GRAPH BASED CAD MODULE FOR BINARY

DISTILLATION COLUMN

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CERTIFICATION

This Thesis titled GRAPH BASED CAD MODULE FOR BINARY DISTILLATION COLUMN meets the regulation governing the award of the degree of M.ENG of the Federal University of Technology, Minna and is approved for its contribution to scientific knowledge and literary presentation.

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This work is dedicated to IMAM ABU HAMID AL-GHAZALI

DECLARATION

I, BUHARI, MUHAMMAD BABA, declare that this project is a result of my personal research work and has not been presented elsewhere for the award of any certificate.

Information derived from published and unpublished works have been dully acknowledged.

DENT SIGNATURE

5-06-2008 DATE

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ABSTRACT

Graph based technique of computer aided design is a new approach of parametric studies of design of process equipments in order to find the most suiatble condition for the equipment design. Graph based technique of computer aided design of binary distillation column has been carried out. The effect of feed condition (temperature, pressure and molar flow rate) on the actual number of stages, optimal feed stage, condenser duty and reboiler duty was investigated. The effect of feed condition (temperature, pressure and molar flow rate) on the actual number of stages, optimal feed stage, condenser duty and reboiler duty were investigated. The effect of external reflux ratio on the actual number of stages, optimal feed stage, condenser duty and reboiler duty was also investigated. The most suitable feed condition obtained for the design of the binary distillation column are feed temperature of 30 oC, feed pressure of 101.3 kPa and molar flow rate of 100 kmol/hr. The external reflux ratio of 4 was obtained as the best value that gave minimum number of stages and reboiler duty.

The equipment design shows that a sieve tray of 1m section diameter was obtained. The column has a sectional height of 4.3m and cross-sectional area of 0.79 m². The design also shows that there is no flooding in the distillation column. The cost estimation was carried out using Hysys spreadsheet. The cost index used is the chemical engineering cost index of 2006. The cost estimation of the column shows that the total bare module cost of the tower, trays, condenser, reboiler and reflux accumulator at 2006 Chemical Engineering index is two hundred and seventy eight million nine hundred and eighty thousand naira (\aleph 278,980,000). the total utility cost (condenser, cooling water, and

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CHAPTER ONE

1.0 INTRODUCTION

Distillation is a process of heating a liquid until its more volatile constituents pass into the vapour phase, and then cooling the vapour to recover such constituents in liquid form by condensation. The main purpose of distillation is to separate a mixture of several components by taking advantage of their different volatilities, or the separation of volatile materials from non-volatile materials. In evaporation and in drying, the purpose usually is to obtain the less volatile constituent; the more volatile constituent, in most cases water, is discarded. In distillation, on the other hand, the principal object of the operation is to obtain the more volatile constituent in pure form.

There are two types of distillation namely binary and multicomponent distillation. Binary distillation is an art of separating mixture of two components by exploring their difference of boiling points using vapourization. Multicomponent distillation is the separation of mixture of more than two components by vapourization (Onifade, 2000).

If the difference in volatility (and hence in boiling point) between the two constituents is great, complete separation may be easily accomplished by a single distillation. Seawater, for example, which contains about 4 percent dissolved solids (principally common salt), may be readily purified by vaporizing the water, condensing the steam thus formed, and collecting the product, distilled water. This product is, for most purposes, equivalent to pure water, although actually it contains some impurities in the form of dissolved gases, the most important of which is carbon dioxide (Onifade, 2000).

If the boiling points of the constituents of a mixture differ only slightly, complete separation cannot be achieved in a single distillation. An important example is the separation of water, which boils at 100° C (212° F), and alcohol, which boils at 78.5° C (173° F). If a mixture of these two liquids is boiled, the vapour that rises is richer in alcohol and poorer in

water than the liquid from which it came, but it is not pure alcohol. In order to concentrate a 10 percent solution of alcohol (such as might be obtained by fermentation) to obtain a 50 percent solution (common for whiskey), the distillate must be redistilled once or twice, and if industrial (95 percent) alcohol is desired, many re-distillations are needed (Lang, 2001).

The design of distillation column usually involves the derivation of long formulae and solution of complex system of equations. This is done manually using graphs and tables. In the past, distillation operation was limited to the separation and purification of simple binary systems (usually in batch). However, the discovery of oil and the rapid expansion of its (oil) industry world wide brought about the need for a more quantitative and qualitative approach to the solution of the various complex design equation that arise from such processes.

In view of the versatility and importance of the distillation column, this research work intends, among other things to undertake a computer aided design module for a binary distillation column.

CAD more widely known as Computer aided design is the use of computer tools to solve complex engineering problems. Computer Aided Design of binary distillation aids the chemical engineer in solving binary distillation problems at lesser time and better efficiency of results when compared to the manual approach of solving binary distillation problems. It is more concerned with the performance of process unit (such as the classical unit operations of chemical Engineering) and the integration of these units into complete, consistent, efficient processes to produce chemical products.

Hysys is a powerful and comprehensive process simulation computational engine, which performs complete heat and material balance calculations for a wide variety of pipeline and processing applications. The simulator's easy-to-create flowsheets allow process engineers to concentrate on engineering, rather than computer operations. Design II aids the chemical engineer in solving binary distillation problems at lesser time and better efficiency of results when compared to the manual approach of solving binary distillation problems. It is more concerned with the performance of process unit (such as the classical unit operations of chemical Engineering) and the integration of these units into complete, consistent, efficient processes to produce chemical products.

1.1 Aim and Objective

The ultimate aim of this work is to develop a Computer Aided Design Module (CAD) that will replace the manual procedures involved in designing a binary distillation column.

1.2 Scope of the Project

The scopes of the project are the following:

- 1. The effect of variation of the feed temperature on the column performance (actual number of trays, optimal feed tray, condenser duty, reboiler duty and product purity.
- The effect of variation of the feed pressure on the column performance (actual number of trays, optimal feed tray, condenser duty, reboiler duty and product purity.
- The effect of variation of the feed molar flow rate on the column performance (actual number of trays, optimal feed tray, condenser duty, reboiler duty and product purity.
- The effect of variation of the column external reflux ratio on the column performance (actual number of trays, optimal feed tray, condenser duty, reboiler duty and product purity.

1.3 Justification of the Project

There are two set back associated to the use of manual approach to solving distillation design problems, they are accuracy and time. Accuracy depends on the state of mind of the

1.3 Justification of the Project

There are two set back associated to the use of manual approach to solving distillation design problems, they are accuracy and time. Accuracy depends on the state of mind of the problem solver which may give error induced results as a result of unfocussed state of mind. Time spent on manual approach of solving problems will be more due to complexity of the distillation problem to be solved. Employing Computer Aided Design in solving distillation problem will eliminate these two setbacks.

CHAPTER TWO

2.0 LITERATURE REVIEW

2.1.0 Distillation and Separation

Variables and definitions used in distillation are best considered in relation to the steady condition of continuous distillation. An acceptable definition of distillation is the separation of a volatile liquid from a non-volatile substance or, more frequently, the separation of two or more liquids of different volatility. Separation here refers to a division into parts, each of different composition as the result of relative differences in volatility of the components of the mixture being separated.

The term volatility is the measure of the liquids vapour pressure at a given temperature or its escaping tendency, which increases as the temperature increases. The lower the temperature at which a liquid boils or the higher its vapour pressure at a given temperature, the more the volatile component will tend to vaporize than the less volatile component (Tatabu, 2001). A typical distillation column is shown below.



Figure 2.1: Schematic diagram of a distillation column

2.1.1 Relative Volatility

If the ratio of the partial pressure to the mole fraction in the liquid is defined as the volatility thus:

Volatility of A =
$$\frac{P_A^O}{x_A}$$
 and Volatility of B = $\frac{P_B^O}{x_B}$ 2.1

The ratio of these two volatility is known as the relative volatility given by

$$\alpha_{AB} = \frac{\frac{P''_{A}}{x_{A}}}{\frac{P''_{B}}{x_{B}}}$$
2.2

From Dalton's law of partial pressure

 $Py_A = P^a{}_A$ 2.3

and

$$Py_{B} = P^{o}{}_{B}$$

$$\alpha_{AB} = \frac{y_A x_B}{y_B x_A}$$
 2.5

or

$$\frac{y_A}{y_B} = \alpha_{AB} \left(\frac{x_A}{x_B} \right)$$
 2.6

Equation 2.6 gives a valuable relation between the ratio of A and B in the vapour and that in the liquid.

Since with a binary mixture

$$y_B = 1 - y_A \tag{2.7}$$

and

$$x_{B} = 1 - x_{A}$$
 2.8

$$\alpha_{AB} = \left(\frac{y_A}{1 - y_A}\right) \left(\frac{1 - x_A}{x_A}\right)$$
 2.9

or

$$y_{A} = \frac{\alpha_{AB} X_{A}}{(1 + (\alpha_{AB} - 1))}$$
 2.10

and

$$x_{A} = \frac{y_{A}}{(1 - (\alpha_{AB} - 1)y_{A})}$$
 2.11

Equation (2.11) enables the composition of the vapour to be calculated for any desired value of X, if α_{AB} is known. For separation to be achieved α_{AB} must not be equal to 1 considering the more volatile component, as α_{AB} increases above unity, Y increases and the separation becomes much easier.

Equation (2.6) is useful in calculation of plate enrichment and finds wide application in multi-component distillation. From the definition of the volatility of a component it could be seen that for an ideal system, the relative volatility is numerically equal to the vapour pressure of the pure component (McCabe, 2002).

2.1.3 Ideal System

This is a special case of normal miscible system where it is assumed that the components have no effect on each other. Each component acts independently and presents a tendency of volatilization only as function of its concentration in the liquid phase and its vapour pressure at the temperature of the system. This is mathematically expressed by Roult's law as

 $P_A = P^a{}_A x_A \tag{2.12}$

Dividing both sides by the total pressure of the system we obtain

$$\frac{P_A}{P} = P_A^o \begin{pmatrix} x_A \\ P \end{pmatrix}$$
 2.13

And applying Dalton's law of partial pressures

 $P_A = y_A P \tag{2.14}$

By substituting (2.14) and (2.13) we have this

$$y_{A} = P_{A}^{o} \left(\frac{x_{A}}{P}\right)$$

$$y_{A} = P_{B}^{o} \left(\frac{x_{B}}{P}\right)$$
2.15
2.16

From 2.6

$$\alpha_{AB} = \begin{pmatrix} y_A \\ x_A \end{pmatrix} \begin{pmatrix} y_B \\ x_B \end{pmatrix}$$

Using 2.15 and 2.16 gives





2.17



Figure 2.2: x-y Diagram for binary mixture

Thus, the relative volatility of an ideal system at any composition is equal to the ratio of the vapour pressure of the two components at the boiling point of the mixture (McCabe, 2002).

Based on this, there are four basic types of vapour-liquid equilibrium of binary distillation system.

- i. Normal complete miscible
- ii. Azeotropic complete miscible
- iii. Partially miscible and
- iv. Completely immiscible.

2.1.4 Methods of Solving Binary Distillation Problems

The methods of solving binary distillation problems include the following:

- 1. McCabe Thiele Method
- 2. Lewis Sorrel's Method
- 3. Thiele Geddes Method
- 4. Smoker Equation

2.1.4.1 McCabe Thiele Method

The McCabe-Thiele approach is a graphical one, and uses the VLE plot to determine the theoretical number of stages required to effect the separation of a binary mixture. It measures constant molar overflow and this implies that:

- molar heat of vaporization of the components are roughly the same
- heat effects (heat of solution, heat losses to and from column, etc) are negligible
- for every mole of vapour condensed, 1 mole of liquid is vaporized.
- The design procedure is simple. Given the VLE diagram of the binary mixture, operating lines are drawn first.

Operating lines defines the mass balance relationship between the liquid and vapour phases in the column

There is one operating line for the bottom (stripping) section of the column, and one for the top (rectification or enriching) section of the columnuse of the constant molar overflow assumption also ensures that the operating lines are straight lines (Perry, 1997).

2.1.4.2 Operating Line for Rectification Section

The operating line for the rectification section is constructed as follows. First the desired top product composition is located on the VLE diagram, and a vertical line produced until it intersects the diagonal line that splits the VLE plot in half. A line with slope R/(R+1) is then drawn from this intersection point. R is the ratio of reflux flow (L) to distillate flow (D) and is called the reflux ratio and is a measure of how much of the material going up the top of the column is returned back to the column as reflux (Tatabu, 2001).

2.1.4.3 Operating Line for the Stripping Section

The operating line for the stripping section is constructed in a similar manner. However, the starting point is the desired bottom product composition. A vertical line is drawn from this point to the diagonal line and a line of slope L_s/V_s is drawn. L_s is the liquid rate down the stripping section of the column while V_s is vapour rate up the stripping section of the column. Thus the slope of the operating line for the stripping section is a ratio between the liquid and the vapour flows in that part of the column (Tatabu, 2001).

2.1.4.4 Equilibrium and Operating Lines

The McCabe-Thiele method assumes that the liquid on a tray and the vapour above it are in equilibrium. A magnified section of the operating line for stripping section is shown in relation to the corresponding n'th stage in the column. L's are the liquid flows while V's are the vapour flows. x and y denote liquid and vapour compositions and subscripts denote the seven theoretical stages are required to achieve the desired separation. The required number of trays (as opposed to stages) is one less than the number of stages since the graphical construction includes the contribution of the reboiler in carrying out the separation. The actual number of trays is given by the formula:

(Number of theoretical trays)/ (tray efficiency)

A typical value for tray efficiency ranges from 0.5 to 0.7 and depends on a number of factors such as the type of tray being used, and internal liquid and vapour flow conditions. Sometimes additional trays are added (up to 10%) to accommodate the possibility that the column may be under-designed (McCabe, 2002).

1.0 0.90 0.80 0.77 Mole fraction alcohol in vapour 0.70 Slope = $L_o/V_o = 0.67$ 0.60 0.50 0.50 X = 0.47 Slope 0.40 0.30 0.20 Slope = $L_m/V_m = 2.92$ 0.16 0.10 0.02 Xw 0 0.10 0.20 0.30 0.40 0.50 0.60 0.70 0.80 0.90 1.0 Mole fraction alcohol in liquid

2.1.4.6 The Feed Line (Q-Line)



Figure 2.4 shows that the binary feed should be introduced at the 4th stage. However, if the fed composition is such that it does not coincide with the intersection of the operating lines, this means that the feed is not a saturated liquid. The condition of the feed can be

Depending on the state of the feed, the feed lines will have different slopes. For example:

q=0 (saturated vapour)

q⁻¹ (saturated liquid)

0<q<1 (mix of liquid and vapour)

q>1 (subcooled liquid)

q<0 (superheated vapour)

The q-lines for the various feed conditions are shown in the diagram on the left (McCabe, 2002)

2.1.4.7 Using Operating Lines and the Feed Line in McCabe-Thiele Design

If we have information about the condition of the feed mixture, then we can construct the q-line and use it in the McCabe-Thiele design. However, excluding the equilibrium line, only two other pairs of lines can be used in the McCabe-Thiele procedure. These are:

- feed line and rectification section operating line
- feed line and stripping section operating line
- stripping and rectification operating lines

This is because these pairs of lines determine the third (McCabe, 2002).

2.1.4.8 Reflux Considerations

The reflux ratio R, is normally defined as:

R = Flow returned as reflux/flow of top product taken off.

The number of stages required for a given separation will be dependent on the reflux ratio use. In an operating column the effective reflux ratio use can be increased by vapour condensed within the column due to heat leakage through the walls. With a wide lagged column the heat loss will be small and no allowances are normally given

for this increase in flow in the design calculation. If a column is poorly insulated, changes in the internal reflux due to sudden changes in the external conditions, such as sudden rainstorms, can have a noticeable effect on the column operation and control (Sinnot, 2000).



Figure 2.5: The plot of vapour-Liquid equilibrium diagram

2.1.4.9 Total Reflux

Total reflux is the condition when all the condensate is returned to the column at reflux: no product is taken off and there is no feed. At total reflux the number of stages required for a given separation is the minimum at which it is theoretically possible to achieve the separation. Throughout a practical operating condition, it is a useful guide to the likely number of stages that will be needed. Column are often started up with no product taken out and operated at total reflux till steady state conditions are attained. The testing of columns is also conveniently carried out at total reflux (Sinnot, 2000).

2.1.4.10 Minimum Reflux

As the ratio is reduced a pinch point will occur at which the separation can only be achieved with an infinite number of stages. This sets the minimum possible reflux ratio for the specified separation (McCabe, 2002).

2.1.4.11 Optimum Reflux Ratio

Practical reflux ratios will lie some where between the minimum for the specified separation and total reflux. The designer must select a value at which the specified separation is achieved at minimum cost, increasing the reflux reduces the number of stages required, and hence the capital cost, but increases the service requirements (steam and water) and the operating cost. No hard and fast rules can be given for the selection of the design reflux ratio, but for many systems the optimum will lie between 1.2 to 1.5 times the minimum reflux ratio (McCabe, 2002).

2.1.4.12 Feed-Point Location

The precise location of the feed point will affect the number of stages required for a specified separation and the subsequent operation of the columns. As a general rule, the feed should enter the column at the point that gives the best match between the feed composition (vapour and liquid if two phases) and the vapour and liquid streams in the column.

10





In practice, it is wise to provide two or three feed-point nozzles located round the predicted feed-point to allow for uncertainties in the design calculation and data, and possible changes in the feed composition after start-up (McCabe, 2002).

2.2 Selection Of Column Pressure

Except when distilling heat-sensitive materials, the main consideration when selecting the column pressure will be to ensure that the dew point of the distillate is above that which can be easily obtained with the plant cooling water. The minimum sensitive materials and why very high temperatures would otherwise be needed to distill relatively non-volatile materials.

When calculating the stage and reflux requirement it is usual to take the operating pressures as constant throughout the column. In vacuum column the column pressure drop will be a significance fraction of the total pressure and the change pressure up the column should be allowed for calculating the stage temperatures. This requires a trial and error calculation, as clearly the pressure drop cannot be estimate of the number of which is made (Sinnot, 2000).

2.3 Dew Point And Bubble Points

To estimate the stage, the condenser and temperatures, procedures are required calculating the dew and bubble points. By definition a saturated liquid is at its bubble point increase in temperature will cause a bubble of vapour and a saturated vapour is at its dew point (any drop in temperature will cause a drop of liquid to form). Dew point and bubble point can be calculated from knowledge of the vapour-liquid equilibrium for the system. In terms of equilibrium constants, the bubble point is defined by the equation

Bubble point :
$$\Sigma Y_i = K_i x_i$$
 2.22
And Dew point : $\Sigma x_i = \frac{\Sigma Y_i}{K_i}$ 2.23

For multi-component mixtures the temperature that satisfies this equation at a given system pressure, must be found by trial and error. For binary systems the equation can be solved more readily because the component compositions are not independent. Fixing one fixes the other (McCabe, 2002).

$$y_A = 1 - y_A \tag{2.24}$$

$$x_B = 1 - x_B \tag{2.25}$$

2.4 Application of Distillation

Continuous distillation may be used when the components involved have adequate volatility differences and these differences extend over the entire concentration range of the intended separation. Under this requirement, no condition must ever exist where vapour and liquid phases in contact have identical composition, or separation will stop at this point. This condition occurs where azeotropic or a constant boiling mixture can form as well as when a pure-product condition is approached. An example is found in the distillation of the ethyl alcohol and water system, where the maximum purity of the alcoholic product is limited to the concentration of the azeotrope. Another limitation can exist if the distillation is set too close to the critical state condition with no separation possible at the critical state. Some distillations have been carried out as close as 25^oF from the critical temperature (Sinnot, 2000).

2.4.1 Single-Stage or Flash Separation

A flash separation takes place when a mixture under partially vaporize condition has composition differences between the vapour and liquid phases. Under complete mixing conditions and over a sufficient duration of time, a state of equilibrium is attained. The phase composition at equilibrium is defined at the pressure and temperature of the system, and the separation is called an equilibrium stage. A single stage separation may be considered as a distillation in itself and may be called a flash separation. The performance of such a distillation compared with the separation obtained under equilibrium condition is described as the efficiency of what is termed the actual stage, to a theoretical stage. Both are compared at the same conditions of temperature and pressure; the efficiency is referred to as stage, plate. or tray efficiency. Alternately, its measurement numerically as fractions of a stage is described in the method which follows (Coulson and Richardson, 1997).

In distillation the state of equilibrium that exists between the vapour and liquid streams as they leave the stage from separate places is the basis of practical measurement in the attainment of stage-equilibrium condition, while the equilibrium stage requires that the phases be in a state of coexistence for its definition. An actual distillation tray may sometimes produce a separation attainable by an equilibrium stage (or tray). The theoretical stage or tray then is not the maximum separation attainable from an actual stage. This is possible because there is a concentration gradient across the tray that is set up from the liquid inlet to the outlet overflow. When the path of the liquid is long and the tray efficiency is normally high, the vapours entering the tray from below are mixed to a uniform composition (the entering gas is the same at both ends of the flow path) and as the gas passes upward through the flowing liquid, equilibrium is attained at each point, just over the surface of the flowing liquid. The apparatus used in a flash separation is mainly a vessel used to hold the partially vapourized mixture charged into the system. The liquid level is usually on control. A heater may be located on the entering charge or within the vessel. A condenser with an appropriately located back-pressure valve is used to permit the conversion of the vapour separated into a liquid product. This is an approximate description for either the small laboratory still or large scale plant separators (Coulson and Richardson, 1997).

Where a vessel is used with no entrainment devices, the separation of the vapour and liquid may be accomplished by allowing sufficient residence time for the passage of both phases through the vessel so that satisfactory separation takes place. This type of design is base on the use of stoke's law and the choice of liquid droplet

diameter for the setting of the liquid phase, with a similar calculation for the rise of bubbles of gas from the liquid layer. In calculatings the relative amounts of vapour and liquid produced from a phase separation when a mixture is partially vaporized, the McCabe-Thiele diagram is used for two component mixtures. The flash separation at equilibrium is an example of a meeting point of three evaluations, since it could be considered as a vapour-liquid equilibrium stage, a theoretical stage, or a minimum stage. In relation to design, the flash separation is usually considered as a single vapour-liquid equilibrium stage, particularly when residence time and mixing are provided and are followed by good separation. There is also reason to refer to this condition as a theoretical stage, since it would be based on the operating conditions (Coulson and Richardson, 1997).

2.4.2 Minimum-Stage and Flash Separation

The McCabe-Thiele diagram used to calculate the vapour and liquid separation shows that the origin of the short operating line starts at the diagonal (at the feed composition point) and then the line is extended to the equilibrium curve. Since the diagonal is used to represent a total reflux condition as a reflux operating line, a flash separation is a minimum stage of separation when taken to equilibrium (Tatabu, 2001).

2.4.3 Multistage Separation by Continuous Distillation

A multistage separation by distillation requires three combined effects from the apparatus; extra flow of internal vapour and liquid streams within, and that the general nature of the vapour and liquid stream is counter current. The apparatus used would include a column or tower, both terms suggesting a vertical cylindrical vessel, within which the multistage effect is produced through the installation of what are called tower trays, these spaced to make possible a series of contacts betwee vapour and liquid streams flowing within the tower. This does not exclude the use of tower packing or other devices, since the basic functions are similar for all.

The general nature of the internal flow of vapour and liquid within the tower is the following. The feed mixture in a partially vaporized state, usually between the bubble point or dew point conditions, enters the tower at some selected stage location and merges into vapour and liquid in excess of the net amount from the feed is generated through the combined effects of the vapourization of some of the liquid at the base of the tower and the return of part of the vapours that are leaving at the top after they have been condensed to a liquid state. The resulting flows of liquid and vapour are counter current, the liquid flowing downward and across each tray, while the vapour is being forced upward through the caps or orifices in the trays, resulting in mixing of the vapour and liquid by the action of the bubbles formed.

The liquid flowing downward from stage to stage passes through a seal at each stage which provides the hydraulic head required to force the upward-flowing gas through the caps or orifices located in the trays. The vapour generation at the base of the tower is reboiling, and the return of condensed liquid to the top of the tower is refluxing. Reboiling is heat addition through vapourization and refluxing is a heatremoval effect from condensed vapours being re evaporated while flowing downward. These two effects, reboiling and refluxing must equate to a heat balance when the heat input of the feed and the heat output of the products and separated streams as well as other minor heat quantities are taken into account.

An examination of the heat and mass transfer taking place during the counteraction of reboiling and refluxing going on from stage to stage will show that the liquid reflux is first depleted of lower boiling components by their vapourisation

2.5 The Feature of CAD

The main feature of CAD is shown in the figure 2.7 below



Figure 2.7: Main features of a CAD system

A typical CAD system is a combination of hardware and software;

2.5.1 The Software

This is the intelligence "Within the mind of Computer. The term is used to refer to both programme and data. Programmes are set of instructions to the computer, indicating to it a series of actions to take "Data" is the term used for the information on which these acts are performed in response to the instruction of the programme.

Programmes can be batch or interactive. In working with a batch programme, the user enters data but does not interact with the computer during the processing of the data. Here the user cannot tell if things went wrong during the entry or processing until the entire analysis is completed. However the interactive software evolved from computer codes that carry out matrix manipulations to comprehensive programs that combine matrix computations, data analysis, equation solving, graphics, and many other features. Interactive programme provides variety of immediate response to the user, the user in turn can respond by modifying earlier actions or performing additional ones.

The software in CAD system consists of six categories mainly:

- The operating systems that control the CPU, it also includes language comp which present a programme written in certain computer language and translate it into machine code that can be executed by the CPU.
- The graphic software, which provides communication between the graphic terminals and the CPU.
- The user interface which relates with the user's command, giving prompt display of result.
- The geometric modeling which may be "2 or 3" dimensional. Application software, which includes drafting and calculation.
- The software, which is developed by the user to suit the existing, purpose.

2.5.2 The Hardware

This consist of the visible part of a system, it is the position of the system that contact the world, the feature of a typical hardware includes compactness, neatly assembled, well interfaced, accurate, stable and reliable. The CAD hardware units consist of the following.

i. The central processing unit (CPU).

ii. Storage devices that store data e.g. Floppy diskettes, disks, and Magnetic tapes.

iii. Input devices that serve and command the system operation e.g. Key board.

iv. The output device that presents the input result to the user.

2.5.3 Guidelines on Basic Programming in CAD Operation

As carlier stated, a programme is a set of instructions to a computer. An instruction in a basic programme in called a "Statement". Each statement is generally written as a separate line with a line number. Any statement starting with the word REM is remark; however each programme has a particular symbol for this. The word END marks end of the programme. There are a large number of versions of various basic Programmes e.g., Q-basic, Visual basic, etc of which there are slight differences and of courses various presentation modifications.

2.5.4 Method of Developing CAD

According to (Onifade, 2000), there are basically two methods of developing CAD flowsheeting in chemical processing industries. These are namely the *Equation Oriented* and *Modular Methods*. In equation oriented methods, the process or system is regarded as unit and the equations, correlation etc, that describe the process are collected together and solved, while the modular regards the design process or system as a collection of subsystems or modules.

Although the modular approach has it's own drawbacks, it is usually preferred because of its inherent advantage of individuality and portability. It employs databank or modules; it stores the process data such as properties, thermodynamic data etc, and the modules for processing algorithms, equation and optimization needed by the design. A master programme synchronizes the passing of information between the databank and the modules (Onifade 1999; Westerberg 1979). Each modules can be developed, tested, and debugged on it's own and incorporated into the overall design or flowsheeting. Furthermore many plants or process consists of the same or similar units that require the same kind of calculations. The modular option therefore allows a module in the design of one plant to be "imported" into the design of another plant in which the module has a similar function.

2.5.5 Source of Data

It is essential for a chemical engineer to be familiar with sources of physical properties data. Accurate values of physical properties are needed in almost all phases of chemical engineering design analysis (Himmelblau 1996). Various ways to obtain data for the physical properties of components are

i) Design software (such as flowsheeting codes)

- ii) On-line databases.
- iii) On-line bulletin boards/e-mail.
- iv) Personal files and handbooks.
- v) Department library.
- vi) Technical magazine/newsletters.
- vii) Reference books and journals.

Much of the data is available, particularly on Internet service.

2.5.6 Importance of Data on Physical Properties

- a. To retrieve an isolated value to be used in a calculation or in the calculation of other property values. Often a value is to be employed in hand calculations or perhaps fed as input to a computer programme for further calculation.
- b. To serve as a subroutine (such as physical properties library), to another computer programme to provide physical property data for process of calculations.
- c. To provide interactive capabilities for the rapid rendering of physical properties of substance of interest for parametric studies of process units.
- d. Such physical properties package is essential in process evaluations, economic evaluation, process safety, unit operations modeling, process simulation and optimization, transportation of materials and pollution studies.
- e. A single system allows for more sophistication and results in some economy by saving duplication effort.

2.5.7 Economic Importance and Engineering Significance of CAD

There are many benefits of computer-aided design. Only some of it can be easily measured. Some of the benefits are intangible, reflected in improving work quality, more pertinent and usable information, and improved control, all of which are difficult to quantify. Other benefits are tangible but the savings from them shows up a downstream in the production process, so that it is difficult to assign any monetary value to them in the design phase. Some of the benefits derived from implementing CAD can be directly measured as follows.

- 1) Improved engineering productivity.
- 2) Reduced engineering personal requirement.
- 3) Customer's modifications are easier to make.
- 4) Faster response to request.
- 5) Avoidance of sub-contracting to meet schedule.
- 6) Minimized transcription errors.
- 7) Improved accuracy of design.
- 8) In analysis, easier recognition of components interaction.
- 9) Provide better functional analysis to reduce prototype testing.
- 10) Assistance in preparation of documents.
- 11) Design has more standardization.
- 12) Better design provided.
- 13) Improved productivity in tool design.
- 14) Better knowledge of cost is provided.
- 15) Reduced training time for routine drafting tasks.
- 16) Fewer errors in "National Control" part programming.
- Helps ensure that designs are appropriate to existing manufacturing techniques.
- 18) Saves materials and machinery's time by optimization of algorithm.
- 19) Provides operational results on the status of work in progress.
- 20) Makes the management of design personnel of project more effective.
Data communication results in greater understanding among engineers, designers, drafters, management and different project groups.

CHAPTER THREE

3.0 Methodology

3.1 Problem Statement

The CAD module will be developed using this problem statement. A mixture of benzene and toluene is to be separated by binary distillation column. The feed has a molar composition of 50% benzene and 50% toluene and is charged into the column at atmospheric pressure. The following results are to be determined:

- 1. The effect of variation of the feed temperature on the column performance (actual number of trays, optimal feed tray, condenser duty, reboiler duty and product purity.
- 2. The effect of variation of the feed pressure on the column performance (actual number of trays, optimal feed tray, condenser duty, reboiler duty and product purity.
- 3. The effect of variation of the feed molar flow rate on the column performance (actual number of trays, optimal feed tray, condenser duty, reboiler duty and product purity.
- 4. The effect of variation of the column external reflux ratio on the column performance (actual number of trays, optimal feed tray, condenser duty, reboiler duty and product purity.

3.2 Process Simulation Procedure

Hysys Process Simulator was used for the simulation and the design of the binary distillation column. Peng Robinson thermodynamic model because it is the most suitable model for light hydrocarbon at pressure below 7 bar (Hyprotech, 1999). The procedures for the simulation using Hysys are shown below.

3.2.1 Shortcut Process Simulation Procedure

The simulation procedure for the shortcut model of the binary distillation column are shown below:

1. The start button was clicked using the mouse

- 2. The cursor placed on the "all programs" menu opened up the pop-out menu.
- From the pop-out menu, Hyprotech was highlighted to further pop-out Hysys 3.1 which was clicked to launch the Hysys program displaying the Hysys windows.
- The "tools" menu was clicked to deep down the menu list and "preference" was clicked to give the "preference" dialogue box.
- On the preference dialogue box, the variable tab was clicked and the units selected to display the system of units available in Hysys.
- 6. A new unit set of SI was selected.

Variables	Ava	ailable Unit	Sels				
i nits ormats	Fie Ho Ho	ld verTextUr verTextUr	utSet1 utSet2		<i></i>		Clone
	Un	ıt Set Na <u>m</u>	e SI			AL IN	
	Elisp	olay Units					
			*****	Unit			⊻iew
	Va	pour Frach	on		Unitless		
	Ter	mperature			C		
	Pre	ssure			kPa	1	
	Ma	w ss Flow			kgmole/h kg/h	-	
		0	100	D	E.A.	011	True Comme

Figure 3.1: Unit Selection Dialog Box

- 7. The preference dialogue box was closed.
- 8. From the file menu, a new case was opened to reveal the task manager window.
- On the task manager window, the "fluid package" tab was clicked and the "Add" button clicked to reveal all the thermodynamic application packages available in Hysys 3.1.

GUEUS General NBTL Graycon Streed Kabadi Danner Lee Nester Plocher Margules MDWR NBS Steam NBTL OUL Electrolista	 All Types EOSs Activity Models Chao Seader Model: Vapour Press Model: Miscellaneou: Type: 	Eguation of State Lee-Kesley Peng Robinson Uphons Hr(S)(S Standard Use EOS Density
Component List Selection		 Smooth Liquid Density Advanced Thermodynamics COMUSer

Figure 3.2: Fluid Package Window

- 10. From the available list, Peng Robinson was selected.
- 11. The view button of the component section was clicked to reveal all the available components in the component library of Hysys 3.1. benzene and toluene, were highlighted and the "add pure" button was clicked to select them from the component library.

Add Component	Selected Component:		Component: Ava-	dable us t	he Component Library	
- Component. Traditional	Tokiene		Haich			View Fillers
Electrolyte			· Sim Name		Full Name / Synonym	Formada
Hypothetical						
Other		Add Dines				and the day
10000000		- TOT PILL	Ethane	1.2		0.340
			Constant	1		C 11110
		Cals Idealar .	1-12-111-041-04	11.4		C4H10
		1.000.177.77	ri buarte	inc. i		C LUI I
			in Containe	N.C.C.		C54115
		Hendse	wither and	CC.		COUL
			o Head war	57		C7H16
			nilictore	1.8		1 204121
		Sout Last	n Nonane	1.14		1.900.00
			n Decane	1.10		C10022
			reC11	C11		C111124
		View Component	n C12	C12		£1.2H26
			r C12	1.15		F 1 364 30
			 Show Synoos 	201	Cluster	
r			211-10-10-10-10-10-10-10-10-			
Selected Compo	send by Uspecial					

Figure 3.3: Component List View Window

- 12. Both the component list windows as well as the fluid package window were closed.
- After this, the simulation has been completely built. Next is to build the process flow diagram.

14. The "Enter Simulation Environment" was clicked

15. On the simulation environment; the "work book" icon on the tool was clicked and the distillation feed steam was created specifying its components molar fraction, its temperature, pressure and volumetric flowrate as shown on Figure 3.4.

Worksheet	Stream Name	l I
c	Vapour / Phase Fraction	0.00000
Londitions	Temperature [C]	.30.000
Properties	Pressure [kPa]	1013.
Composition	Molar Flow [kgmole/h]	100.00
Composition	Mass Flow [kg/h]	8652.8
K Value	Std Ideal Lig Vol Flow [m3/h]	9,8959
User Variables	Molar Enthalpy [kJ/kgmole]	2.867e+004
Mater	Molar Entropy [kJ/kgmole-C]	-114.85
NO(62	Heat Flow [kJ/h]	2.8669e+06
Cost Parameters	Lig Vol Flow @Std Cond [m3/h]	9.8443
	Fluid Package	Basis-1
	4	
	Vachmente Duparrice	
WOIKSHEET A	(achiments) Dynamics	

Figure 3.4: The distillation column feed conditions

16. The shortcut distillation column icon on the PFD pallete was clicked on and the

shortcut distillation column module was displayed.



Figure 3.5: The shortcut distillation column window

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- 17. The design tab was selected and the connection tab was also clicked on to show the shortcut column connections.
- 18. The inlet and outlet connections of the column were entered.
- 19. The parameter tab was selected and the key components, condenser pressure, reboiler pressure and the external reflux ratio were specified as shown in Figure 3.6.

Design	Components	C	oroponent	Mole Fraction	
onnections	Light Key in Bottoms		Benzene	0 1000	
arameters	Heavy Key in Distillate		Toluene	0.1000	
lser Variables	Press <u>u</u> res				
10(62	Condenser Pressure Reboiler Pressure		91.192 kPa 101.325 kPa		
	Beflux Ratios		0.912	bar 6 psia	
	External Reflux Ratio Minimum Reflux Ratio		10.000 1.719		
Design Ra	ting Worksheet Performance	e Dynamic	: [

Figure 3.6: Shortcut distillation column parameters.

- 20. The tool menu was clicked on and the databook was selected from the displayed menu.
- 21. From the databook window, the variable tab was clicked on and the insert button was clicked on and the variable navigator dialog box appears.
- 22. The Feed stream was selected from the object tab and the temperature variable was clicked on. The OK button was selected.
- 23. The same was repeated for feed pressure, molar flow, distillate benzene molar fraction, column actual trays, condenser duty, external reflux, minimum reflux, minimum trays, optimal feed and reboiler duty

Available Data I	Entries				
Object	Variable				
EREAL AND A	Constant Spectra 1	W. B.S. Schups		A FORMATION	Eda
F	Pressure	NYY W ALT I THE LOUGH AND A	ningen under seinen	Di Bentra di Alta della di Conte	C <u>O</u> I
F	Molar Flo	W.		1	Intert
D	Comp M	ole Frac (Benzen	e	1	Insen
T-100	Actual T	rays			-
T-100	Condens	er Duty			Delete
T-100	External	Reflux			
T-100	Minimum	Reflux			
T-100	Minimum	Trays			
T-100	Optimal F	feed			
T-100	Reboiler	Duty			
				N.*	

Figure 3.7: Hysys Databook

- 24. The Process Databook tab was selected and Add button clicked on to enable selection of variable.
- 25. The feed temperature, condenser duty, and reboiler duty were all checked under the show button.
- 26. The Data Recorder tab was selected and Add button was clicked on for selection of variables to be investigated.
- 27. The feed temperature, external reflux ratio and reboiler duty were checked and the record button was clicked.
- 28. The case studies tab was clicked on and the feed temperature was selected as the independent variable, while the condenser duty and reboiler duty were selected as the dependent variable.

Available Case Studies		Case Stu	dies Diata S	election			
物。使用,中的调料	Add	Add Current Case Study		Case Study 1			
	Deleta	Obj	ect	Variable	Ind	Dep	
	Delete		F	Temperatur	eV	Г	
	Constant		F	Fressur	c T	۳ ۲	
	<u>-</u> P_ 77		F	Molar Flov	νΓ	Г	
			DI	Comp Mole Frac (Benzene	э (Г	
			T-100	Actual Tray	\$	Г	
Available Displays			T-100	Condenser Dut	y i	~	
T.L.			T-100	External Reflu	хΓ	Г	
- Grade	Poculto		T-100	Minimum Reflu	x E	5	
• Graph	Testites		T.100	Minimum Trau	e	r	•

Figure 3.8: Hysys Databook

29. The results button was clicked on to display the plot of temperature against condenser



and reboiler duty.



30. The same procedures were repeated for other plots.

3.2.2 Rigorous Process Simulation Procedure

The simulation procedures for the rigorous distillation column design of the binary

distillation column are shown below:

31. The start button was clicked using the mouse

32. The cursor placed on the "all programs" menu opened up the pop-out menu.

- 33. From the pop-out menu, Hyprotech was highlighted to further pop-out Hysys 3.1 which was clicked to launch the Hysys program displaying the Hysys windows.
- 34. The "tools" menu was clicked to deep down the menu list and "preference" was clicked to give the "preference" dialogue box.
- 35. On the preference dialogue box, the variable tab was clicked and the units selected to display the system of units available in Hysys.
- 36. A new unit set of SI was selected.

Variable	s Ava	ilable Unit	Sets				
U nits Formats	Fie Ho Ho	ld verTextUn verTextUn	itSet1 itSet2			^ ب 2018	Clone
	Un	it Set Na <u>m</u> e	e SI				la Al d'antisarativa para
	Uist	play Units		h La			
	Var	DOLY Fractic	00	Unit	Unitless	······ ^	Alem
	Ter	Temperature			C		
	Pre	ssure		i	kPa		
	Flo	w			kgmole/h		e trans en en en en anteretar a
	Ma	ss Flow		1	kg/h		
	_				1	<u></u>	

Figure 3.10: Unit Selection Dialog Box

- 37. The preference dialogue box was then closed.
- 38. From the file menu, a new case was opened to reveal the task manager window.
- 39. On the task manager window, the "fluid package" tab is clicked and the "Add" button clicked to reveal all the thermodynamic application packages available in Hysys 3.1.

operty Package Selectic CEOS eneral NRTL rayson Streed abadi Danner ee-Keder Plock er targules targule	n Property F & All Tyr EOSs Activat Chao Vapor Misce	Package Filte pes y Models Seader Mode ir Press Mode Ilaneou: Typ	r , P dr es es	OS Enthalpy Method Specif • Eguation of State Lee Kesler eng Robinson Options • Hr/S/S Standard Use EOS Density Smooth Liquid Density	ication
omponent List Selection Component List - 1	-	Vie	w.	Advanced Thermodynamic COMThermo	:1
et Up Parameters	Binary Coeffs	StabTest	Phase Order	Rxnt Tabular Notes]
Delete Name	Basis-1	Propert	y Pl.g	Peng Robinton	Edit Properties

re 3.11: Fluid Package Window

40. From the available list, Peng Robinson was selected.

41. The view button of the component section was clicked to reveal all the available components in the component library of Hysys 3.1. benzene and toluene, were highlighted and the "add pure" button was clicked to select them from the component library.

Add Component	Selected Component:		Component: Ava	alable in I	he Component Library	
- Components Traditional	Toluene		Match			View Filters
Electrolyte			 Smillane 		Full Name / Synorym	Formula
Hypothetical						
Other		Sold Fine	C II AND	6.5		C 200
			Electronic	12		1 3408
			Butane	LCA.		C4H10
		 Substitutes 	n Eulane	nis		C 4H(10)
			Pentane	165		C5H12
			n Fentane	n.C5		C5H12
		Flementer	u He care	11.		L 6H14
			n Hectane	C7		C7H16
			n-Octone	13		C8H18
		Soft List	n-Non-arie	0.3		C/9H20
			n-Decane	C10		C10H22
			n C 11	C11		C11H24
		Tiers Fourt-openy	6 C12	C1 '		C12H26
			P.C12	112		פירער די
			 Show Synone 	2015	Charles	

Figure 3.12: Component List View Window

42. Both the component list windows as well as the fluid package window were closed.

43. After this, the simulation has been completely built. Next is to build the process flow diagram.

44. The "Enter Simulation Environment" was clicked

45. On the simulation environment; the "work book" icon on the tool was clicked and the distillation feed steam was created specifying its components molar fraction, its temperature, pressure and volumetric flowrate as shown on figure 3.4.

Worksheet	Stream Name	
Conditions	Vapour / Phase Fraction	0.0000
Continuons	Temperature [C]	30.00
Properties	Pressure [kPa]	1013.
Composition	Molar Flow [kgmole/h]	100.0
	Mass Flow [kg/h]	86521
n Value	Std Ideal Lig Vol Flow [m3/h]	9,895
User Variables	Molar Enthalpy [kJ/kgmole]	2.867e+004
Malas	Molar Entropy [kJ/kgmole-C]	-114 83
L10(62	Heat Flow [kJ/h]	2 8669**0
Cost Parameters	Lig Vol Flow @Std Cond [m3/h]	9.844
	Fluid Package	Elasis-1
	4	
•		
Worksheet	<u>llachments</u> J Dynamics	

Figure 3.13: The distillation column feed conditions

46. The distillation column icon on the PFD pallete was clicked on and the shortcut

distillation column module was displayed.



Figure 3.14: The Distillation Column Input Expert

47. The connections to the distillation column was specified as shown below:



Figure 3.15: The Distillation Column Input Expert showing the Connections

- Distillation Column Input Expert
- 48. The condenser and reboiler duty were specified as shown below:

Figure 3.16: The Distillation Column Input Expert showing the Condenser and Reboiler

Pressure

49. The distillate liquid feed rate and the reflux ratio were specified as:





Ratio

- Distillation Column Input Expert
- 49. The distillate liquid feed rate and the reflux ratio were specified as:

Figure 3.17: The Distillation Column Input Expert showing the Liquid Rate and Reflux

Ratio

50. The Done button was clicked on and the following interface was displayed.

Monitor Condenser Energy Stream Specs CDuty Specs Delta P Subcooling Note: Injet Streams Stream Feed Stream >> Stage Numbering • Top Down Bottom Up	Design Connections	Column <u>N</u> ame T-101	Sub-Flowsheet Tag COL2	Condenser • Total Partial Full Ref
Notes Injet Streams P cond Optional Side Draws Stream Inlet Stage 95.00 kPa Stream Type Draw Stage Feed 5_Mair P reb 101.3 kPa Reboiler Energy Stream Stage Numbering • Top Down Bottom Up • • 1 Delta P Bottoms Liguid Outlet	4onitor Specs Specs Summary Subcooling	Condenser Energy Stream CDuty		Delta P 0.0000 kPa 0⊻hd Liquid Outlet D
Stage Numbering • Top Down Bottom Up Delta P Bottoms Liguid Outlet	lote:	Inlet Streams Stream Inlet Stage Feed 5_Mair Stream>>	→ 2 P cond Num of Stages P reb 101.3 kPa	Optional Side Dr <u>a</u> ws <u>Stream Type Draw Stage</u> << Stream >> Reboiler Energy Stream
Edit Trays		Stage Numbering • Top Down Bottom Up Edit Trays	n In+1 Delta P 0.0000	RDuty + Bottoms Liguid Outlet kPa B +

Figure 3.18: The Distillation Column Input Expert showing the Column Conditions

51. The Run button was clicked on and the converged simulation screen was displayed.

Design Connections	Column <u>N</u> ame T-101 Condenser Energy Stream	Sub-Flowsheet Tag COL2	Condenser • Total	Partial 👘 Full Retl
pecs pecs Summary ubcooling	CDuty 🗸 🔫		0.0000 kPa	O⊻hd Liquid Outlet D
loles	Injet Streams Stream Injet Stage Feed 5_Mair << Stream>>	→ 2 P cond 95.00 kPa n = 10 P reb 101,3 kPa	Optional Side Draw Stream ICC Stream >>	s Type Draw Stage aboiler Energy Stream
	Stage Numbering • Top Down – Bottom Up Edit Trays		a P Bo 000 kPa B	Duty
Design Parar	meters SideOps Bating Works	heet Performance Flowsheet	Reactions Dyna	mics

Figure 3.19: The Distillation Column Input Expert showing the Converged Simulation

3.2.3 Cost Estimation Procedure using Hysys Simulation

The simulation procedures for the cost estimation of the distillation column design of the binary distillation column are shown below:

52. The Hysys spreadsheet icon was clicked on the PFD pallete and the following window was displayed.

SPRDSHT-2					
		Spre	adsheet <u>N</u> ame	SPRDSHT-2	2
Imported ⊻ariable	\$				
Cell	Object	Vari	able Description	Sector Maria Sector Sector	
					Add Import
Exported Variable	S				
Cell	Object	Vari	able Description		
Cell	Object	Vari	able Description		فراط (محمد م
Cell	Object	Vari	able Description	-	Add Expo <u>r</u> t
Cell	Object	Vari	able Description		Add Expo <u>r</u> t
Cell Connections	Object Parameters	Vari Formulas	able Description Spreadsheet	Calculation	Add Expo <u>r</u> t

Figure 3.20: Hysys spreadsheet window.

53. The spreadsheet tab was clicked on to enter the cost equation and text describing what

the equations stand for.

	ent Cell		and the second second second second	and a second state of the second state of			an der nichten eine bestellt die seinen die seinen die seine die seine die seine die seine die seine die seine	Control Constant
, cm	ern c.en							
	A1 Va	iable:			Angles in.	•		
			В	C	D			
						nya matakan panana anaja kanang minana dia		
	Vapour Ma	ass Flow	6273 kg	J/h				
	Vapour Ma	ss Dens	2.519 kg/	m3				
	Molecular	Weight	78.4	41				
	Surface Te	nsion of	<emp< td=""><td>y></td><td></td><td></td><td></td><td></td></emp<>	y>				
	Liquid Ma	tos Flow	4705 kg	l/h				
	Liquid M.	ass Den	814.4 kg/i	m3				
	Liquid Mole	cular W	78.4	11				
	Surface Te	nsion of	21.10 dyne/	cm				
D								
1	Flow Pa	rameter	4.171e-00)2				
2	1							
3								
1								
5								
5								
C	onnections	Parameters	Formulas	Spreadsheet	Calculation Order	User Variables	Notes	
				1				

Figure 3.21: Hysys spreadsheet cost equations window



Figure 3.1: Process Flow Diagram of Binary Distillation Column

CHAPTER FOUR

4.0 RESULTS AND DISCUSSION

4.1 RESULTS

The results of the graph based computer Aided Design of binary distillation column design using Hysys process simulator are shown by the following.



Figure 4.1: The Variation of Feed Pressure with Optimal Feed



Figure 4.2: The Variation of Feed Pressure with Condenser Duty



Figure 4.3: The Variation of Feed Pressure with Minimum Reflux



Figure 4.4: The Variation of Feed Pressure with Molar Flow



Figure 4.5: The Variation of Feed Pressure with Reboiler Duty



Figure 4.6: The Variation of Feed Temperature with Condenser Duty



Figure 4.7: The Variation of Feed Temperature with Component Mole Fraction (Benzene)



Figure 4.8: The Variation of Feed-Temperature with Reboiler Duty



Figure 4.9: The Variation of Feed Temperature with Actual Trays



Figure 4.10: The Variation of Feed Temperature with External Reflux



Figure 4.11: The Variation of Feed Temperature with Minimum Reflux



Figure 4.12: The Variation of Feed Temperature with Minimum Trays



Figure 4.13: The Variation of Feed Temperature with Optimal feed



Figure 4.14: The Variation of Feed Temperature with Pressure



Figure 4.15: The Variation of Feed Molar Flow with Feed Temperature



Figure 4.16: The Variation of Feed Molar Flow with Reboiler Duty



Figure 4.17: The Variation of Feed Molar Flow with Comp Mole Fraction (Benzene)



Figure 4.18: The Variation of Feed Molar Flow with Optimal Feed



Figure 4.19: The Variation of Feed Molar Flow with Minimum Trays



Figure 4.20: The Variation of Feed Molar Flow with Minimum Reflux



Figure 4.21: The Variation of Feed Molar Flow with Condenser Duty



Figure 4.22: The Variation of Feed Molar Flow with Actual Trays



Figure 4.23: The Variation of External Reflux with Reboiler Duty



Figure 4.24: The Variation of External Reflux with Optimal Feed



Figure 4.25: The Variation of External Reflux with Optimal Feed



Figure 4.26: The Variation of External Reflux with Minimum Reflux



Figure 4.27: The Variation of External Reflux with Condenser Duty



Figure 4.28: The Variation of Feed Temperature against Reboiler Duty with Actual Number

of Stages

Financial Indices	Amount (₦)	
Bare module cost of the tower	154,200,000	
Bare module cost of the tray	12,610,000	
Bare module cost of the condenser	205,400,000	
Bare module cost of the reboiler	19,890,000	
Bare module cost of the accumulator	9,919,300	
The total utility cost (condenser, cooling water, and reboiler	143,500,000	
steam)		
The annualized Cost	199,300,000	
The total bare module cost of the tower, trays, condenser,	279,000,000	
reboiler and reflux accumulator	٤.	

Table 4.1: Financial Analysis of the binary distillation Column

4.2 DISCUSSION OF RESULTS

Graph Based Computer Aided design of binary distillation column has been carried out. The components considered for separation are benzene and toluene. Hysys process simulator was used for the computer Aided Design. In this project the effect of feed condition, external reflux ratio on the binary distillation column number of stages, optimal feed stage, condenser duty, reboiler duty product purity were investigated graphically. The best feed condition and minimum reflux ratio were used for designing and costing the distillation column. The design and costing of the column were also carried out in Hysys.

4.2.1 Effect of Molar Flow Rate of the Feed on Column Actual Trays and Optimal Feed Tray

Figure 4.23 showed that there was no visible change in the value of the column actual trays of 6.900 as Molar Flow increases from 100 to 1100. Figure 4.18 showed that there was no visible change in the value of the Component Mole Fraction Benzene at higher purity of 0.995 as Molar Flow increases from 100 to 1100 kmol/hr. Figure 4.19 showed that there was no visible change in the value of the Optimal Feed stage value of 3.80 as molar flow increases from 100 to 1100 kmol/hr. This shows that the column actual stage, optimal feed stage and product purity are not affected by the molar flow of the feed and this is in close agreement with literature.

4.2.2 Effect of Molar Flow on Condenser and Reboiler Duty

The effects of molar flow against the condenser and reboiler duty were also studied. Figure 4.22 indicated that there was a sharp decrease in Condenser Duty from -1.00e007 to -1.50e008 kJ/hr as Molar Flow increases from 100 to 1100 while Figure 4.22 indicated that there was a sharp increase in reboiler duty from 1.10e007 to -1.40e008 kJ/hr as Molar Flow increases from 100 to 1100. This is in agreement with chemical engineering fundamental as more energy is required for vapourizing the increase in molar flow of the feed into the column.

4.2.3 Effect Feed Pressure on Column Actual Trays and Optimal Feed Tray

There was a sharp increase in column actual trays from 5.78 to 6.80 as Pressure increased from 100 to 1100 kPa. This is in close agreement with literature which states that increase in pressure decreases the energy requirement of the reboiler and increases the trays required to effect separation for similar reasons. From, Figure 4.1, there was a sharp increase in optimal feed stage from 3.16 to 3.72 as pressure increases from 100 to 1100 kPa. This shows that product purity was not affected by feed pressure (Hysys, 1999).

4.2.5 Effect of Feed Pressure on Condenser and Reboiler Duty

From Figure 4.3, there was no increase or decrease in Condenser Duty of -1.40 kJ/hr as pressure increased from 100 to 1100 kPa. From figure 4.6, there was a sharp drop in reboiler duty from 1.386e007 to 1.385e007 kJ/hr as pressure increases from 100 to 1100 kPa. This also conform with literature (ASPEN DISTILL, 2003) which states that increase in feed pressure reduces the energy requirement of the reboiler as the boiling point of the mixture are lowered and vaporized at reduced temperature. The condenser duty was not affected by feed pressure.

4.2.6 Effect of Feed Temperature on Condenser and Reboiler Heat Duty

Figure 4.7 shows that there was no visible change in the value of the Condenser duty heat flow of -1.30e007 kJ/hr as feed temperature increases from 30 to120^oC. This shows that the condenser duty is not affected by the feed temperature. Figure 4.9, indicated a continuous drop in reboiler duty heat flow from 1.38e007 to 9.40e006 kJ/hr as feed temperature increased from 30 to 120^oC. Literature states that increase in temperature reduce the heat. This is also in agreement with literature (Hysys, 1999).

4.2.3.2 Effect of Feed Temperature on Product Purity

Figure 4.8, shows that there was no visible change in the value of the Component Mole Fraction of benzene at 0.995 purity as feed temperature increased from 30 to120^oC. Literature (ASPEN DISTILL, 2003) also states that the product purity is not affected by the feed pressure.

4.2.3.3 Effect of Feed Temperature on Column Optimal Feed Tray

From Figure 4.14, the optimal feed tray constant value of 3.16 was obtained as the feed temperature was increased from 30 to 95 °C, a sharp increase in optimal feed tray value from 3.16 to 3.47 was obtained the feed temperature was increased from 95 to 104 °C where it

finally maintained a steady value of 3.47 as the temperature was further increased from 104 to 120 °C. This shows that a feed tray of 3.5 is adequate for the rigorous distillation column design.

4.2.9 Effect of Feed Temperature on Column Actual Trays

From Figure 4.14, the optimal feed tray constant value of 5.78 was obtained as the feed temperature was increased from 30 to 95 °C, a sharp increase in optimal feed tray value from 5.78 to 6.34 was obtained the feed temperature was increased from 95 to 104 °C where it finally maintained a steady value of 6.34 as the temperature was further increased from 104 to 120 °C. This shows that a feed tray of 3.5 is adequate for the rigorous distillation column design. Literature (ASPEN DISTILL, 2003) also states that the column actual tray is affected by the feed temperature.

4.2.10 Effect of External Reflux Ratio on Condenser Duty

From Figure 4.28, there was a sharp drop in the Condenser Duty (kJ/h) when external reflux was increased from 3.00 to 10.00. This is in agreement with literature (ASPEN DISTILL, 2003) which states that increase in reflux ratio decreases the condenser duty. This shows that the condenser is removing less heat as more distillate is returned to column from the accumulator and reduces the enthalpy of the vapour entering the condenser.

While Figure 4.27 shows that there was no visible change in the value of the minimum reflux at 1.8 as external Reflux ratio increased from 3.00 to 10.00. Figure 4.26 shows that there was no visible change in the value of the Minimum Trays (5.995) as External Reflux increases from 3.00 to 10.00.

From Figure 4.25 shows continuous decrease in Optimal Feed stage from 5.400 to 3.65 as External Reflux increased from 3.00 to 10.00. The optimal feed position remains constant at external reflux ratio of 10. Lang also states that the external reflux ratio affects the feed tray and the column actual tray. This is due to the fact that external reflux return cold feed to the

column and adjust the thermodynamics of the column, hence there was adjustment in the position of the feed stage.

Figure 4.24 indicates a sharp linear increase in Reboiler Duty from 5.4e007 to 1.4e008 as External Reflux increases from 3.00 to 10.00. This is also in agreement with literature (Kramer, 1997) which states that increase in reflux ratio increases the reboiler duty. This shows that the condenser is removing less enthalpy as more distillate is returned to column from the accumulator and reduces the enthalpy of the vapour entering the condenser.

Figure 4.26 shows that there was no visible change in the value of the Minimum Trays (5.995) as External Reflux increased from 3.00 to 10.00. This is also in close agreement with literature which states that the external reflux ratio does not affect the minimum number of stages. This is because the reboiler is compensating for the effect caused by the external reflux ratio by increasing its heat duty. There was a continuous decrease in actual tray from 10.00 to 6.800 as external reflux increases from 3.00 to 10.00. This is also in close agreement with literature (ASPEN DISTILL, 2003).

There was no increase or decrease in Component Mole Fraction (Benzene) at 0.995 as External reflux increased from 3.00 - 10.00.

4.2.3 Design of Binary Distillation Column

The optimum feed condition selected for the design of the binary distillation column are feed temperature of 30 °C, pressure of 1 atm, molar flow rate of 100 kmol/hr and molar composition of 50% benzene and 50% toluene.

The design parameters used for the rigorous distillation column design are: 8 actual nu number of trays, optimal feed stage of 6, external reflux ratio value of 4, distillate rate of 37.5 kPa, condenser pressure of 95 kPa and reboiler pressure of 101.3 kPa. These parameters were obtained from shortcut distillation column simulation.
The rigorous distillation column design shows that 99% of the benzene was recovered in the distillate. The column temperature profile dropped from 81.43 oC to 104.4 oC from the condenser to the reboiler. The column pressure profile dropped from 95 kPa to 101.3 kPa from the condenser to the reboiler. The distillate and bottom withdrawn from the column is 37.50 kmol/hr and 62.495 kmol/hr respectively.

Hysys simulation carried out for the design of distillation column shows that a sieve tray of 1m section diameter was used. The column has a section height of 4.3m and cross-sectional area of 0.79 m^2 . The design shows that there is no flooding in the column.

The cost estimation was carried out using Hysys spreadsheet. The cost index used is the chemical engineering cost index of 2006. The estimation shows that the bare module cost s of the tower and the sieve trays are one hundred and fifty-four million one hundred and eighty thousand naira (¥154,180,000) and twelve million six hundred and twelve thousand naira (\$12,610,000) respectively. The bare module cost of the tower plus the trays is two hundred and five million four hundred thousand naira (N205,400,000). The total utility cost which is dominated by the steam cost is one hundred and fourty three million and five hundred and twenty thousand naira (¥143, 520,000). The bare module cost of the condenser and the reboiler are nineteen million eight hundred and ninety thousand naira (N19, 890,000) and nine million nine hundred and nineteen thousand naira ($\frac{199,919,0000}{190,0000}$) respectively. The bare module cost of the accumulator is (149, 919, 0000). The cost estimation of the column shows that the total bare module cost of the tower, trays, condenser, reboiler and reflux accumulator at 2006 Chemical Engineering index is two hundred and seventy eight million nine hundred and eighty thousand naira (N 278,980,000). The total utility cost (condenser, cooling water, and reboiler steam) from above is one hundred and fourty three million five hundred and twenty thousand naira (\mathbb{N} 143,520,000/yr). The annualized cost is one hundred and ninety nine million two hundred and ninety thousand naira (N 199,290,000).

CHAPTER FIVE

5.0 Conclusions and Recommendations

5.1 Conclusions

The following conclusions may be drawn from the results of the analysis.

- Graph based CAD module for binary distillation column gave a better parametric studies of the distillation column design than manual CAD module for binary distillation column.
- The design column has a sieve tray of 1m section diameter, column section height of
 4.3m and cross sectional area of 0.79 m².
- The cost estimation of the column shows that the total bare module cost of the tower, trays, condenser, reboiler and reflux accumulator is two hundred and seventy eight million nine hundred and eighty thousand naira (N 278,980,000).
- 4 The total utility cost is one hundred and fourty three million five hundred and twenty thousand naira (N 143,520,000/yr).

5.2 Recommendations

Based on the analysis carried out the followings have been recommended:

- The binary distillation column optimization should be carried out using Hysys optimizer.
- 2. The graph based distillation design of binary distillation column should be carried out using components that form an azeotrope at higher purity.

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TEAM LND Calgary, Alberta CANADA

Case Name: C:\Program Files\Hyprotech\HYSYS 3.1\Cases\Project\Tempt. Vs Op Unit Set: SI Date/Time: Fri Jun 08 18:21:11 2007

		Conne	ctions		
Feed	Condensor Duty	Disti	stillate Reboiler Duty		Bottoms
F	Cduty	· C	D Rduty		В
		Param	ieters		
,		Comp	onent	Mole F	raction
Light Key			Benzene	ene 0.1	
Heavy Key			Toluene		0.1000 *
\$					
P	ressures (kPa)			Reflux Ratios	
Condenser Pressure		91.19 *	External Reflux Ratio		10.00
Reboiler Pressure		101.3 *	Minimum Reflux Ratio		2.795
		User Va	riables		
		Results S	ummary		and the second second
Tray	s / Temperatures			Flows	1
Minimum # of Trays		5.147	Rectify Vapour	(kgmole/h)	412.5
Actual # of Trays		6.343	Rectify Liquid	(kgmole/h)	375.0
Optimal Feed Stage		3.470	Stripping Vapour	(kgmole/h)	312.5
Condenser Temperature	(C)	78.76	Stripping Liquid	(kgmole/h)	375.0
Reboiler Temperature	(C)	105.9	Condenser Duty	(kJ/h)	-1.287e+007
			Reboiler Duty	(kJ/h)	9.368e+006



Case Name: C:\Program Files\Hyprotech\HYSYS 3.1\Cases\Project\Temp. VsRdu Unit Set: SI

Date/Time: Fri Jun 08 18:20:40 2007

		Cor	nne	ctions			
Feed	Condensor	Duty Distillate		llate Re	boiler Duty	Bottoms	
F	Cduty		C	C Rduty		В	
		Pa	ram	neters			
		C	omp	onent	Mole Fraction		
Light Key				Benzene	0.10		
Heavy Key				Toluene		0.1000 •	
Pressures (kPa)				Reflux Ratios			
Condenser Pressure		91.19 *		External Reflux Ratio		10.00 *	
Reboiler Pressure		101	.3 *	Minimum Reflux Ratio		2.795	
		User	· Va	riables			
		Resul	ts S	Summary			
Tray	s / Temperatures				Flows		
Minimum # of Trays		5.14	17	Rectify Vapour	(kgmole/h)	412.5	
Actual # of Trays		6.34	13	Rectify Liquid	(kgmole/h)	375.0	
Optimal Feed Stage		3.47	0	Stripping Vapour	(kgmole/h)	312.5	
Condenser Temperature	(C)	78.7	6	Stripping Liquid	(kgmole/h)	375.0	
Reboiler Temperature	(C)	105	.9	Condenser Duty	(kJ/h)	-1.287e+007	
				Reboiler Duty	(kJ/h)	9.368e+006	



Case Name: C:\Program Files\Hyprotech\HYSYS 3.1\Cases\Project\Pressure Vs 0
Unit Set: SI

Date/Time: Fri Jun 08 18:20:10 2007

		Conne	ctions		
Feed	Condensor Duty	Dist	Distillate Reboiler Duty Bottoms D Rduty B		Bottoms
F	Cduty				В
		Paran	neters		
		Comp	onent	Mole F	raction
nt Key		,	Benzene		0.1000 •
avy Key			Toluene		0.1000 *
P	ressures (kPa)			Reflux Ratios	
ndenser Pressure	Indenser Pressure 91 19 *				10.00 *
boiler Pressure		101.3 *	Minimum Reflux Ratio		1.719
		User Va	iriables		
		Results S	Summary		
Tray	vs / Temperatures			Flows	and the second
nimum # of Trays		5.906	Rectify Vapour	(kgmole/h)	412.5
tual # of Trays		6.790	Rectify Liquid	(kgmole/h)	375.0
timal Feed Stage		3.714	Stripping Vapour	(kgmole/h)	412.5
ondenser Temperature	(C)	78.76	Stripping Liquid	(kgmole/h)	475.0
boiler Temperature	(C)	105.9	Condenser Duty	(kJ/h)	-1.287e+007
			Reboiler Duty	(kJ/h)	1.385e+007



Case Name: C:\Program Files\Hyprotech\HYSYS 3.1\Cases\Project\Molar Flow V: Unit Set: SI

Date/Time: Fri Jun 08 18:19:28 2007

		Conne	ctions			
Feed	Condensor Duty	Disti	Distillate Rel		Bottoms	
F	Cduty	C)	Rduty	В	
		Param	neters			
		Comp	onent	Mole Fraction		
t Key			Benzene	Benzene		
vy Key			Toluene		0.1000 *	
p	ressures (kPa)			Reflux Ratios		
denser Pressure		91.19 *	External Reflux Ratio		10.00 *	
oiler Pressure		101.3 *	Minimum Reflux Ratio		1.719	
		User Va	riables			
		Results S	Summary			
Tray	vs / Temperatures			Flows		
imum # of Trays		5.906	Rectify Vapour	(kgmole/h)	4125	
ual # of Trays		6.790	Rectify Liquid	(kgmole/h)	3750	
timal Feed Stage		3.714	Stripping Vapour	(kgmole/h)	4125	
ndenser Temperature	(C)	78.76	Stripping Liquid	(kgmole/h)	4750	
boiler Temperature	(C)	105.9	Condenser Duty	(kJ/h)	-1.287e+008	
			Reboiler Duty	(kJ/h)	1.385e+008	

n	
DDO	TEAN
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Unit Set:

C:\Program Files\Hyprotech\HYSYS 3.1\Cases\Project\External Reflu

Date/Time: Fri Jun 08 18:18:37 2007

SI

Shortcut Column: T-100

		Conne	ctions		
Feed	Condensor Duty	Disti	Distillate Reboiler Duty		Bottoms
F	Cduty	D		Rduty	В
1		Param	neters		
		Comp	onent	Mole F	raction
Key			Benzene		0.1000
vy Key			Toluene 0.1		
Pi	essures (kPa)			Reflux Ratios	and a second
denser Pressure		91.19 *	9 * External Reflux Ratio		10.00
oiler Pressure		101.3 •	3 • Minimum Reflux Ratio		1.719
		User Va	riables		
		Results S	Summary		
Tray	s / Temperatures			Flows	n aan ar har ah daaraa dahaa ah ay ah daaraa ah iyo
imum # of Trays		5.906	Rectify Vapour	(kgmole/h)	4125
ual # of Trays		6.790	Rectify Liquid	(kgmole/h)	3750
imal Feed Stage		3.714	Stripping Vapour	(kgmole/h)	4125
denser Temperature	(C)	78.76	Stripping Liquid	(kgmole/h)	4750
oiler Temperature	(C)	105.9	Condenser Duty	(kJ/h)	-1.287e+008
			Reboiler Duty	(kJ/h)	1.385e+008

Case Name: