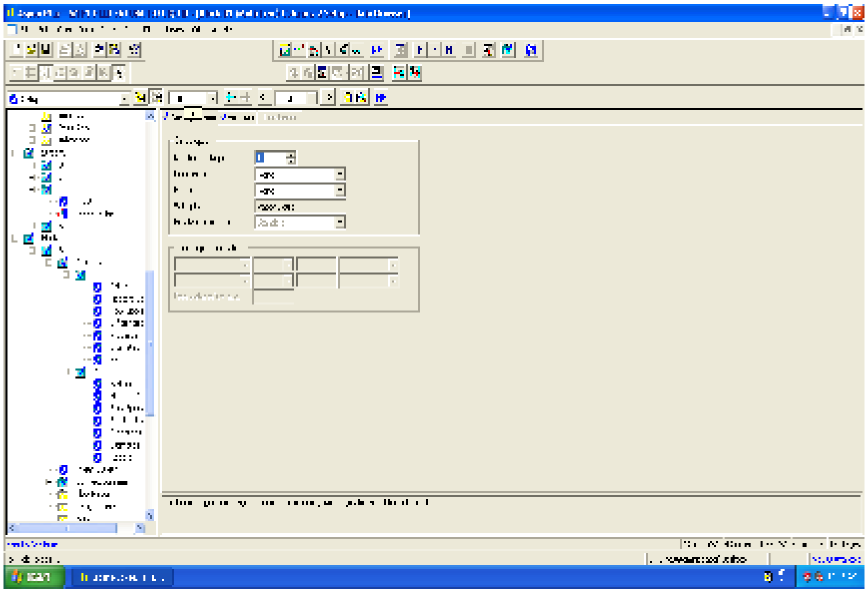


Figure 3.11: Column 2 specifications

Set the pressure for column 2 (section 2 of main column) as shown in figure 3.12

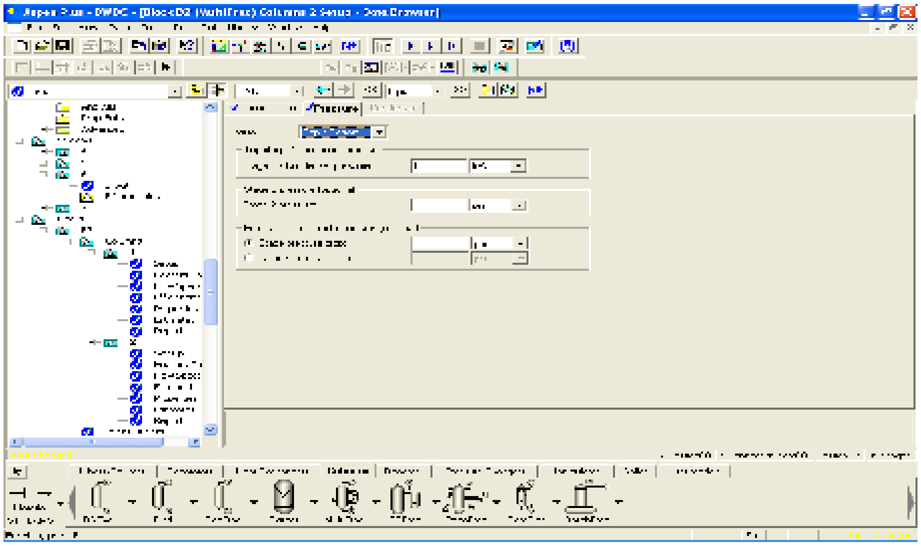


Figure 3.12: Condenser specifications for column 2

The temperature of top and bottom stage is specified as shown in figure 3.13

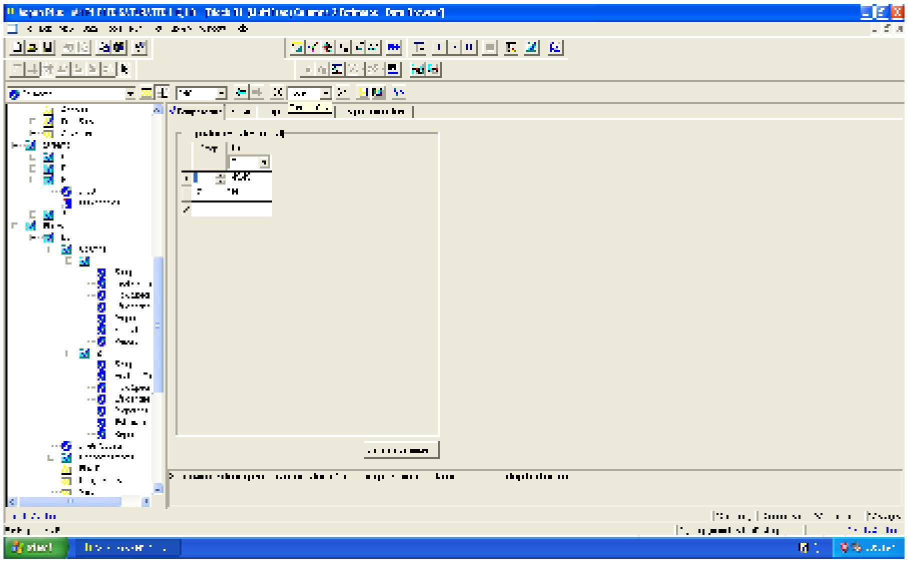


Figure 3.13: Top and bottom stage temperature of column 2

Now, specify the feed in stage and product out stages in the columns as shown in figure 3.14.

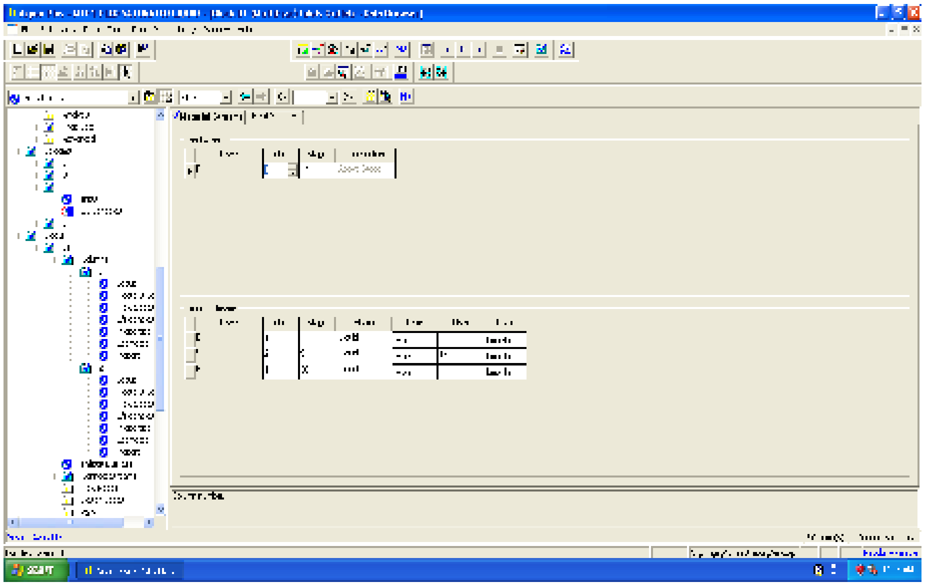


Figure 3.14: Feed and product stage specifications.

Now in block of column, add the four connect stream, which makes the thermally coupled arrangement between two column. Figure 3.15 shows the connect stream 1. The liquid flow rate from the main column should be specified with this stream.

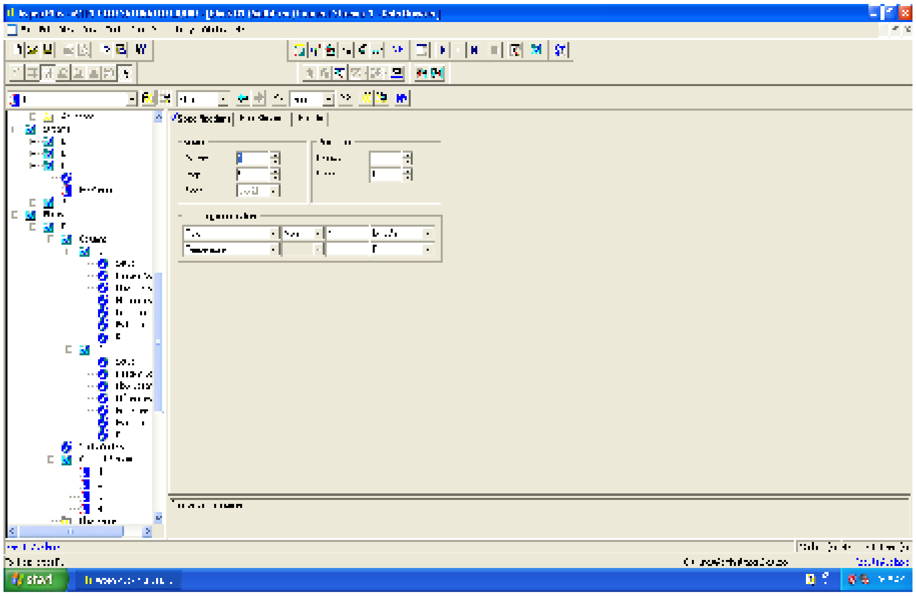


Figure 3.15: Specification of connect stream 1

The connect stream 2 specify the vapor flow from the column 2 to column 1. The flow rate of vapors is not known as shown in figure 3.16.

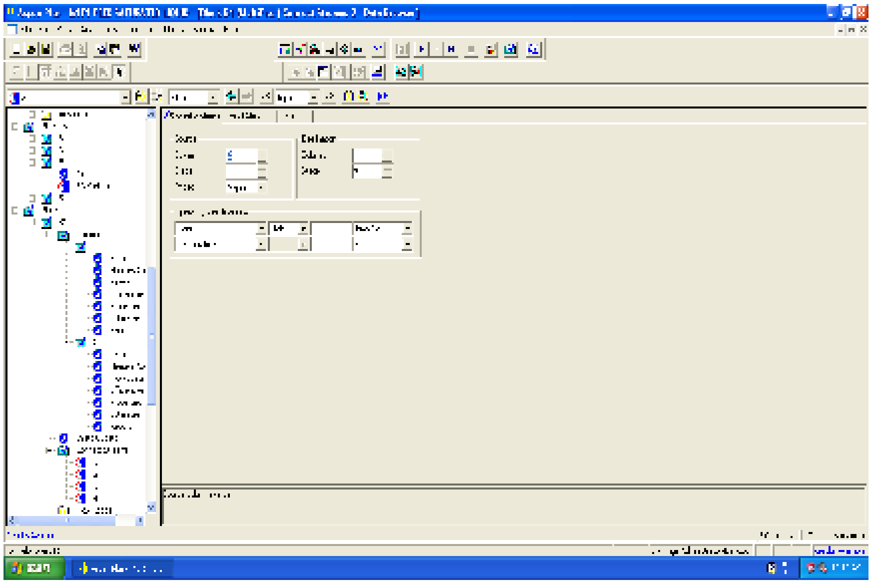


Figure 3.16: specification of connect stream 2

The vapor flow from column 1 to column 2 is specified with connect stream 3 as shown in figure 3.17.

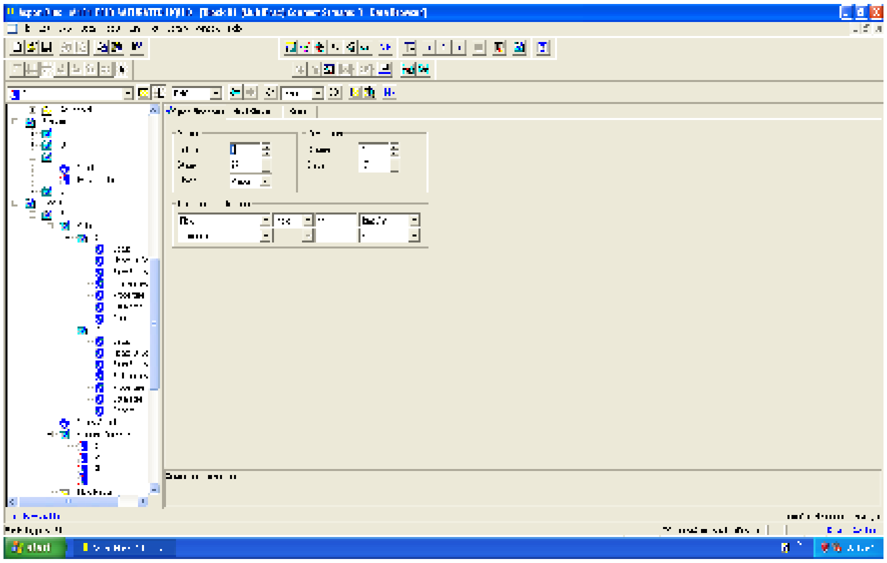


Figure 3.17: Specification of connect stream 3

Now specify the vapor flow rate from column 1 to column 2 as shown in figure 3.18.

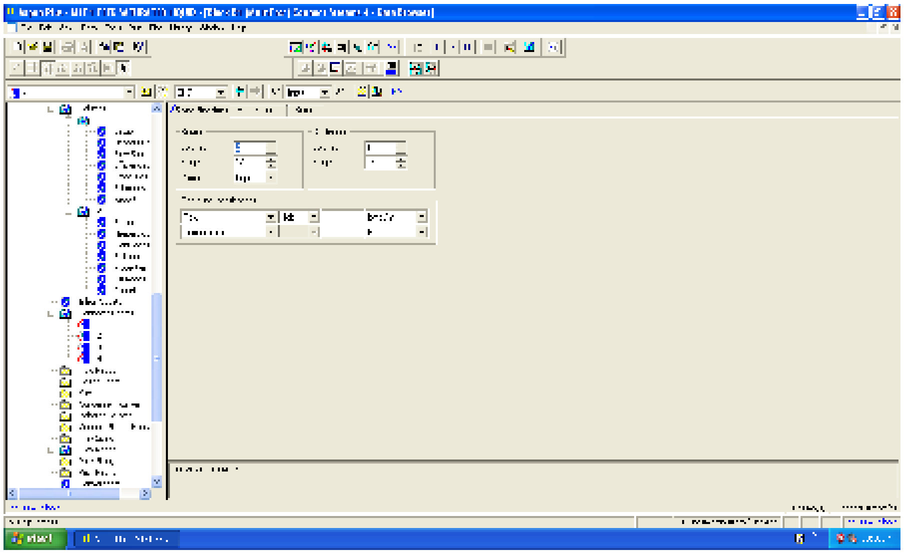


Figure 3.18: Specification of connect stream 4

Now from the *Tray Rating* features of ASPEN Plus, provide the data for hydrodynamic calculation as shown in figure 3.19.

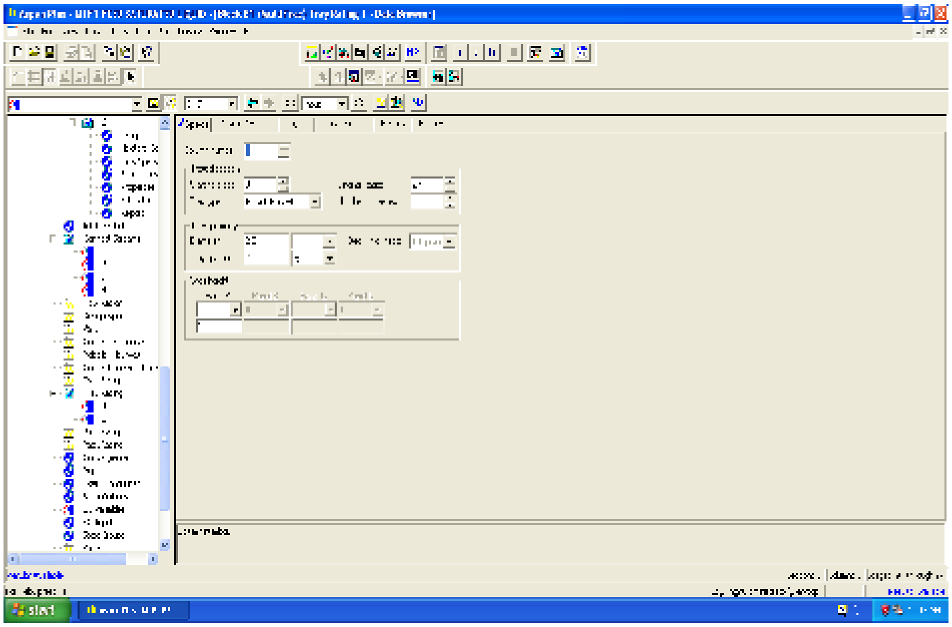


Figure 3.19: Tray rating for column 1

Tray rating for column 2 is given in figure 3.20.

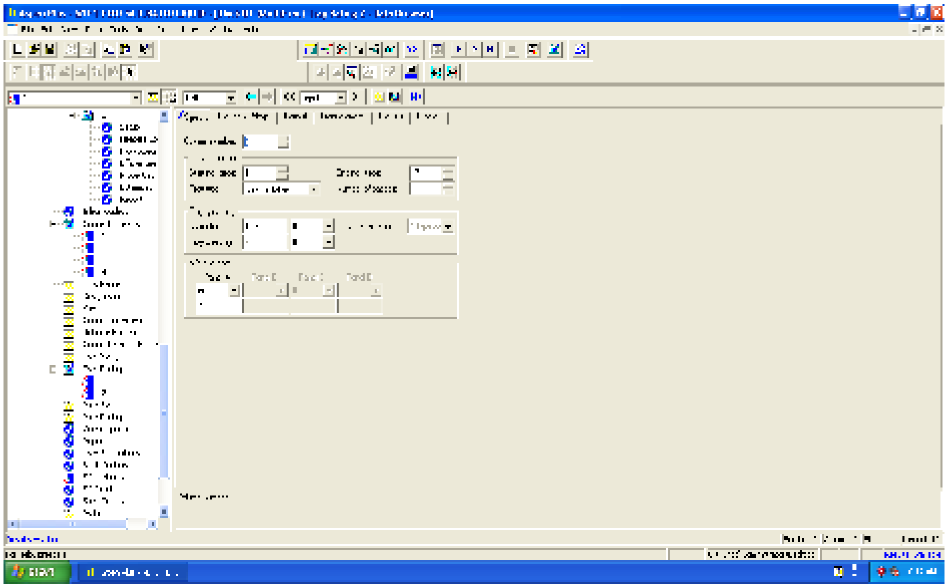


Figure 3.20: Tray rating for column 2

After completing all the specifications, run the simulation to get the results as shown in figure 3.21.

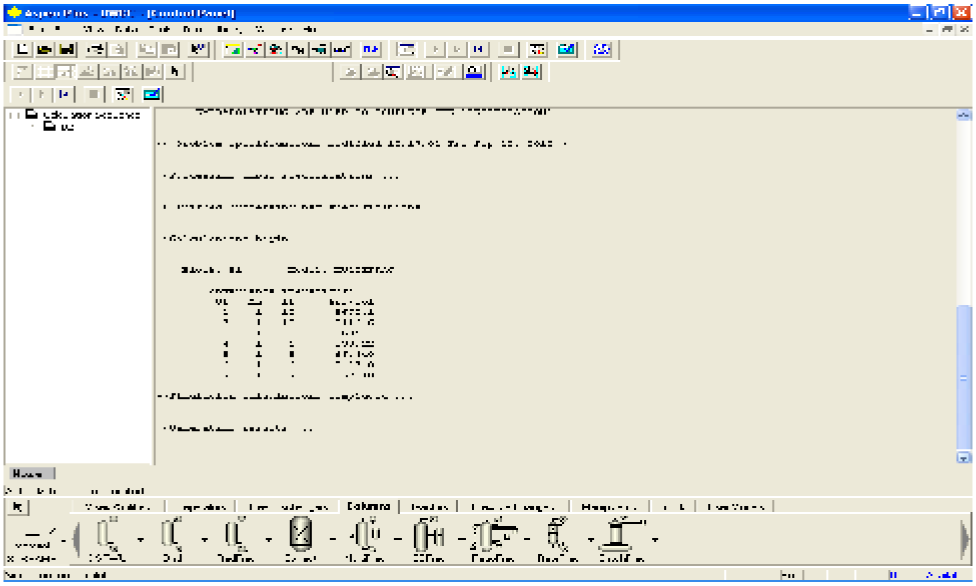


Figure 3.21: Simulation results

CHAPTER 4
RESULTS AND DISCUSSIONS

The performance of divided wall column is affected by varying structural and operational variables. The energy duty, purity of products and pressure drop across the divided wall are affected by varying structural and operational variables such as location of feed, location of side draw, number of trays in main column, number of trays in post fractionator, reflux rate, vapor split, liquid split, position of wall, height of wall.

The thermodynamic efficiency of divided wall distillation column and direct sequence columns is calculated by using second law of efficiency. The sizing and costing of divided wall distillation column is done by computer programming in C language.
We take a ternary system for the separation of hydrocarbon mixture, as shown in Table 4.1 with its specifications.

Table 4.1 Feed and product specifications, operating pressure and fluid package for mixture

components	composition	Feed conditions	Product specifications	Operating conditions	Fluid package
BPH		100lbmol/hr		Total condenser	PR
n-Butane	0.4	24.8psi	D=99mol% Butane	Pcond= 21.08 psi	
n-Pentane	0.2	Saturated	B=98mol Pentane		
n-Hexane	0.4	liquid	S=97mol% Hexane		

4.1 Effect of Structural Variables

The effect of structural variables such as location of feed, location of side stream, locations of liquid and vapor splits, number of stages in main and post fractionator column, on product purities, reboiler duty and on pressure drop across the wall are discussed in this study.

4.1.1 Effect of feed location

The distillate purity will decrease by varying feed location as shown in figure 4.1 or by decreasing number of stages in stripping section. The purity of bottom product will increase because as number of stages in stripping section decreases, the purity will increased. The purity of side product firstly increase by increasing number of stages in rectifying section then it will decrease because of the less separation of side product on the bottom of the dividing wall and the purity will decreases.

The variation in feed location have no effect on reboiler duty as shown in figure 4.2, because the column reflux rate and the feed flow rate are same. The duty will vary by varying the flow rates in the column.

Feed locations have a very small effect on the pressure drop as shown in figure 4.3. Pressure drop will decrease by increasing number of stages in rectifying section by moving upward, the pressure will decrease because of condenser pressure. Due to this reason the pressure drop firstly increase then decreased due to reboiler pressure. The optimum feed stage obtained from following results is 17.

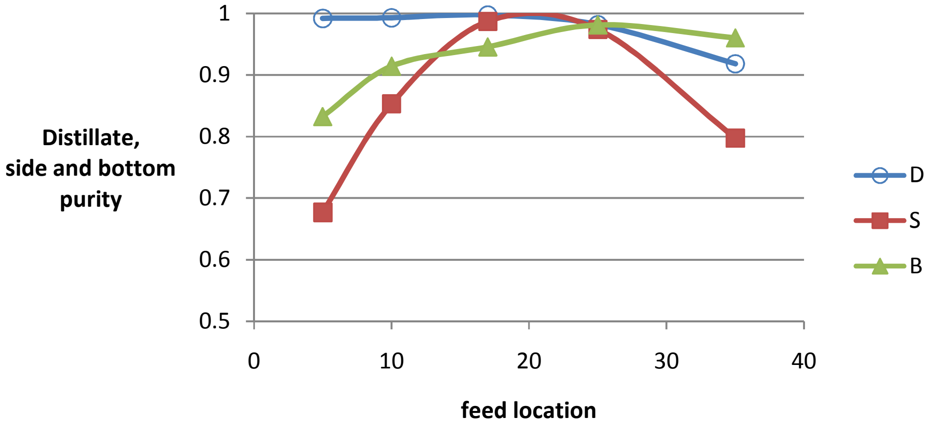


Figure 4.1: Effect of feed location on product purity

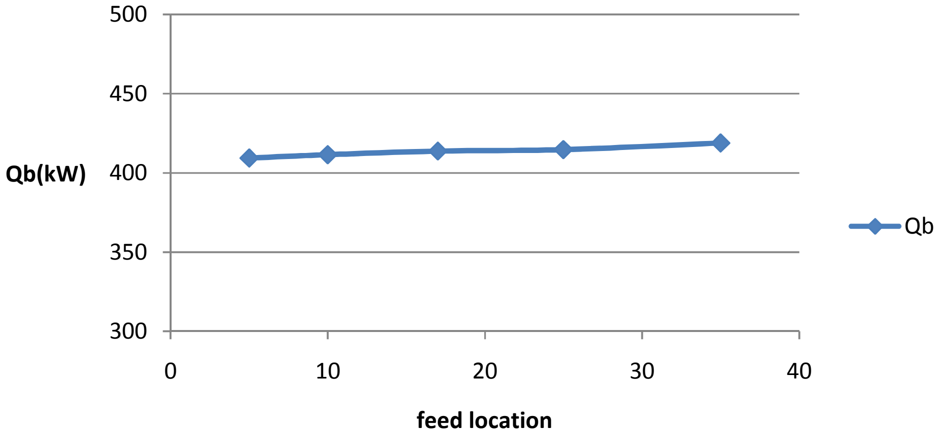


Figure 4.2: Effect of feed location on reboiler duty.

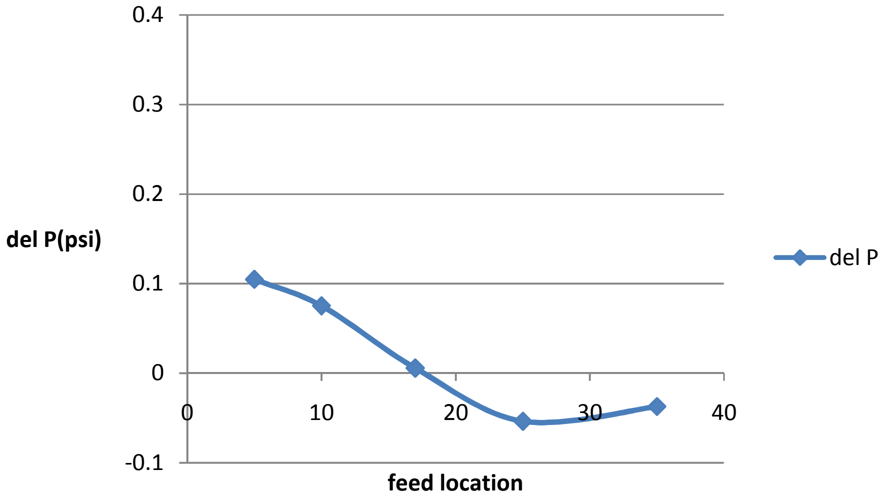


Figure 4.3: Effect of feed location on the pressure drop

4.1.2 Effect of Side location

The purity of distillate will increase by shifting the side location towards the bottom section of column, as shown in figure 4.4, if side product is recovered from rectifying section then due to early recovery the purity will be less and if we recover from the middle of the wall then it will recovered at its maximum concentration.

The location of side stage have no effect on reboiler duty as shown in figure 4.5 because side stream is recovered from post fractionator and the flow rate of connect streams are same. The side location has a great effect on pressure drop. The pressure drop will decrease as shown in figure 4.6 because reboiler pressure is more than the condenser pressure. The following result shows that the optimum side stage is 9.

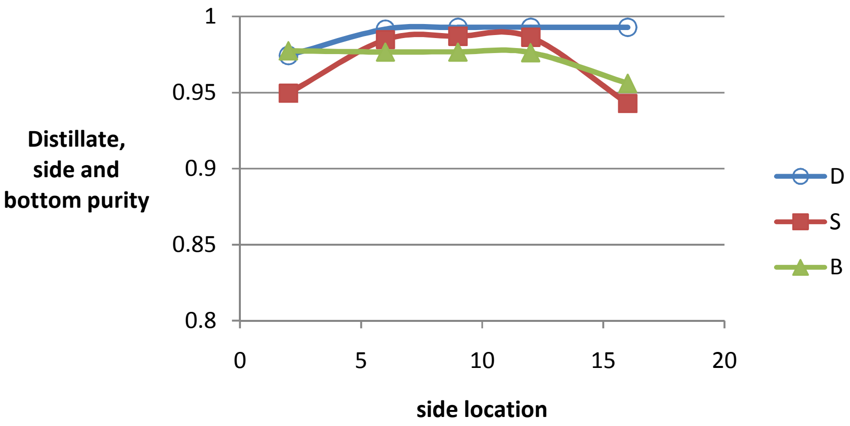


Figure 4.4: Effect of side location on product purity

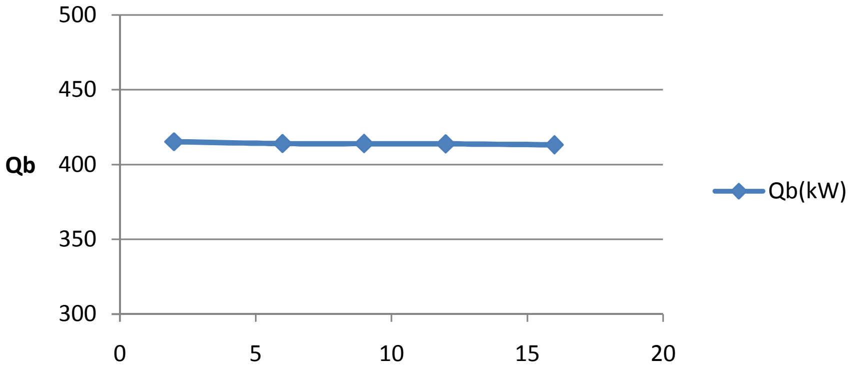


Figure 4.5: Effect of side location on reboiler duty

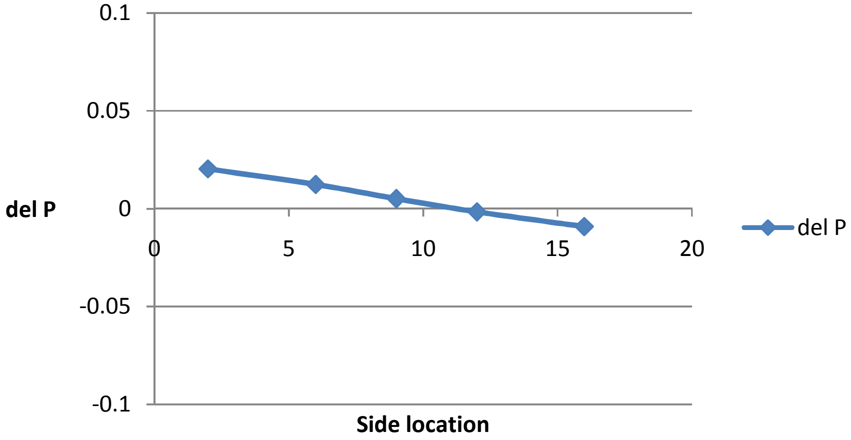


Figure 4.6: Effect of side location on pressure drop

4.1.3 Effect of Number of Stages in Main Column

The variation in number of stages have no effect on product purity as shown in figure 4.7 because the connect streams flow rates and reflux rate are same.

The variation in number of stages have no effect on reboiler duty as shown in figure 4.8 because location of connect streams are same.

The pressure drop will increase by increasing number of stages in main column as shown in figure 4.9 because as height will increase pressure in main column will decrease and in postfractionator, it will remain same. As a result, pressure drop will increase. The optimum numbers of stages in main column are 38, as obtained from the following results.

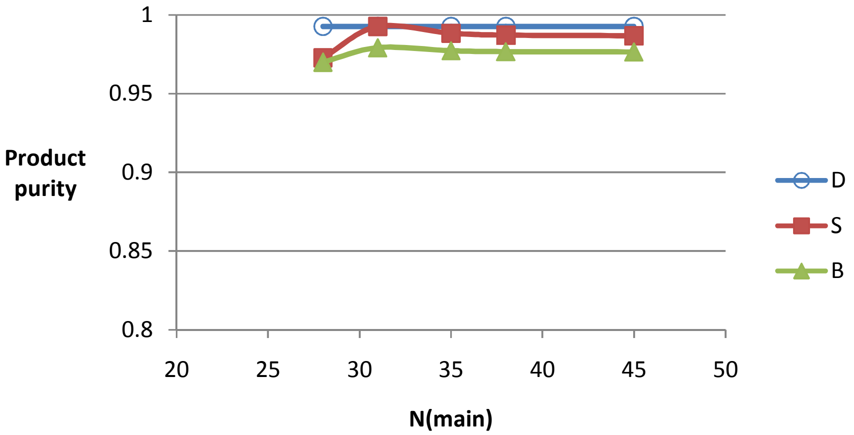


Figure 4.7: Effect of number of stages (main column) on product purity

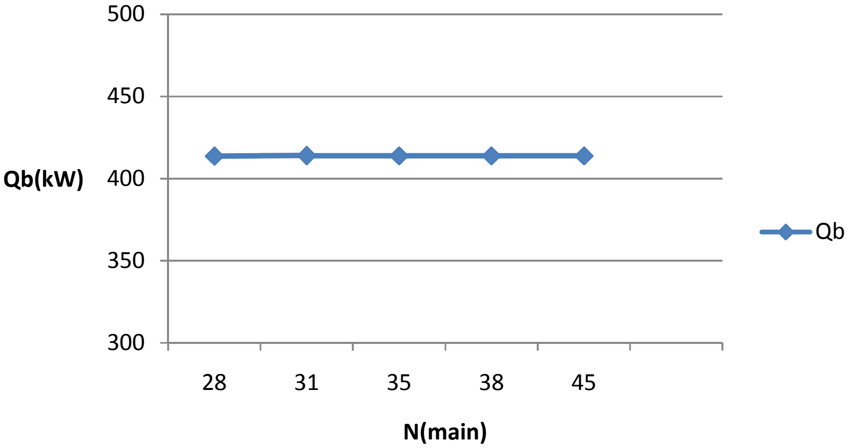


Figure 4.8: Effect of number of stages (main column) on reboiler duty

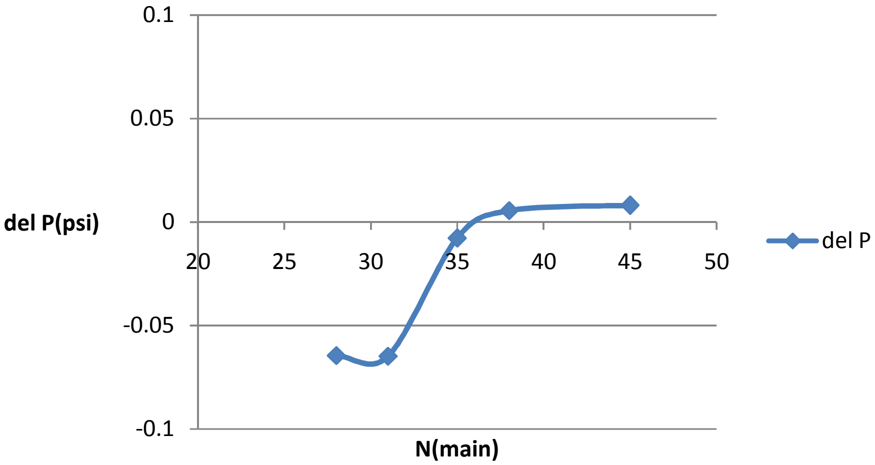


Figure 4.9: Effect of number of stages (main column) on pressure drop

4.1.4 Effect of Number of stages in postfractionator

The variation in number of stages in post fractionator affect the product purities as shown in figure 4.10. The distillate purity will decrease by increasing number of stages in postfractionator because of change in the connect streams location or because of the increase in the height of the wall. The bottom purity will increase because the HK will be separated easily at the end of the wall. The side purity will decrease because the side location is same. If we recover side product from the middle of post fractionator then the purity will be more. The number of stages in postfractionator have no effect on reboiler duty as shown in figure 4.11 because connect stream flow rates and column reflux rates are same. The pressure drop will decrease by varying the number of stages in postfractionator as shown in figure 4.12. The optimum stages obtained in postfractionator are 17.

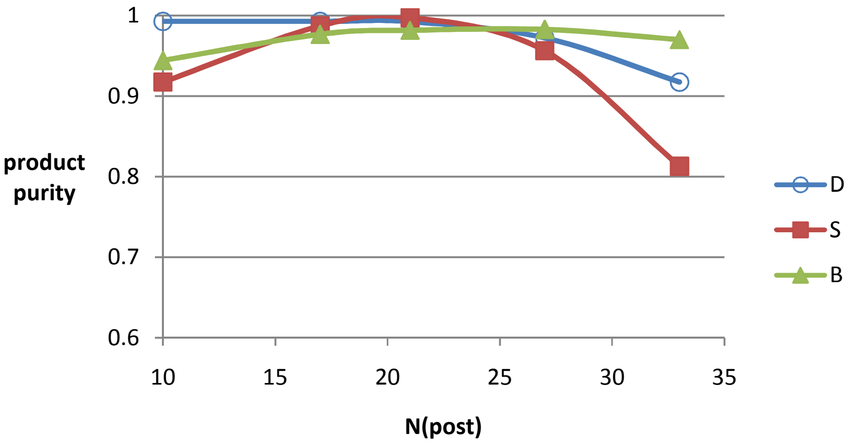


Figure 4.10: Effect of number of stages (postfractionator) on product purity

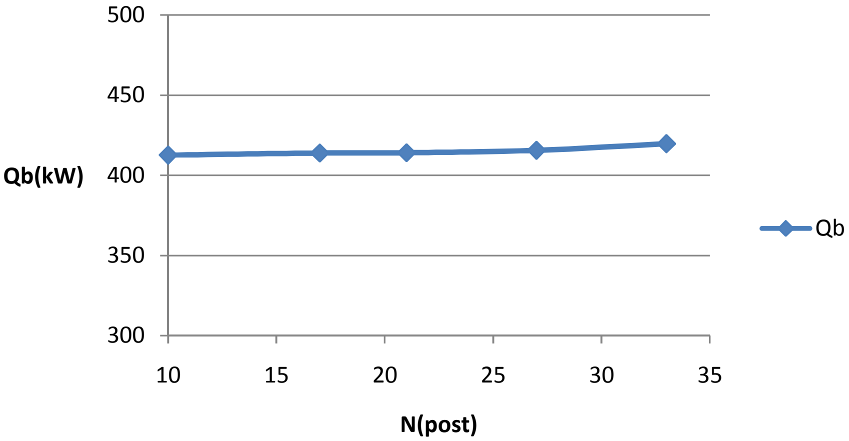


Figure 4.11: Effect of number of stages (postfractionator) on reboiler duty.

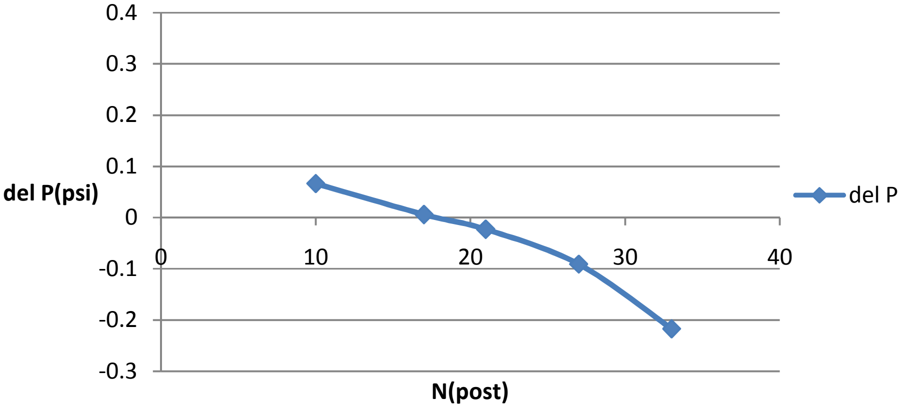


Figure 4.12: Effect of number of stages (postfractionator) on pressure drop

4.1.5 Effect of Wall Position

The effect of wall position in column on product purity as shown in figure 4.13. The distillate purity increases and then remains same by lowering wall position because, as the wall position decreases towards the bottom, the number of stages on upper side of wall increases. The bottom purity decreases because as wall position decreases toward the bottom, the number of stages below the wall end decreases, the product purity decreases. The side purity is maximum when wall is in middle position

The position of wall have a very small effect on reboiler duty as shown in figure 4.14. The reboiler duty decreases by lowering wall position because as number of stages decreases below the wall end, the less separation will takes place and duty will decreases. As shown in figure 4.15, the pressure drop across the wall increases by lowering wall position. The wall position is optimum when it will start at 9th stage.

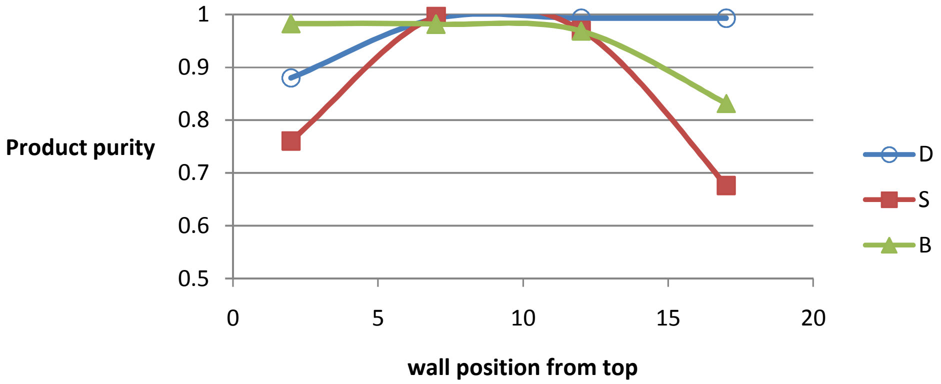


Figure 4.13: Effect of wall position on product purity

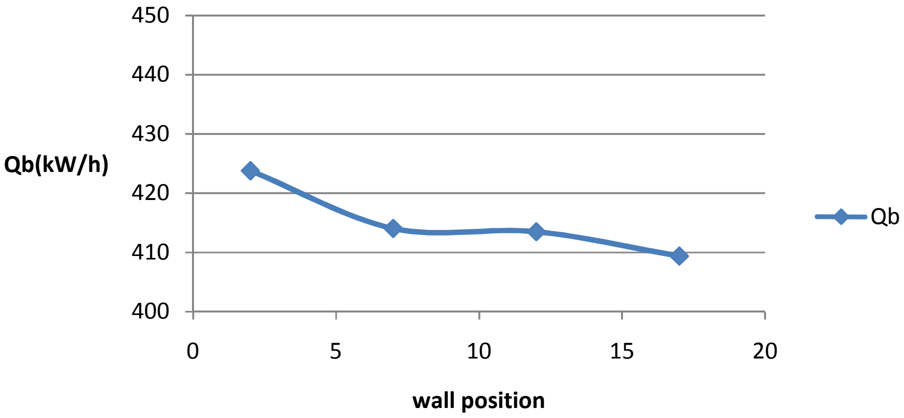


Figure 4.14: Effect of wall position on reboiler duty

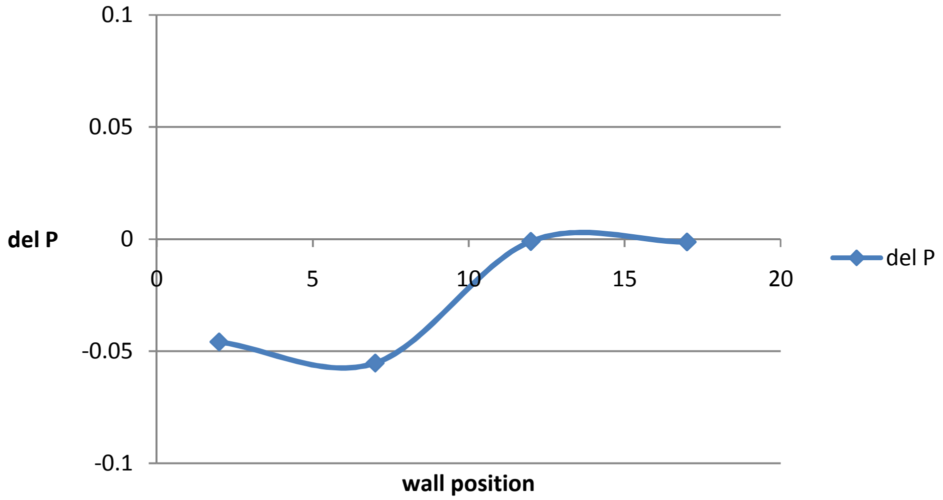


Figure 4.15: Effect of wall position on pressure drop

4.1.6 Effect of liquid split location

As shown in figure 4.16, by lowering the liquid split location towards bottom, the product purity decreases. The reboiler duty is not much effected by liquid split location as shown in figure 4.17. The pressure drop decreases by changing liquid split location as shown in figure 4.18, because as going down in column, the pressure increases due to reboiler pressure. The stage 9 is the optimum liquid split location analysed from the following results.

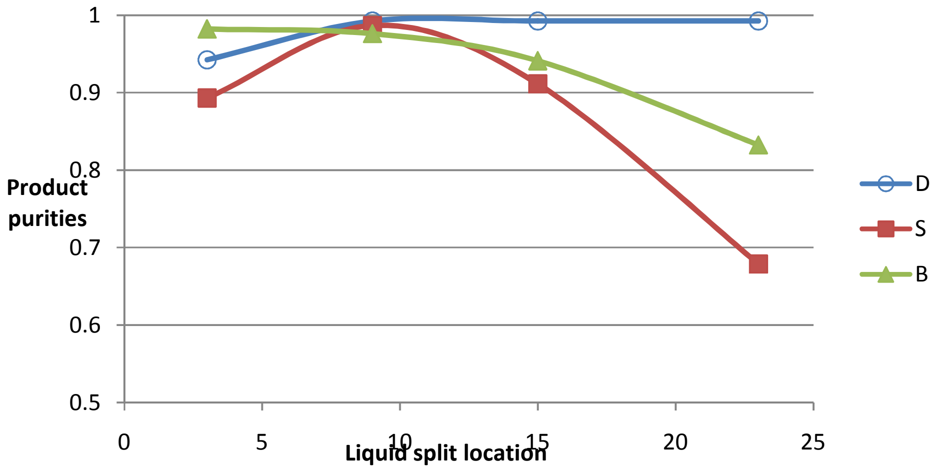


Figure 4.16: Effect of liquid split location on product purity

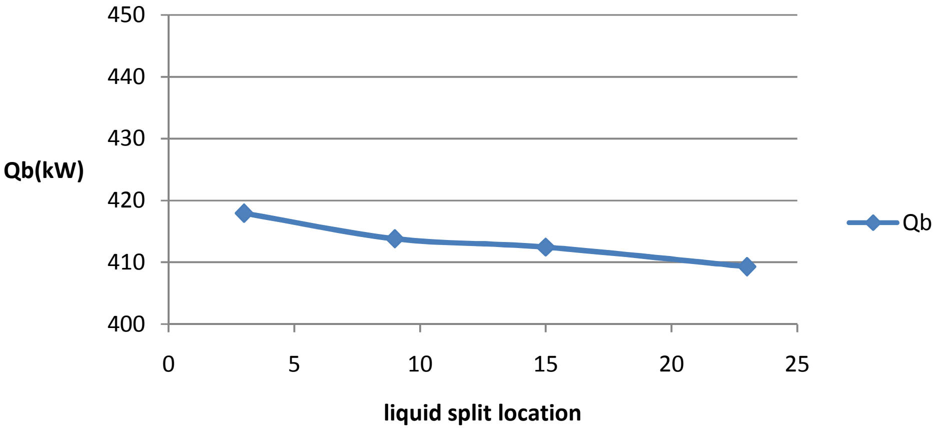


Figure 4.17: Effect of liquid split location on reboiler duty

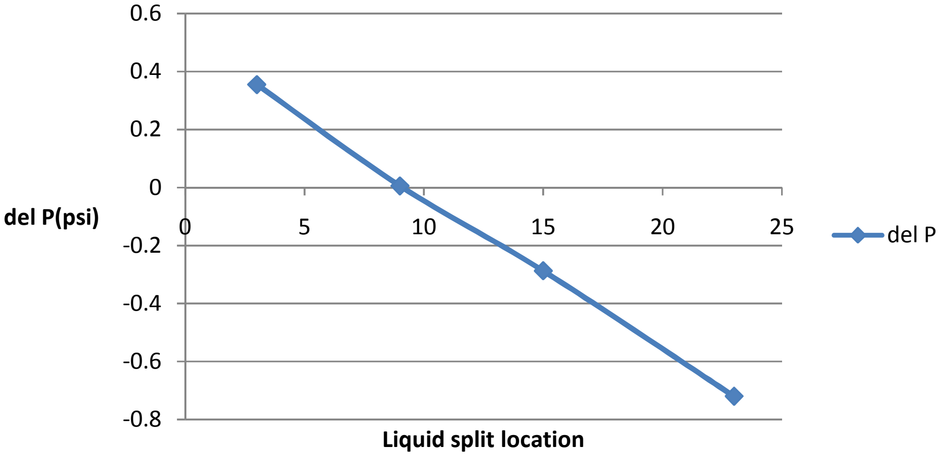


Figure 4.18: Effect of liquid split location on pressure drop

4.1.7 Effect of Vapor Split Location

The product purity increases by lowering the vapor split location to bottom as shown in figure 4.19. The reboiler duty decreases by varying liquid split location as shown in figure 4.20. The pressure drop increases by changing liquid split location as shown in figure 4.21. The optimum vapor split stage obtained from following results is 27.

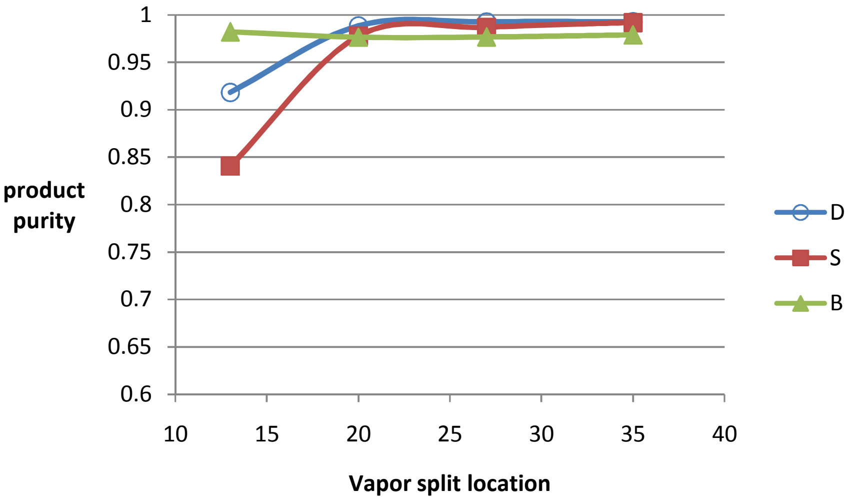


Figure 4.19: Effect of vapor split location on product purity

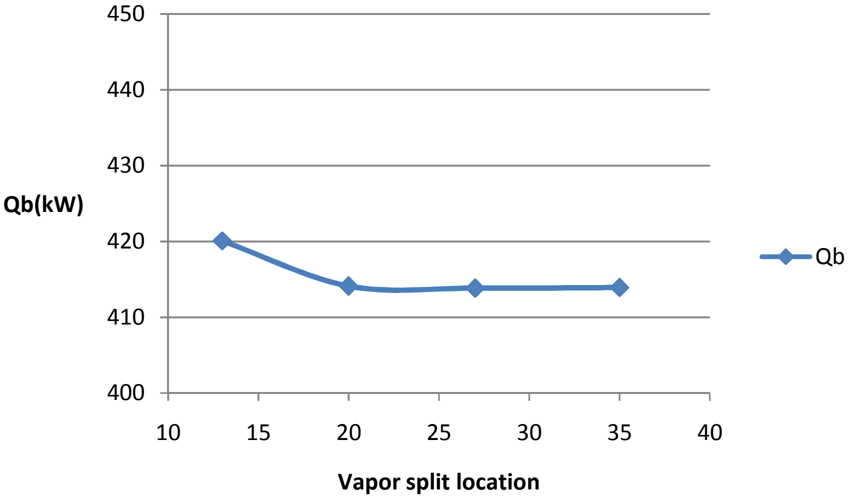


Figure 4.20: Effect of vapor split location on reboiler duty

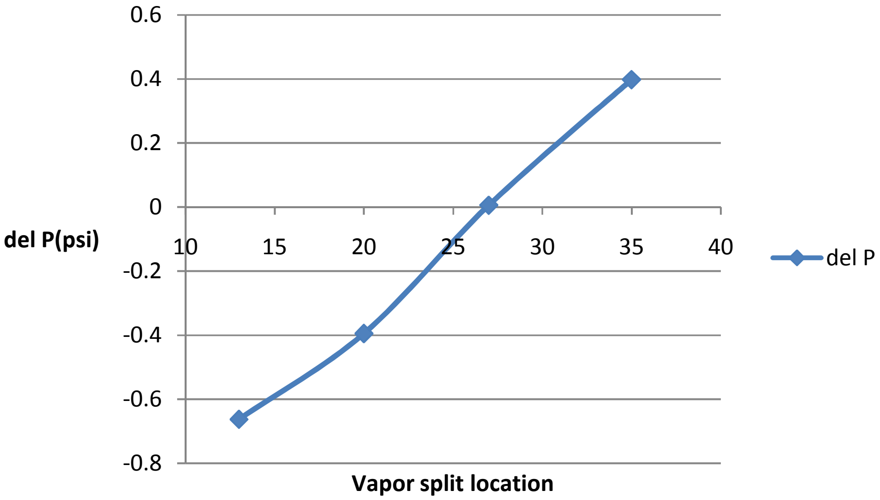


Figure 4.21: Effect of vapor split location on pressure drop

4.2 Effect of operational variables

The effect of operational variables such as reflux ratio and liquid and vapor flow rate from main column, on product purity, reboiler duty and pressure drop across the wall are discussed.

4.2.1 Effect of Liquid split ratio

The liquid split affects the side and bottom purities as shown in figure 4.22. The liquid split is basically the liquid flow rate in main column to liquid flow rate in postfractionator. By increasing the flow rate in postfractionator the side purity will firstly increases then decreases because as liquid flow rate in post fractionator will increase then separation efficiency will decrease and purity will decrease. There is a very minor effect on reboiler duty by variation in liquid split ratio as shown in figure 4.23. The liquid split affects the pressure drop as shown in figure 4.24. The pressure drop will decrease because of variation in flow rates.

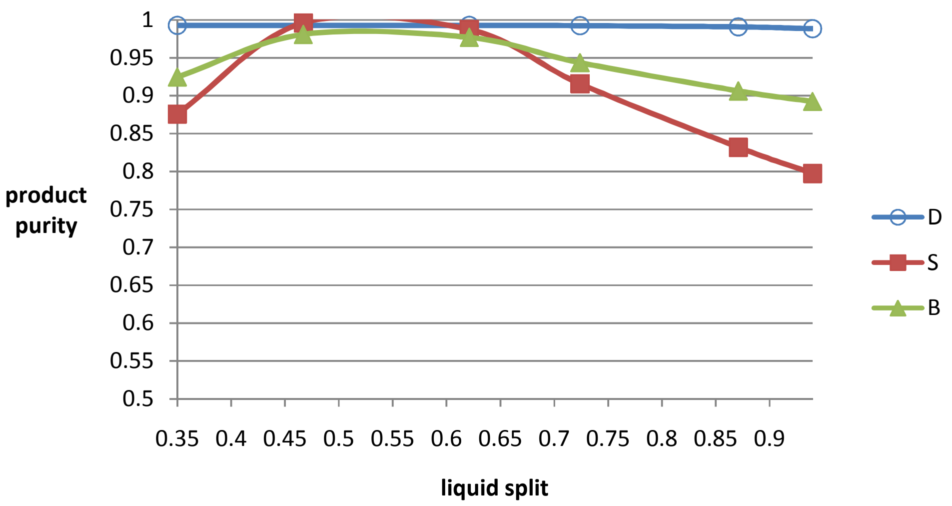


Figure 4.22: Effect of liquid split on product purity.

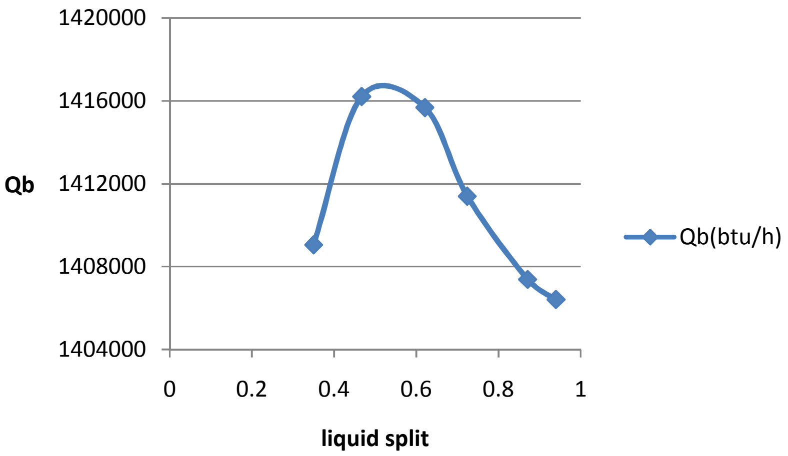


Figure 4.23: Effect of liquid split on reboiler duty

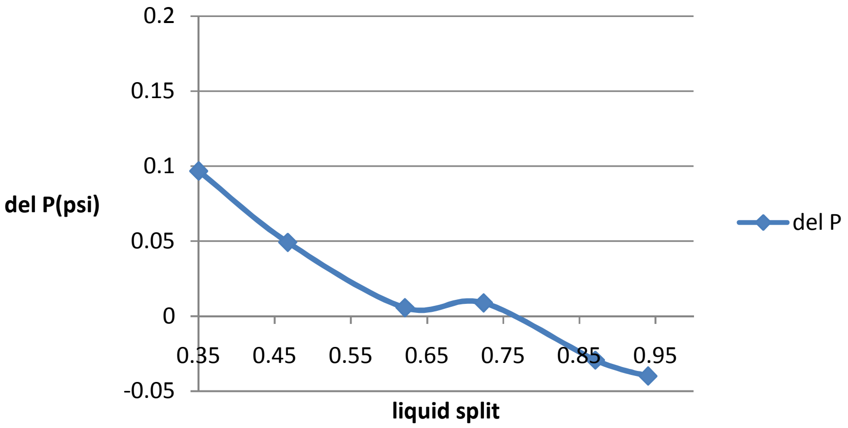


Figure 4.24: Effect of liquid split on pressure drop

4.2.2 Effect of vapor split ratio

As shown in figure 4.25, the vapor splits have a great effect on product purities. The major effect of vapor split is on side product purity. The purity of side stream will increase when vapor split is up to 0.4 , if we further increase the vapor flow rate then side product purity will start decreasing because the vapor flow rate much is more than the liquid flow rate. The reboiler duty will firstly decrease then increases as shown in figure 4.26. The vapor split affects the reboiler duty because as vapor flow increases, the duty also increases. The pressure drop will decrease by increasing vapor flow rate as shown in figure 4.27 because as the vapor flow rate decreases the pressure in postfractionator will decrease and pressure in main will remain same, as a result, the pressure drop will decrease.

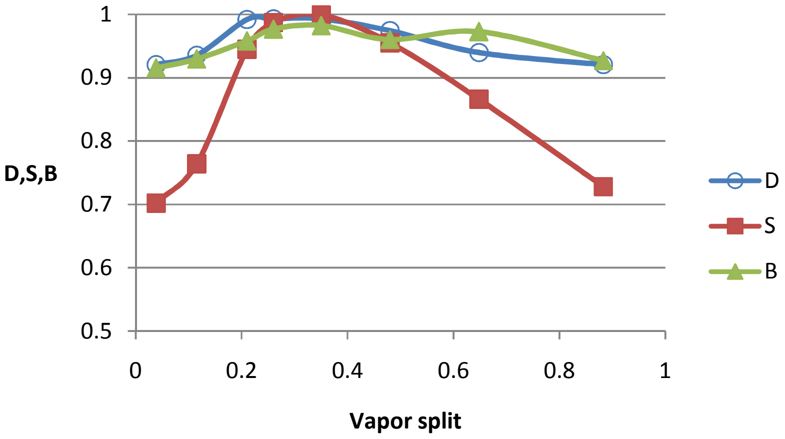


Figure 4.25: Effect of vapor split on product purities

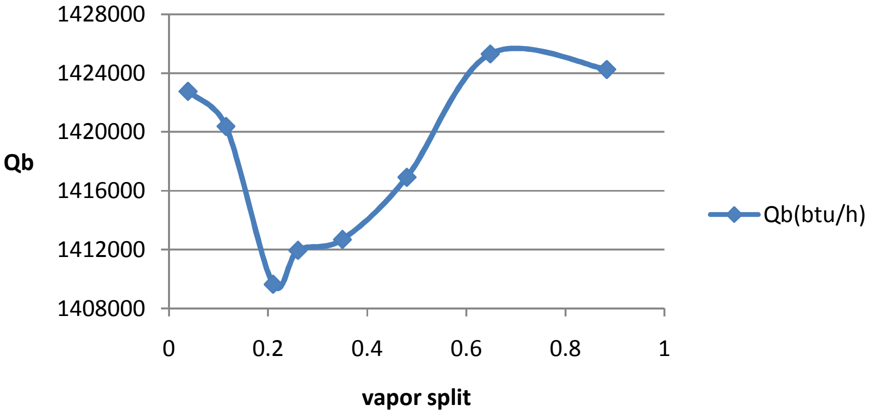


Figure 4.26: Effect of vapor split on product purity

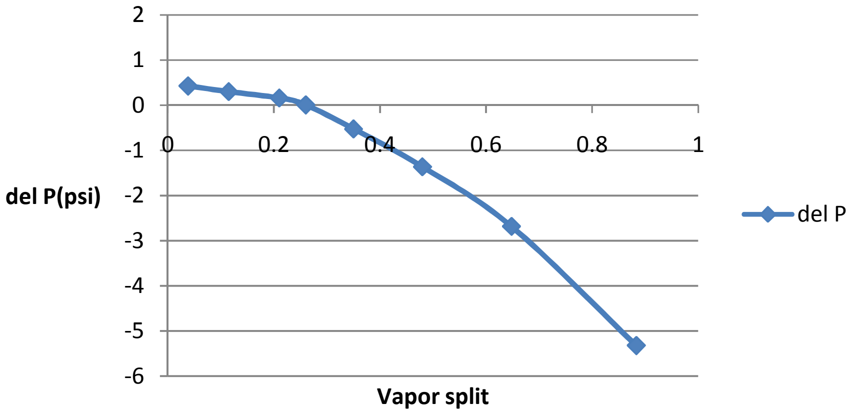


Figure 4.27: Effect of vapor split on pressure drop

4.2.3 Effect of reflux ratio

As shown in figure 4.28, the side and bottom purities will increase by increasing reflux ratio because as liquid flow rate in column will increase then the product purities will also increases.

The reboiler duty will increase by increasing reflux ratio as shown in figure 4.29 because as liquid as well as vapor flow rate in column will increase then the heat load on condenser as well as on will reboiler increase.

The pressure drop will increase by increasing reflux ratio as shown in figure 4.30 because as the liquid and vapor flow rates will increase then reboiler and condenser heat load will increase due to increase in condenser and reboiler heat load the pressure in main column will increase. So, as a result , pressure drop wil increases.

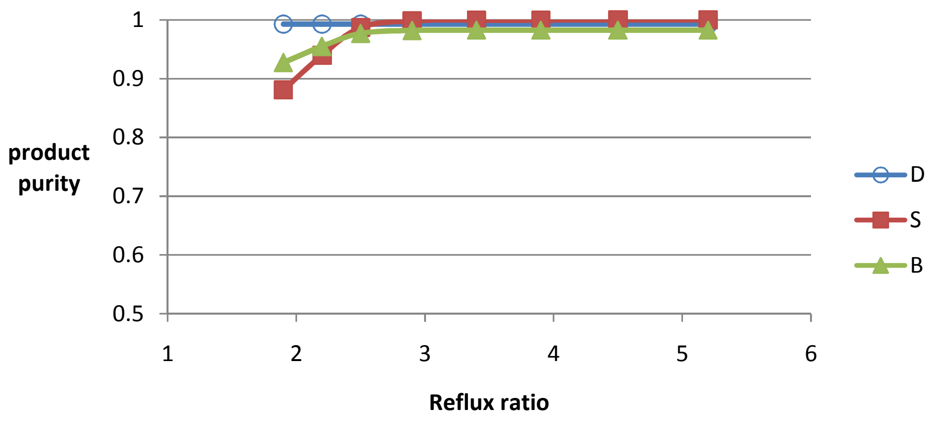


Figure 4.28: Effect of reflux ratio on product purities

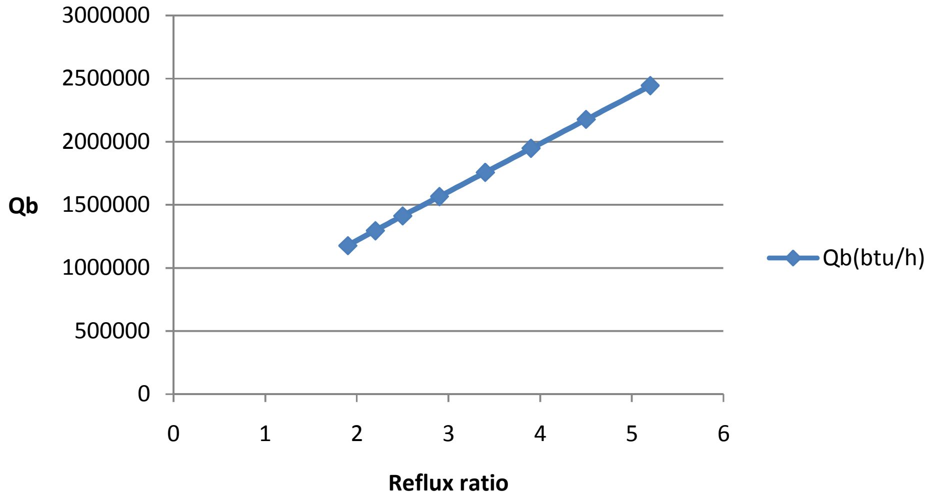


Figure 4.29: Effect of reflux ratio on reboiler duty

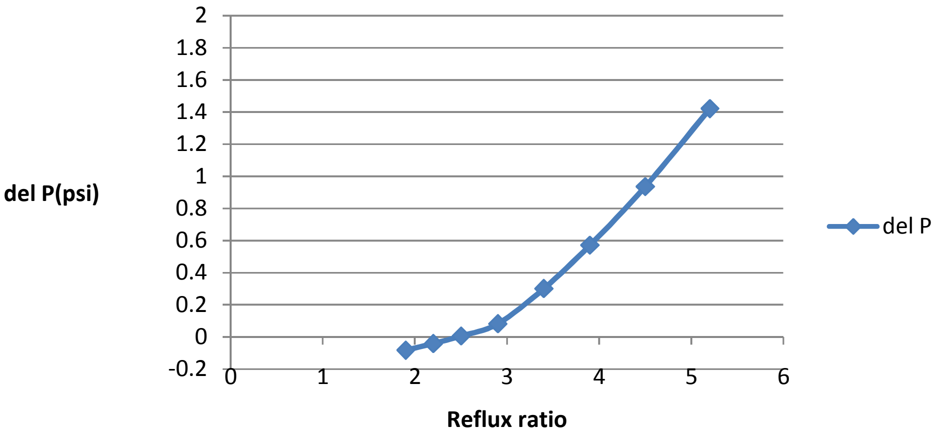


Figure 4.30: Effect of reflux ratio on pressure drop

The optimum results obtained from the above study are given in Table 4.2:

Table 4.2

Number of stages in main column	38
Number of stages in post fractionator	17
Main Lout stage	9
Main Vout stage	27
Feed location	17
Side location	9
Main Lout flow (kmol/hr)	23.85
Main Vout flow(kmol/hr)	15.075
Liquid split ratio	0.621
Vapor split ratio	0.26

4.3 Estimation of Thermodynamic efficiency of distillation column

At present, distillation remains one of the most widely used separation methods in the chemical engineering industry. However, this separation process conveys a significant disadvantage; it requires high amounts of energy. In fact, the cost of stream has the highest contribution to the total annual cost of a distillation column. Moreover, the distillation process has inherent low thermodynamic efficiency. Several attempts have been made to reduce energy consumption in distillation sequence. The thermally coupled distillation column or divided wall distillation column can give significant energy savings. Thermally coupled distillation sequences, consisting of implementation of vapor-liquid interconnections, achieving heat transfer by direct connect between the streams of the columns, and resulting in elimination of condensers and reboilers of columns. The systems can produce significant energy savings over conventional distillation sequences. The thermodynamic efficiencies of Petlyuk columns are greater than the columns in sequence.

The thermodynamic efficiencies can be computed using the laws of thermodynamics. Most industrial separation operations utilize large quantities of energy in form of heat. The energy consumed by distillation separation in petroleum, chemical, and natural-gas process plants are 2.7% of total energy consumption. Thus, it is of considerable interest to know the extent of energy consumption in separation process, and to what degree energy requirements might be reduced. Such energy estimates can be made by applying the first and second laws of thermodynamics.

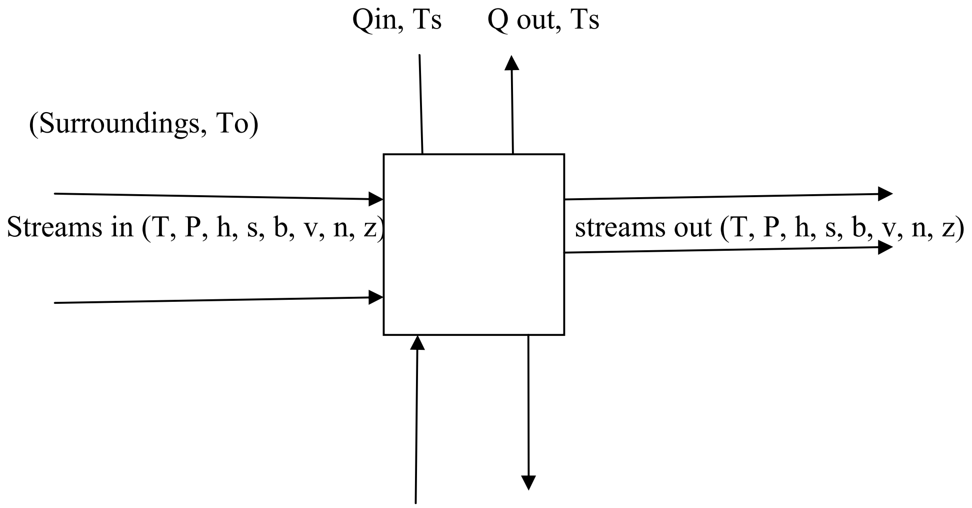


Figure 4.31: General separation system

Consider the continuous, steady-state, flow system for a general separation process as shown in figure 4.31. One or more feed streams flowing into the system are separated into two more product streams that flow out of the system

For all these streams we denote the molar flow rates by n, the component mole fraction by z, the temperature by T, the pressure by P, the molar enthalpies by h, the molar entropies by s, the molar availabilities by b. Heat flows in or out of the system are denoted by Q, and shaft work crossing the boundary of system is denoted by W. At steady state, if kinetic, potential, and surface energy changes are neglected , the first law of thermodynamic states that the sum of all forms of energy flowing into the system equals the sum of energy flows leaving the system:

$$(\text{stream enthalpy flows} + \text{heat transfer} + \text{shaft work})_{\text{leaving system}} - (\text{stream enthalpy flows} + \text{heat transfer} + \text{shaft work})_{\text{entering system}} = 0$$

In terms of symbols, the energy balance is given by equation 1 in Table 4.3, where all flow rate, heat transfer, and shaft work terms are positive. Molar enthalpies may be positive or negative depending on the reference state.

All separation processes must satisfy the energy balance. Inefficient separation processes require large transfers of heat and /or shaft work into and out of the process; efficient processes require smaller levels of heat transfer and/or shaft work. The first law of thermodynamics provides no information on energy efficiency, but second law of thermodynamics given by equation 2 in Table 3, the steady state entropy balance is

(stream entropy flows + entropy flows by heat transfer)$_{\text{leaving system}}$ - (stream entropy flows + entropy flows by heat transfer)$_{\text{entering system}}$ = production of entropy by the process

Although ΔS_{irr} is a measure of efficiency. The stream availability function, b, as defined by

$$b = h - T_0 s$$

is measure of maximum amount of stream energy that can be converted into shaft work if stream is taken to the reference state.

Table 4.3: Equations for calculation of thermodynamic efficiency

Energy balance:

$$\sum(nh + Q + Ws)out - \sum(nh + Q + Ws)in = 0 \qquad (1)$$

Entropy balance:

$$\sum\left(ns + \frac{Q}{Ts}\right)out - \sum\left(ns + \frac{Q}{Ts}\right)in = \Delta Sirr \qquad (2)$$

Availability balance

$$\sum\left|nb + Q\left(1 - \frac{T0}{Ts}\right) + Ws\right]in - \sum\left|nb + Q\left(1 - \frac{T0}{Ts}\right) + Ws\right]out = LW \qquad (3)$$

Minimum work of separation

$$Wmin = \sum nb\ out - \sum nb\ in \qquad (4)$$

Second-law efficiency:

$$\eta = Wmin/(LW + Wmin) \qquad (5)$$

where b = h-T0s = availability function.

LW = T0ΔSirr = Lost work

4.3.1 Case study

A mixture of 45 kmol/hr of n-butane, n-pentane and n-hexane is considered. The feed conditions are shown in Table 4.1.

4.3.2 Simulation of DWC by using ASPEN for hydrocarbon mixture

Develop a design model to describe the steady state behavior of a divided wall column is not an easy task. We take Petlyuk column which is a rigorous model, available in Aspen model library. Petlyuk column consists of main column and postfractionator as shown in figure 4.32. The number of trays in main column is taken as 38 and postfractionator consists of 17 trays. The distillate rate is taken as 40.49 lbmol/h and reflux ratio is taken as 2.5. The main Lout and V_{out} stages are respectively 9 and 27. The flow rates of vapor and liquid from main column are 33.5 lbmol/hr and 53 lbmol/hr. The mixture is fed at 17th stage of the main column and side product is obtained from the 9th stage of postfractionator.

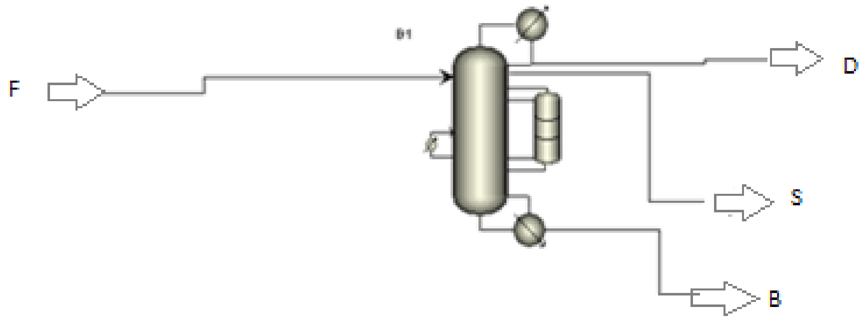


Figure 4.32: Petlyuk column

4.3.3 Simulation of direct sequence columns by using ASPEN

The direct sequence column arrangement is made by taking two RADFRAC columns in sequence as shown in figure 4.33. The feed mixture is fed in the first column at 17th tray. In this arrangement the light key component is obtained from the top of the first column and from the bottom the mixture is fed to the second column. For distillate rate for both columns is respectively 40.29 lbmol/hr and 19 lbmol/hr. The reflux ratios for both columns are taken as 2.5 and 2.84 respectively. The feed in second column is fed at 9th stage.

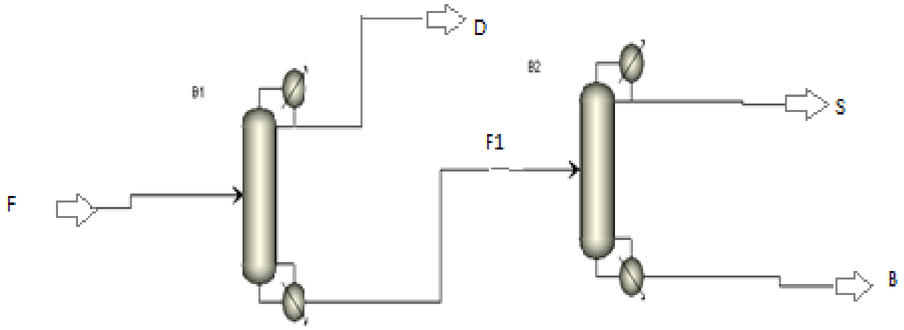


Figure 4.33: Columns in Direct sequence

4.3.4 Simulation results

For divided wall distillation column	**For direct sequence columns**
Reboiler duty of DWC, Q1= 413.819 kW	Reboiler duty of Direct sequence columns = 647.391 kW
Condenser duty of DWC, Q2=-391.387 kW	Condenser duty of Direct sequence columns=-624.992 kW

Top stage temperature, T1=282.798 K

Bottom stage temperature, T2=352.776 K

Enthalpy of distillate, h1= -148720 kJ/kmol

Enthalpy of bottom product, h2= -186770 kJ/kmol

Enthalpy of side product, h3 = -169000 kJ/kmol

Enthalpy of feed, h4= -170430 kJ/kmol

Entropy of distillate, s1=-452.76 kJ/kmol-K

Entropy of bottom product, s2= -614.44 kJ/kmol-K

Entropy of side product, s3= -537.09 kJ/kmol-K

Entropy of feed, s4= -531.30 kJ/kmol-K

4.3.5 Thermodynamic efficiency calculation by using C programming

By using ASPEN simulation results, the thermodynamic efficiency of both column arrangements is calculated. A Computer program in C language is written by using equations as discussed in appendix A 8.

The efficiency obtained by using Petlyuk column is 32.3% where the efficiency obtained from direct sequence columns is 4.09%.

The thermodynamically efficiency in direct sequence columns is less because of the mixing effects that occur due to miss-matches between the composition of the column feed and the composition on the feed tray and reduction of the re-mixing of middle component, as a result, a non-sharp split in the prefractionator, where in DWC, the remixing of components will not takes place and will lead to increase in thermodynamic efficiency.

Table 4.4: Energy consumption and thermodynamic efficiency comparison

Sequence	Energy consumption(kW/h)	η[%]
Direct sequence	647.391	4.09
DWC	413.819	32.3

The comparison shows that the Petlyuk or DWC are more energy efficient as compare to columns in sequence as shown in Table 4.3. The Thermodynamic efficiency of Petlyuk column arrangement is 28% more than the direct sequence arrangement. The similar observation for thermodynamic efficiency was observed by many researchers (Hernandez et al., 2008; Agrawal et al., 1998).

4.4 Sizing of Divided Wall Distillation Column

The capital cost for major equipments (namely, the condenser, reboiler, and the tray column) and the operating cost for a DWC are calculated based on module costing technique. The total annual cost, which includes both capital and operating costs, is then calculated.

4.4.1 Column sizing –Diameter, Tray spacing and Column height

In principle, the cross sectional area of a column has to be large enough to handle the vapor and liquid flow rates within a satisfactory operation region and to avoid excessive liquid entrainment in the column (Treybal, 1980). For conservative design, the minimum diameter required for a column is calculated based on a smaller value of the vapor velocity, *Vact*, typically 80 percent of the flooding vapor velocity for non-foaming liquids (Treybal, 1980).

DWC involves housing of two columns within a single shell, adjustment on the diameter calculations is required. The cross sectional area of the middle section of DWC is divided into two portions, and hence the corresponding diameters, D1 and D2, can be calculated separately based on the respective flooding vapor velocity, V1 and V2. Nonetheless, each section of the column has to be sized based on the maximum vapor load available from ASPEN. As distillation columns are conventionally fabricated with 0.5 ft increment in the diameter, the calculated diameter is rounded up to the nearest 0.5 ft for conservative design.

In general, the minimum tray spacing of 0.5 m is required for convenience of tray cleaning (Treybal, 1980). According to Ulrich (1984), the tray spacing should be a function of diameter for the columns with diameter larger than 1 m and should be calculated as follows:

$$S = 0.5 \text{ m} \qquad \text{for } D \leq 1 \text{ m}$$

$$S = 0.5D^{0.3} \text{m} \qquad \text{for } D \geq 1 \text{ m}$$

The column height can be determined by multiplying the tray spacing by the number of real trays required, which refers to the number of trays required for the particular separation when tray efficiency of 70% is assumed. On top of that, additional column height of 3 m should also be included to account for the space at the top and the bottom of the column for vapor disengagement and liquid sump respectively (Ulrich, 1984). Hence, the column height is given by:

$$H = (N\,act/0.70) + 3\text{m}$$

A computer program in C language is written by using above equations to calculate column diameter and height given in Appendix A 1.

Results:

Diameter column=2.48 ft
Height of column=100.46 ft

4.4.2 Condenser and reboiler sizing

Sizing of heat exchanger is mainly affected by the temperature of the process streams to be heat exchanged and the associated duty requirement. For the sizing of condenser, an average value of 510 W/m^2 K for U and minimum driving force of 10oC are assumed for all simulations in this study. On the other hand, driving force in the reboiler is also constrained within 45 F to ensure nucleate boiling, and a conservative heat flux (*U* × *LMTD*) of 35,490 W/m2 is used for reboiler sizing based on Douglas's (1988) recommendation.

The computer programs are made to calculate the condenser and reboiler area are given in Appendix A 2 & 3 and results are given below:

Results:
Area of condenser=406.035m^2
Area of reboiler=8.65 m^2

4.5 Capital cost

Capital cost refers to the investment required for all the equipments in the plant including installation and auxiliaries that are needed for complete process operation. As such, the factored-cost methods introduced by Guthrie are employed for the calculation of capital cost which includes direct project expense, indirect project expense, contingency and contractor fees (Turton et al., 2003). Detailed information on the related cost coefficients discussed in the following section is from Turton et al. (2003).

4.5.1 Costing of column and trays

By considering a distillation column as a vertical pressurized vessel with sieve trays as internals, the purchase cost of the vessel and the trays can be calculated separately. Purchase cost of a vertical pressurized vessel made of carbon steel under ambient pressure is given as:

$$\log C_{purchase=} K_1 + K_2 \log H + K_3 (\log H)^2$$

where K_1, K_2 and K_3 are the cost coefficients ($K_1 = 3.4974$; $K_2 = 0.4485$; $K_3 = 0.1074$). When the pressure at which an equipment operates increases, the purchase cost of the particular equipment increases as well due to the increase in the wall thickness. Hence, pressure factor has to be incorporated into the calculation of equipment capital cost.

In addition, different material of construction results in different bare module cost for a particular piece of equipment; thus, this effect must be considered for the costing calculation using the following correlations:

$$C_{BM,\ Column}= C_{purchase}(B_1+B_2F_MF_P)$$

Where, B_1 and B_2 are coefficients ($B_1 = 2.25$; $B_2 = 1.82$).

For the trays, the bare module cost is independent of pressure as they are surrounded by liquid and hence not subjected to significant differential pressure. However, the bare module cost of trays is affected by the quantity of trays purchased and the material of construction. The common, sieve tray is considered in this study and the quantity of trays used in the following calculations is the number of actual trays obtained after considering tray efficiency of 70%. Purchase cost and bare module cost for trays in a vertical pressurized vessel are given as follow:

$$\log C_{purchase}=K_1+K_2 \log A+K_3 (\log A)^2$$

where $K1$ (= 2.9949) $K2$ (= 0.4465) and $K3$ (= 0.3961)) are cost coefficients, and

$$C_{BM,\ Tray}= C_{purchase} N_{act}\ F_M F_q$$

A computer program in C language is made by using above equations to calculate cost of column and trays is given in Appendix A 4 & 5 and results are given below:

Results:
$C_{BM,\ column}$=\$595.16
$C_{BM,\ Tray}$=\$991.27

4.5.2 Costing of condenser and reboiler

In this study, floating-head heat exchanger is considered for both the condenser and the reboiler. Purchase cost of both these constructed of carbon steel for ambient operating pressure is given by:

$$\log C_{purchase}=K_1+K_2 \log A+ K_3 (\log A)^2$$

where K_1, K_2 and K_3 are the cost coefficients ($K_1 = 4.8306$; $K_2 = -0.8509$; $K_3 =0.3187$).

Similar to the bare module cost of a pressure vessel, the bare module cost of a heat exchanger should also include the pressure factor and the material factor.

The pressure factor, *Fp* of heat exchanger is given as follow.

$$\log F_P = C_1 + C_2 \log P + C_3 (\log P)^2$$

where, P is the pressure in bar gauge, and C_1, C_2 and C_3 are coefficients ($C_1 = 0.03881$; $C_2 = -0.11272$; $C_3 = 0.08183$). Value of the pressure factor should always be greater than unity. However, for condenser and reboiler, effect of pressure on the bare module cost is not as significant as that for a pressure vessel. This is because majority cost of a heat exchanger is due to numerous tubes in it. Bare module cost of the heat exchanger is given by:

$$C_{BM,condenser/reboiler} = C_{purchase}(B_1 + B_2 F_M F_P)$$

where, B_1 and B_2 are coefficients ($B_1 = 1.63$; $B_2 = 1.66$). Stainless steel is used as the material of construction for costing purposes for all trays, column, condenser, and reboiler in this study because such material offers higher resistance to corrosion. Moreover, it is more costly and hence provides a more conservative economic evaluation for DWC. Considering that the bare module cost of the major equipments, namely the column, the condenser and the reboiler, contribute to the majority of the capital cost, the unadjusted capital cost or the total module cost for the column, which includes the associated installation cost of the equipments, can be calculated as follows.

$$Unadjusted\ capital\ cost = 1.18(C_{BM,\ column} + C_{BM,\ tray} + C_{BM,cond} + C_{BM,reb})$$

A computer program in C language is made to to calculate the cost of condenser and reboiler, is given in Appendix A 6 and results are given below:

Result:

$C_{BM,reboiler}$= \$248.515

$C_{bm,condenser}$=\$395.045

Unadjusted capital cost=\$2631.809

4.5.3 Cost Escalation

Cost of materials and labour usually vary due to inflation. Hence, it is necessary to update the estimated cost to present or future time for realistic economic evaluation. The appropriate adjustment can be performed by (Turton et al., 2003):

$$C_{BM,present} = C_{BM,past} \, (I_{present}/I_{past})$$

Where, $C_{BM,present}$ and $C_{BM,past}$ are the present and past bare module costs respectively, and $I_{present}$ and I_{past} are the present and past cost indices respectively. The costing methods and related correlation coefficients mentioned above are based on historical data during the period of May to September of 2001, so an average Chemical Engineering Plant Cost Index (CEPCI) of 397 over this period is used when accounting for inflation. To update the capital cost, CEPCI of 550.8 is used in this study. The CEPCI of 550.8 for May 2010 reported in Chemical Engineering.

$$C_{BM,\ present} = \$\ 3745.73$$

4.5.4 Operating Cost

Operating cost mainly consists of raw material cost, labour cost and utilities cost for day-to-day operation of the plant. However, raw material cost and labour cost are relatively independent of DWC design, and hence only the utility cost is considered for the operating cost. Similarly, compression cost is not considered in this study as it is often negligible compared to the utility cost. There are two main types of utilities considered in this study, namely, process steam as the hot utility, and cooling water or refrigerant as the cold utility. For each application, type of the utility used can either be specified in the problem definition or determined by the temperature of the process streams to be heat exchanged. The cost of process steam is taken as $ 5.50/1000 lb and cost of cooling water is taken as $0.05/1000 gal (Seader, 2009). The computer program in C language is made to calculate the operating cost is given in Appendix A 7 & 8 and results are given below:

Results:
Process steam cost= $ 207,617/yr
Cooling water cost= $1064.34/yr
Total operating cost=$208,681/yr

4.5.5 Annualization

A fixed percentage of the total capital cost is chargeable for depreciation, maintenance and interest annually. As such, using the Annualization factor of 20 %, the annualized capital cost can be calculated and later add to the operating cost to obtain the total annual cost.

Total annual cost =$ 212,427

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

Conclusions:

Based on the present work, the following conclusions can be drawn:

1. The structural variables feed location, liquid split location, vapour split location, number of stages in postfractionator and divided wall position affects the side stream purities where distillate and bottom product purities affects are less pronounced.
2. The structural variables such as feed location, side location, number of stages in column and liquid and vapour split locations have no significant effect on reboiler duty. Only the position of divided wall plays some significant role on energy efficiency of DWC.
3. Liquid split location, vapour split location and number of stages in postfractionator greatly affects the pressure drop across the wall as compare number of stages in main column. Difference in pressure drop across the divided wall (Δp_1-Δp_2) decreases by varying liquid split location towards the bottom of column where opposite results are obtained by varying vapour split location. The difference in pressure drop across the wall increases by lowering the vapour split location towards the bottom of the column.
4. The operational variables liquid split ratio and vapour split ratio affects the side stream purity significantly as compared to distillate and bottom product purities.
5. The product purities increase by increasing reflux ratio up to 2.5. After that there is no change in product purities with increasing reflux ratio for C_4, C_5 and C_6 ternary separation.
6. The operational variables such as reflux ratio, liquid split and vapour split ratio affects have significant effect on reboiler duty as compare to structural variables.
7. The operational variables, reflux ratio and vapour split shows a great effects on pressure drop across the divided wall as compare to liquid split ratio.
8. In order to maximize potential gain on energy saving, the thermodynamic efficiency of DWC is calculated by second law of efficiency and compares with

direct sequence columns. The thermodynamic efficiency of DWC is 28.3% more than the columns in direct sequence.

9. The sizing and costing of DWC was done to calculate the capital cost, operating cost and total annual cost of the column. The total annualized cost of DWC is calculated as $ 212,427 which is 28% less than the column in direct sequence.

Recommendations:

1. Mixture with different relative volatilities will be investigated for simulation study of DWC.
2. The investigations of quaternary and higher-order systems in DWCs with more than one wall represent an interest for future research.

REFERENCES

Agrawal, R., 1996 Synthesis of Distillation Column Configurations for a Multicomponent Separation., Ind. Eng. Chem. Res., Vol. 35, pp. 1059-1071.

Abdul Mutalib, M.I. and Smith, R., 1998, Operation and Control of Dividing Wall Distillation Columns, Part 1: Degrees of Freedom and Dynamic Simulation, Trans. IChemE, Part A, Vol. 76, pp. 308-318.

Agrawal, R. and Fidkowski, Z. T., 1998a, Are Thermally Coupled Distillation Columns Always Thermodynamically More Efficient for Ternary Distillations, Ind. Eng. Chem. Res. 37, pp.3444-3454.

Agrawal, R. and Fidkowski, Z. T., 1998b, More Operable Arrangements Of Fully Thermally Coupled Distillation Columns, AICHE J. 44, pp.2565-2568.

Agrawal, R. and Fidkowski, Z.T., 1999, New Thermally Coupled Schemes for Ternary Distillation, AIChE Journal, Vol. 45, pp. 485.

Agrawal, R., 2000a, A method to Draw Fully Thermally Coupled Distillation Column Configurations for Multicomponent Distillation. Trans. Inst. Chem. Eng. 78, Part A, pp.454-464.

Agrawal, R., 2000b, Thermally coupled distillation with reduced number of intercolumn vapor transfers. AIChE J. 46(11), pp.2198–2210.

Agrawal, R., 2000c, Multieffect distillation for thermally coupled configurations. AIChE J. 46(11), pp.2211.

Agrawal R., 2003, Synthesis of multicomponent distillation column configurations, AIChE J. 49, pp.379–401.

Amminudin, K.A., Smith, R., Thong, D.Y.C. and Towler, G.P., 2001, Design and Optimization of Fully Thermally Coupled Distillation Columns. Part 1: Preliminary Design and Optimization Methodology, Trans. IChemE, Part A, Vol. 79, pp. 701- 715.

Caballero, J.A., Grossmann, I.E., 2003, Thermodynamically equivalent configurations for thermally coupled distillation, AIChE *J.*, 49 (11), pp. 2864-2884.

Caballero J. A.; Grossmann I. E., 2004, Design of distillation sequences: from conventional to fully thermally coupled distillation systems, Computers and Chemical Engineering, 28, pp.2307-2329.

Christiansen, A. C., Skogestad, S., and Lien, K., 1997, Complex distillation arrangements: Extending the petlyuk ideas*,* Comp. Chem. Eng. 21, pp.237-242.

Douglas, J.M., 1988, Conceptual Design of Chemical Processes, McGraw-Hill, New York.

DÜnnebier, G. and Pantelides, C.C., 1999, Optimal Design of Thermally Coupled Distillation Columns, Ind. Eng. Chem. Res, Vol. 38, pp. 162-176.

Ennenbach, F., Kolbe, B. and Ranke, U., 2000, Divided-Wall columns – A Novel Distillation Concept, PTQ, Autumn, pp. 97-103.

Errico M., Tola G., and Mascia M., 2009, Energy saving in a crude distillation unit by a preflash implementation, Applied Therm. Eng., Vol. 29, pp. 1642-1657.

Fidkowski, Z.T. and Krolikowski, L., 1987, Minimum Energy Requirements of Thermally Coupled Distillation Systems, AIChE Journal, Vol. 33, pp. 643-653.

Friday, J. R., Smith, B. D., 1964, An Analysis of the Equilibrium Stage Separation general systems of interlinked, multistaged separators, AIChE J. 24, pp.1131–1134.

Gomez-Castro, F. I., Segovia-Hernandez, J. G., Hernandez, S., Gutierrez-Antonio, C., and Briones-Ramirez, A., 2008 Dividing Wall Distillation Columns: Optimization and Control Properties*,* Chem. Eng. Technol. 31 (2008) 1246-1260.

Halvorsen, I. J., Skogestad, S., 2003, Minimum energy consumption in multicomponent distillation. 1. Vmin diagram for a two-product column, Ind. Eng. Chem. Res., pp.596-604.

Halvorsen, I. J., and Skogestad, S., 2003, Minimum energy consumption in multicomponent distillation. 2. Three-product Petlyuk arrangements*,* Ind. Eng. Chem. Res. 42, pp.605-615.

Hernández, S., Pereira-Pech, S., Jiménez, A., and Rico-Ramírez, V., 2003, Energy

Efficiency of an Indirect Thermally Coupled Distillation Sequence, The Can. J.Chem. Eng. 81, pp.1087.

Hernandez-Gaona, C. G., Cardenas, J. C., Segovia-Hernandez, J. G., Hernandez, S., and Rico-Ramirez, V., 2005, Second Law Analysis of Conventional and Nonconventional Distillation Sequences, Chem. Biochem. Eng. Q. 19, pp.235-241.

Hess, F. E., Holland, C. D., 1977 Solve more distillation problems, Hydrocarbon Process, pp. 241–249.

Hewitt, G., Quarini, J. and Morrell, M., 1999, More Efficient Distillation, The Chemical Engineer, pp. 16-19, 21 Oct.

Hofeling, Seader, J. D., 1978, A modified Naphtali-Sandholm method for general System interlinked, multistaged separators, AIChE J. 24, pp.1131–1134.

Holland, C.D., 1981, Fundamentals of Multi-component Distillation, McGraw- Hill, New York.

Juan G. S. H.; Vargas E. A. H.; Munoz J. A. M, 2007, Control properties of thermally coupled distillation sequences for different operating conditions, Computers and Chemical Engineering, 31, pp.867-874.

Kaibel, G., 1987, Distillation Columns with Vertical Partitions. Chem. Eng. Tech., Vol. 10 (2), pp. 92-98.

Kaibel, B., Jansen, H., Zich, E., and Olujic, Z., 2006, Unfixed dividing wall technology for packed and tray distillation columns, IChemE, symposium series no. 152

Kim Y.H., 2001a, Rigorous design of fully thermally coupled distillation column, J. Chem. Eng. Japan 34, pp.236–243.

Kim, Y. H., 2001b, Structural design of extended fully thermally coupled distillation columns. Industrial and Engineering Chemistry Research, 40, pp.2460–2466.

Kim Y. H, 2002, Structural design and operation of a fully thermally coupled distillation column, Chem. Eng., J. 85, pp. 289-301.

Kim, Y. H., 2002, Rigorous design of extended fully thermally coupled distillation columns, Chem. Eng. J. 89, pp.89-99.

Kolbe, B. and Wenzel S., 2004, Novel distillation concepts using one-shell columns, Chemical Engineering and Processing, Vol. 43, pp. 339-346.

Kim, Y. H., 2005 Structural design of fully thermally coupled distillation columns using a semirigorous model, Comp. Chem. Eng. 29, pp.1555-1559.

Kim Y. H., 2006a, A New thermally coupled distillation column with postfractionator, Chemical Engineering and Processing, 45, pp.254-263.

Kim, Y.H., 2006b, Operability improvement in a fully thermally coupled distillation system with separated main columns Journal of Chemical Engineering of Japan, 39 (3), pp.284-291.

N. Asprion, G. Kaibel, Dividing wall columns: Fundamentals and recent advances, Chem. Eng. Process.: Process Intensification, 49 (2010) 139-146.

Lockett, M. J., 1986 Distillation Tray Fundamentals, Cambridge University Press Linearization, AIChE J. 17, pp.148–153.

Mueller, I., Pech, C., Bhatia, D., Kenig, E. Y., 2007, Rate-based analysis of reactive distillation sequences with different degrees of integration, Chem. Eng. Sci., 62, pp.7327-7335.

Muralikrishna, K., Madhavan, V. K. P. and Shah, S. S., 2002 Development of Dividing Wall Distillation Column Design Space for a Specified Separation, Chem. Eng. Res. Des. 80, pp. 155-166.

Mutalib, M. I. A., Smith, R., 1998 Operation and Control of Dividing Wall Distillation Columns: Part 1: Degrees of Freedom and Dynamic Simulation, Chem. Eng. Res. Des. 76, pp.308-318.

Naphtali, L. M., Sandholm, D. P., 1971 Multicomponent Separation Calculations by Linearization, AIChE J. 17, pp.148–153.

Olujic, Z., Sun, L., Rijke, A., and Jansens, P. J., 2006, Conceptual design of an internally heat integrated propylene-propane splitter, Energy 31, pp.3083-3096.

Olujic, Z., Jödecke, M., Shilkin, A., Schuch, G., and Kaibel, B., 2009 Equipment improvement trends in distillation, Chem. Eng. Process. 48, pp.1089-1104.

Parkinson, G., 2005, Distillation: New Wrinkles for an Age-Old Technology, Chemical

Engineering Progress, July, pp. 10-12.

Parkinson, G., 2007, Dividing-Wall Columns Find Greater Appeal, Chemical Engineering Progress, May, pp. 8-11.

Premkumar, R. and Rangaiah, G.P., 2009, Retrofitting Conventional Columns Systems to Dividing-Wall Columns, Chemical Engineering Research and Design, Vol. 87, pp. 47-60.

Petlyuk, F. B., Platonov V. M., Slavinskii, D. M., 1965, Thermodynamically optimal method for separating multicomponent mixtures*,* International Chem. Eng. 5, pp.555-561.

Rangaiah, G.P., Chan T.S.J. and Hidajat, K., 2006, Optimization of Complex Distillation Columns, Chemical Engineering, September, pp. 60-64.

Rangaiah, G. P., Ooi, E. L., Premkumar, R., 2009, Procedure for quick design of dividing wall columns, Chem. Product and Process Modeling, 4(1) Article 7.

Robles-Zapiain, S., Segovia-Hernández, J. G., Bonilla-Petriciolet, A., Maya-Yescas, R., 2008, Energy-efficient complex distillation sequences: Control properties, Can. J. Chem. Eng., 86, 46 , pp.249-259.

Rong, B. G., Turunen, I., 2006, A new method for synthesis of thermodynamically equivalent structures for Petlyuk arrangements, Chem. Eng. Res. Des., 84, pp.1095-1116.

Seader, J. D., 1989 The Rate-Based Approach for Modelling Staged Separations, Chem Eng. Prog., 85(10), pp. 41.

Seader, J. D., Henley, E. J., 2009, Separation process principles.

Schultz, M.A., Stewart, D.G., Harris, J.M., Rosenblum, S.P., Shakur, M.S. and O'Brien, D.E., 2002, Reduce Costs with Dividing Wall Columns, Chemical Engineering Progress, May, pp. 64-71.

Segovia-Hernández, J.G., Hernández, S., Jiménez, A., 2005, Analysis of dynamic properties of alternative sequences to the Petlyuk column, Comput. Chem. Eng., 29, pp.1389-1399.

Serra, M., Espuna, A., and Puigjaner, L., 1999 Control and optimization of the divided wall column, Chem. Eng. Process. 38, pp.549-562.

Serra, M., Espuna, A., and Puigjaner, 2001, Analysis of different control possibilities for the divided wall column: feedback diagonal and dynamic matrix control, Comp. Chem. Eng. 25, pp.859-866.

Serra, M., Espuna, A., and Puigjaner, 2002, Study of the divided wall column controllability: influence of design and operation, Comp. Chem. Eng. 24, pp.901-907.

Serra, M., Espuna, A., and Puigjaner, L., 2003 Controllability of different multicomponent distillation arrangements, Ind. Eng. Chem. Res. 42, pp. 1773-1782.

Shah, P.B., 2002, Squeeze More out of Complex Columns, Chemical Engineering, Progress, July, pp. 46-55.

Sotudeh, N., Shahraki, B. H., 2007 A method for the design of divided wall columns, Chem Eng. Technol. 30(9), pp.1284-1291.

Tamayo-Galvan, V.E., Segovia-Hernandez, J.G., Hernandez, S., Cabrera-Ruiz, Alcantara-Avila, J. R., 2008, Controllability analysis of alternate schemes to complex column arrangements with thermal coupling for the separation of ternary mixtures, Comput. Chem. Eng., 32, pp.3057-3066.

Tomich, J. F., 1970, A New Simulation Method for Equilibrium Stage Processes, AIChE J. 16 , pp.229–232.

Treybal, R. E., 1980, Mass-Transfer Operations, Third Edition, McGraw-Hill, New York.

Triantafyllou, C. and Smith, R., 1992, The design and optimization of fully thermally coupled distillation columns, Trans. IChemE, Part A, Vol. 70, pp.118.

Turton, R., Bailie, R. C., Whiting W. B., Shaeiwitz J. A., 2003, Analysis, Synthesis and Design of Chemical Processes, Second Edition, Prentice Hall PTR., Upper Saddle

River, N.J.

Ulrich, G. D., 1984, A Guide to Chemical Engineering Process Design and Economics, Wiley, New York.

Wang San-Jang, Wong David S. H., 2007, Controllability and energy efficiency of a high-purity divided wall column, Chemical Engineering Science 62, pp.1010 – 1025.

Wang San-Jang, Lee Chi-Ju, Jang Shi-Shang, Shieh, 2007, Plant wide design and control of acetic acid dehydration system via heterogeneous azeotropic distillation and divided wall distillation, J. of Process Control, 18, pp.45-60.

APPENDIX A

Computer Programs in C language

1. Height of column:

```
#include<stdio.h>
  #include<conio.h>
  void main()
  {
  clrscr();
  float k=0.07,pl1,pl2,pv1,pv2,Vmax1,Vmax2,Vact1,Vact2,d1,d2,G1,G2,D,R,V,
  NA1,NA2,DA1,DA2,s=0.5,H,Nact;

  Vmax1=k*((pl1-pv1)/pv1)^0.5;// maximum velocity for section 1//
  Vmax2=k*((pl2-pv2)/pv2)^0.5;//maximum velocity for section 2//
  Vact1=0.8*Vmax1;//actual velocity for section 1//
  Vact2=0.8*Vmax2;//actual velocity for section 2//
  V=D*(1+R);//vapor rate//
  G1=(V*F1)/(pv1*3600);//maximum flow rate for section 1//
  G2=(V*F2)/(pv2*3600);//maximum flow rate for section 2//
  NA1=G1/Vact1;//net area for section 1//
  NA2=G2/Vact2;//net area for section 2//
  DA1=NA1/0.88;//downcomer area of main column//
  DA2=NA2/0.88;//downcomer area of postfractionator//
  d1=((DA1*4)/3.14)^0.5;//diameter of main column//
  d2=((DA2*4)/3.14)^0.5 ;//diameter of postfractionator//
  printf("%f%f",d1,d2);
  H=((Nact*s)/0.70)+3;//height of column//
  printf("%f",H);
  getch();
  }
```

2. Condenser sizing:

```
#include<stdio.h>
#include<conio.h>
#include<math.h>
int main()
{
float
Q,q=391.387,hv=127600,hL=149720,m,Thi=352.826,Tho=282.801,Tci=298,Tco=238.67,cpw=75.2,FT=0.92,Ui=900,Nt=992,Pt=25,Db=954,Nr=38,SS=317.813,TS=268.335,TA,Tw,Tm,delT,pv,LMTD,th,l,hc,Nr1,k=0.136,pl=601.4,u=0.000682,At,Vt,pw,hi,kw=50,hod=6000,hid=6000,Uo,d0=20,di=16.8,A;
Q=(q/3600)*(hv-hL);//volumetric flow rate//
m=Q/((Thi-Tho)*cpw);//mass flow rate//
LMTD=((Tho-Tci)-(Thi-Tco))/ln((Tho-Tci)/(Thi-Tco));//logarithmic mean temperature difference//
delT=FT*LMTD;//temperature difference, FT= correction factor//
TA=(Q*1000)/(Ui*delT);//TRIAL AREA//

//shell side coefficient//
SS=(Tci+Tco)/2;//Shell side mean temperature//
TS=(Thi+Tho)/2;//tube side mean temperature//
Tw=-((((SS-TS)*Ui)/1500)-SS);//tube wall temperature//
Tm=(SS+Tw)/2;//mean temperature condensate//
pv=(58/22.4)*(273/(273+SS))*21.08;//density of vapor//
th=(q/3600)*(1/(l*Nt));//tube loading//
Nr1=(2/3)*Nr;//average number of tubes in vertical tube row//
hc=0.95*k*pow((pl*(pl-pv)*9.81)/(u*th),0.99);//shell side coefficient//
//tube side coefficient//
At=0.055;//tube cross sectional area//
Vt=m/(pw*At);//tube velocity//
hi=4200*(1.35+0.02*TS)*pow(Vt,0.8)/(16.8*16.8);//tube side coefficient//
Uo=1/((1/hc)+(1/hod)+((d0*ln(d0/di))/(2*kw))+((d0/di)*(1/hid))+((d0/di)*(1/hi)));//overall heat transfer coefficient//
```

```
A=Q/(Uo*delT);//area of condenser//
printf("%f",A);
getch();
}
```

3. Reboiler sizing:

```
#include<stdio.h>
#include<conio.h>
#include<math.h>
void main()
{
float
SH,Tb=69,Tf=37.79,cp=2.18,HL,LH=365,Q,Ui=1,delT,Ts=115.2,L=4.8,Nt,A1,OD=0.03
,SP,
q,hnb,pc=30.2,p=1.45,Uo,od=0.03,id=0.025,kw=55,A,a,b,c,d,e,f,l,n;
clrscr();
SH=(Tb-Tf)*cp;//sensible heat//
HL=(SH+LH);//total heat load//
Q=1.05*HL;//maximum heat load//
delT=Ts-Tb;
A1=(Q)/(1*Tb);//area required//
Nt=A1/(OD*3.14*L);//number of U tubes//
SP=1.5*OD;//square pitch arrangement//
q=Q*1000/A1;//heat flux//
a=p/pc;
b=pow(a,0.17);
c=pow(a,1.2);
d=pow(a,10.0);
e=pow(pc,0.69);
f= pow(q,0.7);
hnb=(0.104*e*f*(1.8*b+4*c+10*d));//heat transfer coefficient//
l=(1/hnb);
n =(od*0.182)/(2*kw);
```

```
Uo=1/(l+0.0001+n+1.2*(0.0002+0.000125));//overall heat transfer coefficient//
A=(Q*1000)/(Uo*delT);//area of reboiler//
printf("a=%f",a);
printf("b=%f",b);
printf("c=%f",c);
printf("d=%f",d);
printf("e=%f",e);
printf("Q=%f",Q);
printf("Uo=%f",Uo);
printf("hnb=%f",hnb);
printf("q=%f",q);
printf("area1=%f",A1);
printf("area=%f",A);
getch();
}
```

4.costing of column and trays

```
#include<stdio.h>
#include<conio.h>
void main()
{
float
Cp1,k1=3.4974,k2=0.4485,k3=0.1074,H,Fp,Cbm1,B1=2.25,B2=1.82,Fm,Cp2,K1=2.9949,K2=0.4465,K3=0.3961, d,Cbm2,Nact,Fm,Fq;
clrscr();
logCp1=k1+k2*logH+k3*(log H)^2;//purchase cost of column, H=height of column//
Cbm1=Cp1(B1+B2*Fm*Fp);//bare module cost of column, Fm= material factor, Fp= pressure factor//
log Cp2=K1+K2*log((3.14*d^2)/4)+K3*((log*3.14*d^2)/4)^2;//purchase cost of trays//
Cbm2=Cp2*Nact*Fm*Fq;//bare module cost of trays, Nact= actual number of trays, Fm= material factor//
printf("%f%f",Cbm1,Cbm2);
```

```
getch();
}
```

5. costing of reboiler and condenser

```
#include<stdio.h>
#include<conio.h>
void main()
{
floatCp1,k1=4.8306,k2=0.8509,k3=0.3187,Fp,Cbm1,B1=1.63,B2=1.66,Fm,C1=0.03881,
C2=-0.11272,C3=0.08183;
clrscr();
logCp1=k1+k2*logA+k3*(log A)^2;//purchase cost of reboiler and condenser//
logFp=C1+C2*log P+C3(log P)^2;//pressure factor//
Cbm1=Cp1(B1+B2*Fm*Fp);//bare cost module for reboiler and condenser//
printf("%f%f",Cbm1);
getch();
}
```

6. Operating cost of process steam

```
#include<stdio.h>
#include<conio.h>
void main()
{
Float  Qb=413.819, Sr, S, Cp=5.50, Asc;
Sr=Qb/365;//steam requirement, Qb= reboiler duty//
S=Sr*24*365*0.9;//steam requirement per year//
Asc=S*Cp/1000;//annual steam cost, Cp= purchase cost of steam//
Printf("%f", Asc);
getch();
}
```

7. Operating cost of cooling water

```
#include<stdio.h>
```

```
#include<conio.h>
void main()
{
float Tin=41, Tout=147.63, Qc= 1335412.4, cpw=1,den=8.33, TGPY,Cp=0.05, TAC,M;
M=Qc/(cpw*(Tout-Tin));//Mass flow rate, cpw=heat capacity of water, Tout=outlet
temperature, Tin=inlet temperature of water//
TGPY=M*60*24;//Total gallons per year//
TAC=(Cp*TGPY)/1000;//total annual cost, Cp= purchase cost of water//
Printf(“%f”, TAC);
getch();
}
```

8. Thermodynamic efficiency

```
#include<stdio.h>
#include<conio.h>
int main()
{
floatn1=18.1305,n2=26.8695,n4=45,s1=-452.76,s2=-587.72,s4=-531.30,q1=-
1408942.8,q2=1466593.2,T1=282.801,T2=339.523,T0=298,b1,b2,b4,h1=-149720,h2=-
182270,h4=-170990,
N,Wmin,LW,delS;
 clrscr();
//printf("enter the value of n1,n2,n3,n4,s1,s2,s3,s4,q1,q2,T1,T2,T0,h1,h2,h3,h4");
//scanf("%f",&n1,"%f",&n2,"%f",&n3,"%f",&n4,"%f",&s1,"%f",&s2,"%f",&s3,"%f",&
s4,"%f",&q1,"%f",&q2,
//"%f",&T1,"%f",&T2,"%f",&T0,
//"%f",&h1,"%f",&h2,"%f",&h3,"%f",&h4);
delS=(n1*s1+(q1/T1))+(n2*s2+(q1/T1))-(n4*s4+(q2/T2));//production of entropy by
process,n1 and n2 are mass output, n3 is
the mass input, s1 &s2 are the entropy ouput, s4 is the entropy input//
b1=h1-T0*s1;//stream availability for output component//
b2=h2-T0*s2;//stream availability for output component//
b4=h4-T0*s4;//stream availability for input component//
```

```
LW=(n4*b4+q2*(1-(T0/T2)))-(n1*b1+q1*(1-(T0/T1)))-(n2*b2+q1*(1-(T0/T1)));//loss
of work//
Wmin=n1*b1+n2*b2-n4*b4;//minimum work done//
N=Wmin/(LW+Wmin);//energy efficiency//
//printf("the value of delS,b1,b2,b3,b4,LW,Wmin,N= %f %f %f %f %f %f
%f",delS,b1,b2,b3,b4,LW,Wmin,N);
printf("%f",N);
getch();
}
```