Design and Development of Multicomponent Distillation Design and Simulation Software

by

Anthony Marc Botha

Dissertation submitted in partial fulfilment of

the requirements for the

Bachelor of Engineering (Hons)

(Chemical Engineering)

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CERTIFICATION OF APPROVAL

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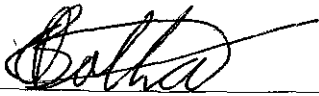(Dr. Mohanad El-Harbawi)
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JUNE 2009

CERTIFICATION OF ORIGINALITY

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

ANTHONY MARC BOTHA

ACKNOWLEDGEMENTS

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CHAPTER 1

INTRODUCTION

Since 2005, there has been a rapid increase in the price of crude oil and the resulting consumer shock at the petrol stations have forced the scientific and engineering communities to re-evaluate and analyze the current crisis.

Energy is the real problem that faces the world, and it will not be solved by the recent biotechnology or nanotechnology trends. Energy consumption is the main producer of carbon dioxide, so it is directly linked with the problem of global warming. Therefore, a thorough evaluation of our energy supply and consumption systems is required. Our inefficient use of energy in all aspects of our modern society must be stopped.

One of the most important technologies in our energy supply system is distillation. Basically, all our transportation fuel goes through at least one distillation column on its way from crude oil to the petrol pump.

Eventually, we will probably switch to renewable sources of energy such as biomass, and the most likely transportation fuel will be methanol. The most probable process to methanol will be the production of synthesis gas (a mixture of hydrogen, carbon monoxide, and carbon dioxide), which is formed by the partial oxidation of biomass, and the subsequent reaction of these components will produce methanol and water. Still, distillation will be utilized for these processes. Distillation is used to separate methanol from water, which is an important part of this process. Furthermore, distillation is used to produce the oxygen used in the partial oxidation reactor.

Therefore distillation is, and will remain in the twenty-first century, the conventional separation method in the chemical and petroleum industries. It is involved in supplying much of our energy needs (Luyben, 2006).

The separation of liquid mixtures by distillation depends on differences in volatility between the components. The greater the relative volatilities, the easier the separation of components. Vapor flows up the column and liquid counter-currently down the column. The vapor and liquid are brought into contact on plates, or packing. Moreover, distillation could either be a batch or a continuous process. Distillation can be categorized according to the number of components to be separated, where binary distillation is the separation if two components and multicomponent separation is the separation of more than two components (Sinnott, 2005).

Components in the unrefined state are of limited value and of limited use to society. Refining is therefore required to produce products that are useful to society. Refining can be defined as a series of steps by which components are converted into saleable products in desired qualities and in the quantities dictated by the market (Priestley, 1973).

1.1 Problem Statement

Develop software capable of performing multicomponent distillation product prediction and column design. This software should be able to save time and improve the accuracy of multicomponent distillation problems. This will ultimately lead to the improvement in multicomponent distillation operation, therefore contributing to the maximization of saleable product yields at lower costs.

1.2 Objectives of the Study

The main objectives of this study are:

i)   Develop a stand alone user-friendly software package using Visual Basic application for multicomponent distillation simulation and design.

ii)   Perform product prediction and the preliminary design of a multicomponent

distillation tower given the relevant operating conditions/variables of the distillation process.

iii) Confirm the validity of the software and verify it by comparing the results from the current software with results from established data, published literature, laboratory, numerical data sets or multicomponent distillation simulation software.

1.3 Scope of Study

- The Fenske, Underwood and Gilliland calculations are used for the product prediction and preliminary design of the distillation columns. The equations and methods of solving them will be obtained from Chemical Process Design and Integration by R. Smith.

- Visual Basic is the programming language which will be used to design and develop the simulation software. Visual basic enables the user to apply programming skills, and creative interface design, to develop a useful product. Therefore, basic programming skills are a prerequisite to using Visual Basic.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

The objective of distillation is to separate compounds that have different vapor pressures at any given temperature. In other words, distillation is the physical separation of a mixture into two or more product fractions that have different boiling points. The larger the relative volatilities, the easier the separation.

Vapor will flow up the column and liquid will flow counter-currently down the column. The vapor and liquid come into contact on plates, or packing. A fraction of the condensate from the condenser is returned to the top of the column to provide liquid flow above the feed point, this is known as reflux, and some of the liquid from the bottom of the column is vaporized in the reboiler and returned to the tower to provide the vapor flow (Sinnott, 2005).

If a mixture containing two volatile materials is heated, then the vapor that is produced will have a higher concentration of the lower boiling point material from the liquid. However, if a vapor mixture is cooled, the higher boiling point component will condense faster than the lower boiling point material. Distillers that produce alcohol used to apply these principles in the early days. Commercially, distillation was developed and practiced by Coffey in 1832. Later, in 1893, the theoretical functioning of distillation was studied by Sorel, Lord Rayleigh and Lewis followed by making theoretical advances in this field. Modern day technology has enabled large scale separations of components with very similar properties, such as benzene and xylene separation (Holland, 1997).

2.2 Structure of Distillation Towers

2.2.1 Columns

Distillation columns (distillation towers) are made up of several components, each of which is used either to transfer heat energy or promote mass transfer. A typical distillation column consists of the following major parts:

1. Vertical shell where separation of the components is carried out.

2. Column internals such as trays, plates, or packing that are used to enhance component separation.

3. Reboiler to provide the necessary vaporization for the distillation process.

4. Condenser to cool and condense the vapor leaving the top of the column.

5. Reflux drum to hold the condensed vapor from the top of the column, so that liquid (reflux) can be recycled back to the column.

Basically, a vessel, with column internals together with a condenser and reboiler makes up a distillation column.
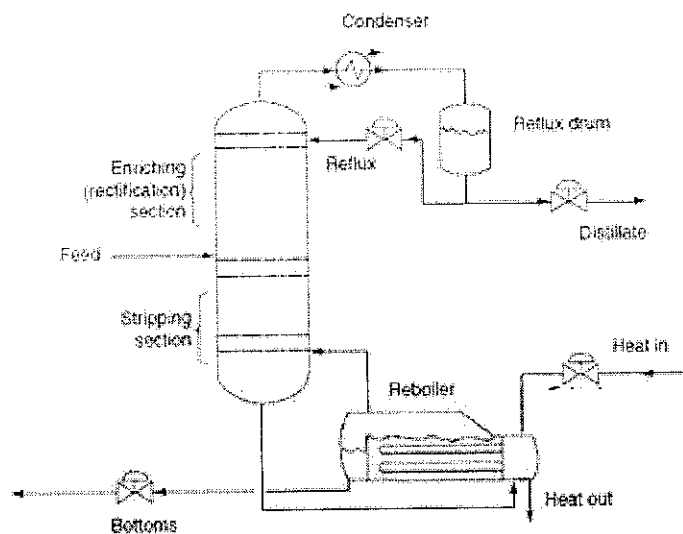
Figure 2. 1: Components of Distillation Tower

2.2.2 Packing

The packing in a distillation column creates a surface for the liquid to spread on, therefore providing a high surface area for mass transfer between the liquid and the vapor (Speight, 2006).

2.2.3 Trays

Usually, trays are horizontal, flat, specially pre fabricated metal sheets, which are placed at a regular distance in a vertical cylindrical column. Trays have two main parts:

1. Contacting area, which is the area where vapor and liquid are contacted.
2. The down comer area, thus the area where vapor and liquid are separated after they come into contact.

Classification of trays is based on:

1. The type of plate used in the contacting area.
2. The type and number of downcomers making up the downcomer area.
3. The direction and path of the liquid flowing across the contacting area of the tray.
4. The vapor flow direction through the holes in the plate.
5. If baffles, packing or anything else is used to improve the separation performance of the tray.

Common plate types are as follows:

1. Bubble cap tray- This tray has caps mounted over risers fixed on the plate (Figure2.2). The caps come in a wide variety of sizes and shapes (round, square, and rectangular).

2. Sieve trays-This tray can be found with different hole shapes (round, square, triangular, rectangular, star), various hole sizes (from about 2 to 25 mm) and a number of punch patterns (triangular, square, rectangular).

3. Valve tray-This tray has a number of valve shapes (round, square, rectangular, triangular), valve sizes, valve weights (light and heavy), orifice sizes and the valves can either be fixed or floating.

Trays usually have one or more downcomers. The type and number of downcomers used depends on the downcomer area required to handle the liquid flow.

Single pass trays are trays with one downcomer, delivering the liquid from the next higher tray, to contact the vapor and one downcomer for the liquid to the next lower tray. Trays with multiple downcomers, have multiple liquid passes and can have a number of layout geometries. The downcomers may be rotated 90 degrees on successive trays. The downcomer layout pattern determines the liquid flow path arrangement and liquid flow direction in the contacting area of the trays.

The most important parameter of a tray is its separation performance. Four factors are of importance in the design and operation of a tray-column:

1. The level of tray efficiency in the normal operating range.
2. The vapor rate at the upper limit (which is the maximum vapor load).
3. The vapor rate at the lower limit (which is the minimum vapor load).
4. The tray pressure drop.

The separation performance of a tray ultimately determines the performance of a column as a whole.

It is evident that tray efficiency is influenced by:

1. The type of components being separated (this generally applies to multicomponent. systems in which the efficiency can be different for each

component, because of different diffusivities, diffusion interactions, and different stripping factors).

2. The vapor flow rate- usually increasing the vapor flow rate increases the effective mass transfer rate, while at the same time it decreases the contact time. These counteracting effects lead to a roughly constant efficiency value for a tray in its normal operating range. Upon approaching the lower operating limit, a tray starts weeping and loses efficiency (Speight, 2006).
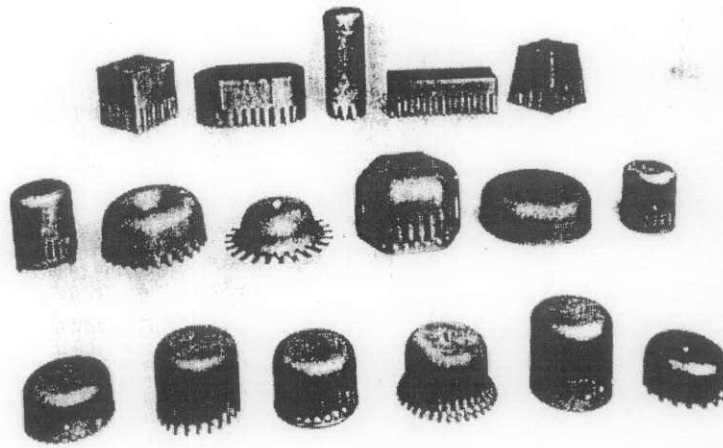
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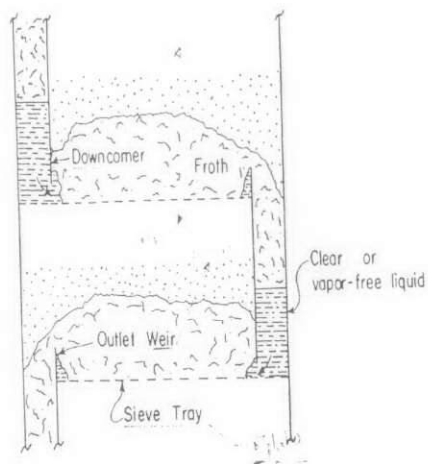
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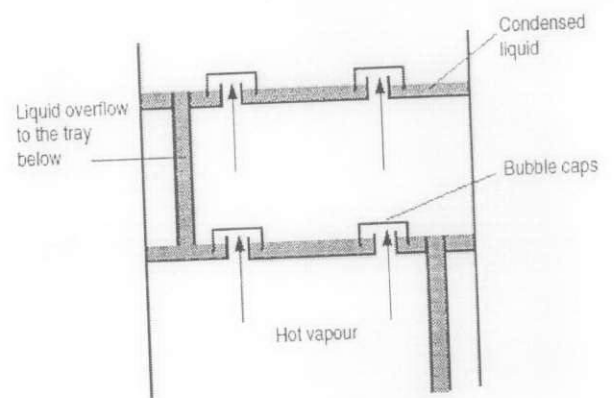
Developed by: Anthony Marc Botha

2.3 Operating Variables

2.3.1 Reflux considerations

The reflux ratio, $R = \dfrac{\text{flowrate of liquid returned as reflux}}{\text{flowrate of top product taken off}}$

The reflux ratio can be utilized to determine the number of stages which will be required for the separation. Typically, the reflux ratio will increase as the vapor condensed increases due to heat loss. With a well-insulated column, the heat loss will be small and therefore the reflux flowrate increase is taken as negligible. If a column is not insulated properly, changes in the internal reflux due to sudden changes in external conditions, such as snow, can have an effect on the column operation and control (Sinnott, 2005).

2.3.2 Total reflux

This condition occurs when all the condensate produced from the top condenser is returned to the column as reflux. Therefore, no product is taken off and there is no feed. At the total reflux condition, the minimum number of stages needed for a separation (which is theoretically possible) can be determined. Although, this is not a practical operating condition, it is a useful method to determine the approximate number of stages that will be needed for a given separation. The towers are often started up with no product draw-off and operated at total reflux until steady conditions are reached (Sinnott, 2005).

2.3.3 Minimum reflux

As the reflux ratio becomes less, a pinch point occurs where the separation can only be achieved with an infinite number of stages. This is the minimum possible reflux ratio for a given separation (Sinnott, 2005).

2.3.4 Optimum reflux ratio

Realistic reflux ratios will be within the range of the minimum and total reflux. The optimal reflux ratio is where the minimum cost for a specific separation is achieved. Increasing the reflux ratio reduces the number of stages required of the column, and the capital cost, but increases the operating costs of the system. The optimum reflux ratio is the ratio that gives the lowest operating cost. Typically, the optimum reflux ratio will lie between 1.2 to 1.5 times the minimum reflux ratio. For new designs (where the ratio cannot be decided) the effect of reflux ratio on the number of stages can be determined using the short-cut design methods which will be discussed later in the report.

At low reflux ratios, the calculated number of stages is strongly dependent on the accuracy of the vapor-liquid equilibrium data available (Sinnott, 2005).

2.3.5 Feed-point location

The location of the feed point affects the number of stages needed for a separation. Generally, the feed should enter the tower at the point where the best match between the feed composition and the vapor and liquid streams in the column can be found. It is wise to provide multiple feed-point nozzles around the calculated feed point, to allow for uncertainties in the design calculations and data, and any possible changes in the feed composition that could occur (Sinnott, 2005).

2.3.6 Selection of column pressure

Other than when heat-sensitive materials are involved, the main consideration when selecting the column operating-pressure is to ensure that the dew point of the distillate is above the dew point that can be easily obtained with the cooling water. The maximum temperature of cooling water is typically 30 ^{0}C. This means that if high pressures will be required, refrigerated brine cooling can be used. When distilling heat-sensitive materials, vacuum operation is used to reduce the column temperatures.

Generally, when performing calculations to determine the stage and reflux requirements, the column operating pressure is taken as constant throughout the column. However, in vacuum distillation, the column pressure drop is a large fraction of the total pressure and a change in pressure moving up the column should be allowed for the calculation of stage temperatures. This could possibly require a trial and error calculation, since the pressure drop cannot be determined, before the number of stages are approximated (Sinnott, 2005).

2.4 Distillation Simulation

Simulation can be used to predict the effect of changing operating conditions. This can be used to optimize operation quickly and safely. Simulation methods come in two types, namely, digital and analogue simulation. Of these two types, digital simulation (which involves the use of code and programme) is commonly used since they can be implemented on modern computers with exceptional speed and accuracy (Koutitas, 1988; Alhassan and Jimoh, 2006).

The analysis, design, operation, control, and optimization of distillation columns have been studied for almost a century. Until the invention of computers, hand calculations and graphical methods were developed and widely used in these studies. Since about 1950, analog and digital computer simulations have been used to solve many engineering problems. Distillation analysis involves iterative vapor–liquid phase equilibrium calculations and tray-to-tray component balances, which are ideal for digital computation.

Initially most engineers wrote their own programs to solve both the nonlinear algebraic equations that describe the steady-state operation of a distillation column and the nonlinear ordinary differential equations that describe its dynamic behavior. Commercial steady-state simulators took over around the mid-1980s and now dominate the field. Commercial dynamic simulators were developed a bit later. In today's day and age, both steady-state and dynamic simulations of distillation columns are widely used in industry and in universities.

There are three steps in developing a process design. The steps are follows:

i.   Conceptual design- Simple approximate methods are used to develop a preliminary flowsheet.

ii. Preliminary design- Rigorous simulation methods are used to evaluate both steady-state and dynamic performance of the proposed flowsheet.

iii. Detailed design-Hardware is specified in great detail, with specifics such as types of trays, number of sieve tray holes, feed and reflux piping, pumps, heat exchanger areas, and valve sizes.

2.5 Published Distillation Simulation

There are a number of people and companies that have developed distillation simulation software. This section of the report will highlight some distillation software (although, the software might not be multicomponent distillation) that has been developed.

Harry Kooijman (Shell Global Solutions International BV, Amsterdam) and Ross Taylor (Kodak Distinguished Professor, Dept. of Chemical Engineering, Clarkson University, USA) developed ChemSep, a software system for simulation of distillation, absorption, and extraction operations. This software is capable of handling flash calculations, equilibrium stage column model and non-equilibrium (rate-based) column models. ChemSep is diverse in allowing you to simulate any problem and export the results in a variety of formats. In the non-equilibrium mode ChemSep provides a large number of mass transfer correlations and flow models, liquid-liquid extraction and three phase distillation.

On the January 8th, 1996, Krzysztof Alejski and Francoise Duprat (from the Institute of Chemical Technology and Engineering, Poznan University of Technology, Poland), designed a dynamic mathematical model of multicomponent reactive distillation in case of kinetically controlled chemical reactions. The accuracy of the dynamic simulation results is verified by comparing the results with results of actual experiments on a pilot-

scale distillation column. The observed differences in the results are from the simplification of the mathematical model and the inaccuracy of the kinetic & vapor-liquid equilibrium description data for highly nonideal multicomponent systems.

Moreover, in 1996, T. S. Cantos, J. Moshi, D. Willcox and J. K. Floess developed a discrete relaxation method for solving multicomponent distillation problems. This is a computational method which is used to solve multi-component distillation problems. The method solves for the composition profiles of a column under steady state conditions. This is determined by using the Rachford-Rice equation, to solve stage by stage, the vapor-liquid equilibrium problem. This equation is applied at each stage until the column temperature profile converges to the steady state solution. The advantage of this method is that it is relatively easy to conceptualize and it is easy to program.

Microchannel technology developed by M. Fanelli of the Battelle Memorial Institute has being applied in simulating a microchannel distillation process. The results of this simulation model were validated with experimental data. The simulation software serves optimize and refine the design of multiphase mircochannel processes. Research in this field has been conducted since the year 2000.

Lastly, a design method, based on the quasi-binary method, to simplify the design process of multicomponent distillation was developed by Wu Lianying, Hu Yangdong and Wen Ya (College of Chemistry and Chemical Engineering, Ocean University of China, Qingdac, China) (published 1 December, 2006). The software integrator method used with Visual C++ language and it has the capability to determine the minimum reflux ratio (R_{min}), the liquid-vapor ratio $\left(\dfrac{L}{V}\right)_{min}$, and the minimum numbers of stage

(N_{min}).

CHAPTER 3

METHODOLOGY

3.1 Introduction

This chapter will focus on the development of the multicomponent distillation design and simulation software (MDDSS). There are many types of software produced in the market but not all software is suitable for use, due to the fact that environments (PC environments) differ, software differs and prices are high. Therefore, the aim of this study is to develop a stand alone user-friendly software package using Visual Basic to simulate multicomponent distillation and to estimate the product process variables (composition, flowrate) and the preliminary design of the column such as height, number of stages, feed point entry, diameter of the column and reflux ratio given the feed and distillation operating conditions.

The methodology of this project is divided into two sections.
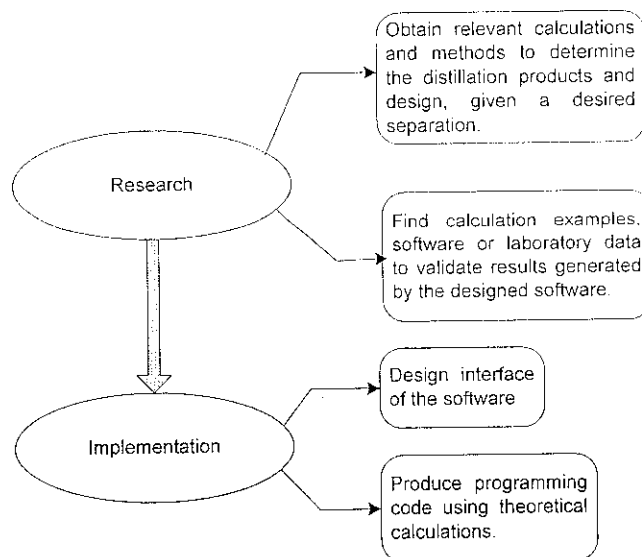
Figure 3. 1: Proposed methodology to complete the project

3.2 Multicomponent Distillation Equations

Main Reference: Chemical Process Design and Integration, Robin Smith, 2005

(See Appendix A for Sample Calculation)

All equations were taken from the main reference above, unless otherwise stated.

In multicomponent distillation, one must establish the two key components between which it is desired to make the separation.

For example: Consider 6 components in descending order of relative volatility. The objective of the separation is to recover C at the overhead product by certain % together with D at the bottom product by certain %.
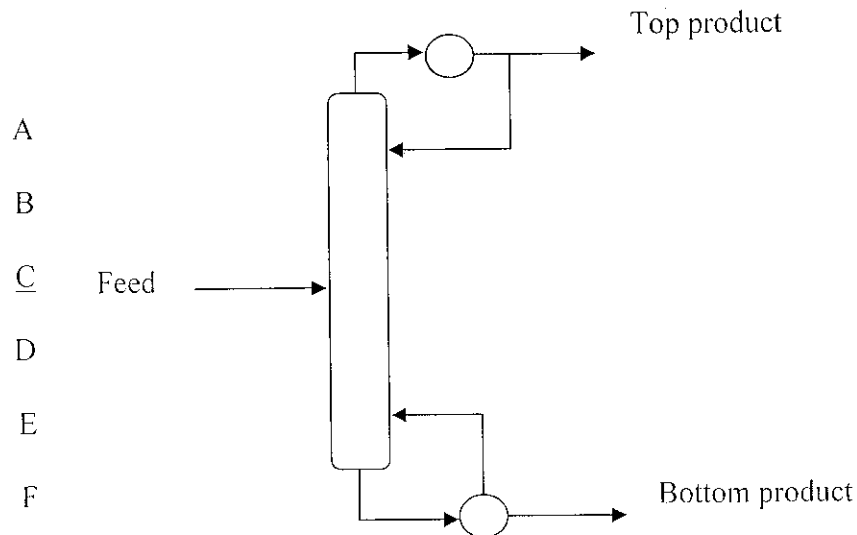
Figure 3. 2: Multicomponent distillation with C as the LK (recovered in top product) and D as the HK (recovered in bottom product) components.

- o component C as LIGHT KEY (LK) – a component that must be kept out of the bottom product according to the specification

- o component D as HEAVY KEY (HK) – a component that must be kept out of the top product according to the specification
- o components A,B as Non-Keys, or specifically: Lighter than Light Key (LLK). A component that tends to go predominantly with the top product
- o components E,F as Non-Keys, or specifically: Heavier than Heavy Key (HHK).A component that tends to go predominantly with the bottom product

The shortcut method equations (Fenske, Underwood, Gilliland) for distillation tower preliminary design will be the utilized. The equations are as follows:

3.2.1 Fenske Equation

The Fenske Equation (1) below, solves for the minimum number of stages of a distillation process given the recovery and relative volatility of the light and heavy keys. This equation is based on total reflux conditions.

Assumptions: -Component Distributions do not depend on reflux ratio

-Relative Volatility is constant

-Pressure drop through the column is neglected

-Constant molar overflow

$$N_{min} = \frac{\ln\left(\frac{r_{L,D}}{1-r_{L,D}} \cdot \frac{r_{H,B}}{1-r_{H,B}}\right)}{\ln\alpha_{L,H}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

Where,

$r_{L,D}$ = recovery of LK comp in the distillate

$r_{H,B}$ = recovery of HK comp in the bottom

$\alpha_{L,H}$ = relative volatility between LK and HK

N_{min} = minimum number of theoretical stages

The Fenske equation can also be used to estimate the composition of the product streams by,

$$\log\left[\frac{d_i}{b_i}\right] = N_{min} \log \alpha_{ij} + \log\left[\frac{d_j}{b_j}\right] \quad \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2)$$

Where,

d_i = molar distillate flow for component i

d_j = molar distillate flow for component j

b_i = molar bottom flow for component i

b_j = molar bottom flow for component j

α_{ij} = relative volatility between comp i and j

N_{min} = minimum number of theoretical stages

Equation (2) demonstrates that a $\left[\frac{d_i}{b_i}\right]$ vs. $\log\alpha_{ij}$ plot will be a straight line, with N_{min} as the gradient. This therefore allows the compositions of the nonkey components to be estimated. Therefore, by specifying the distribution of the light and heavy components and knowing the relative volatilities of the non key components will enable their compositions to be determined by combining equation (2) with the overall component balance:

$$f_i = d_i + b_i \quad \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (3)$$

Where,

f_i = component i in the feed

d_i = component i in the distillate or top product

b_i = component I in the bottom product

From the combination of equations, more convenient equations are obtained in order to determine the product compositions.

$$d_i = \frac{\alpha_{ij}^{N_{min}} f_i \left(\dfrac{d_j}{b_j} \right)}{1 + \alpha_{ij}^{N_{min}} \left(\dfrac{d_j}{b_j} \right)} \qquad \ldots\ldots\ldots\ldots\ldots\ldots (4)$$

$$b_i = \frac{f_i}{1 + \alpha_{ij}^{N_{min}} \left(\dfrac{d_j}{b_j} \right)} \qquad \ldots\ldots\ldots\ldots\ldots\ldots (5)$$

The relative volatility can be calculated using the feed condition, however, this might be valid throughout the column. Typically, the relative volatility varies as you move along the distillation column, hence an average needs to be determined. Calculations should be conducted using the average temperature of the tower. In order to determine the average relative volatility, assume that $\ln P_i^{SAT}$ changes with $\dfrac{1}{T}$ in a linear manner.

If this is the case, then the two key components should both change in a linear manner, and therefore the difference $\left(\ln P_i^{SAT} - \ln P_j^{SAT} \right)$ also changes as $1/T$ changes, which means $\ln \left(\dfrac{P_i^{SAT}}{P_j^{SAT}} \right)$ changes as $\dfrac{1}{T}$ does. Assuming that Raoult's Law is applicable (meaning that the solution behaves ideally), then the relative volatility α_{ij}

is the ratio of the saturated vapor pressures $\left(\dfrac{P_i^{SAT}}{P_j^{SAT}}\right)$. Therefore, $\ln \alpha_{ij}$ changes as $\dfrac{1}{T}$

does .Therefore, the average temperature in the column is:

$$T_{mean} = \frac{1}{2}\left(T_{top} + T_{bottom}\right) \qquad \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots(6)$$

Moreover, by assuming that $\ln \alpha_{ij}$ is proportional to $\dfrac{1}{T}$, the following equation to

determine the average relative volatility is obtained.

$$\left(\alpha_{ij}\right)_{mean} = \exp\left[\frac{2\ln\left(\alpha_{ij}\right)_{top}\ln\left(\alpha_{ij}\right)_{bottom}}{\ln\left(\alpha_{ij}\right)_{top} + \ln\left(\alpha_{ij}\right)_{bottom}}\right] \qquad \dots\dots\dots\dots\dots\dots\dots (7)$$

The less ideal the behavior of a mixture to separate (it does not obey Raoult's Law); the more difficult it will be to predict the properties of the mixture and components to be separated. Moreover, the larger the change of relative volatility is as you move across the column, the larger the error would be when utilizing the averaging equation 7. A more accurate relative volatility can be determined by the use of iteration. First calculate the relative volatility using the feed conditions. Thereafter, the Fenske equation can be used to determine the product compositions. The average relative volatility is then estimated using the top and bottom products. However, the calculated relative volatility will result in new estimates of the product compositions, and therefore the calculation should iterate to convergence. The accuracy of the approximations strongly depends on the ideality of the mixture. Typically, the less ideal the mixture, the greater the error.

3.2.2 Underwood equations

Assumptions
- All of the lighter than light key components go to the overheads.
- All of the heavier than heavy key components go to the column bottoms.

- If the light and heavy key components are adjacent in volatility, there are no components between the keys.

- Constant molar overflow

- Constant relative volatility

The Underwood Equations can be used to determine the minimum reflux for multicomponent distillation. The first Underwood equation is as follows:

$$\sum_{i=1}^{NC} \frac{\alpha_{ij} \cdot x_{i,F}}{\alpha_{ij} - \theta} = 1 - q \qquad \dots\dots\dots\dots\dots (8)$$

Where:

$x_{i,F}$ = mole fraction of component i in the feed

θ = root of equation

q = feed condition = $\dfrac{\text{heat required to vaporize one mole of feed}}{\text{molar latent heat of vaporization of feed}}$

= 1 for a saturated liquid feed, 0 for a saturated vapor feed

NC = number of components

The objective when solving the equation 8 is to find the positive roots, θ and each of these roots lies between the $\alpha's$ of the components. Start by first assuming a feed condition in order to obtain a fixed q value. Saturated liquid feed (i.e. = 1) is a conventional assumption in an initial design as it decreases the minimum reflux ratio as opposed to a vaporized feed. Moreover, liquid feeds are preferred because the operating pressure can easily be increased by merely pumping the liquid to a higher pressure. In contrast, increasing the pressure of a vapor feed more expensive since a compressor. Having a subcooled liquid or a superheated vapor results in an inefficient separation, since the feed must first return to saturated conditions in order for the distillation process to occur. Equation (8) refers to all the components of the feed and the values of θ should be determined.

The second Underwood Equation

$$R_{min} + 1 = \sum_{i=1}^{NC} \frac{\alpha_{ij} \cdot x_{i,D}}{\alpha_{ij} - \theta} \qquad \dots\dots\dots\dots\dots\dots\dots (9)$$

Where,

$x_{i,D}$ = mole fraction of component i in the distillate (unknown)

R_{min} = minimum reflux ratio (unknown)

In order to solve for the equation, the values of α_{ij}, θ and $x_{i,D}$ should be known. However, the values of $x_{i,D}$ for each component in the distillate (at minimum reflux) are unknown. Therefore, Equation (9) above should be written (NC-1) times to solve simultaneously for R_{min} and (NC-2) values for $x_{i,D}$ (nonkey).Thereafter, and the two equations can be solved simultaneously. This equation (9) can not only be utilized to solve for R_{min}, but it can be used to determine the distribution of nonkey components at the minimum reflux conditions given the key component separation. This is similar to the Fenske Equation which is used to determine the component distribution at total reflux. The true component distribution is most likely to be between the estimate at minimum reflux and the estimate at total reflux.

By making the assumptions stated at the beginning of this section regarding the component distribution to approximate $x_{i,D}$, the calculation can be simplified. By making these assumptions, equation 8 can be solved using trial and error for the single value of θ (which should lie between the relative volatilities of the key components). This value of θ can then be used in Equation (9) to-solve for R_{min}, since all $x_{i,D}$ are known.

By maintaining the assumptions that the Underwood equation is based on, then for separations where the light and heavy key components to be separated are not

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adjacent in volatility, then one more value of θ is required than there are components between the keys (therefore if there is one component between the LK and HK in terms of relative volatility, then 2 values of θ should be calculated for). This will result in the $x_{i,D}$ of the components between the keys being unknown. After the θ values have been solved for, Equation (9) is used for each value of θ by having $x_{i,D}$ of the components between the keys as unknowns. Thereafter, R_{min} and $x_{i,D}$ are solved for each components between the keys using the equations which are solved simultaneously. In order to simplify matters even further, the Fenske equation can be used to calculate $x_{i,D}$. However, these values of $x_{i,D}$ will be for total reflux rather than minimum reflux.

3.2.3 Gilliland Equation

After utilizing the Fenske Equation to determine the minimum number of stages and the Underwood Equations to determine the minimum reflux ratio, the Gilliland equation can be utilized to calculate the number of stages (theoretical).

Assumptions:

- Constant molar overflow
- Constant relative volatility

$$Y = 0.2788 - 1.3154 \cdot X + 0.4114 \cdot X^{0.2910} + 0.8268 \cdot \ln X + 0.9020 \cdot \ln\left(X + \frac{1}{X}\right) \dots (10)$$

Where:

$$Y = \frac{N - N_{min}}{N + 1}, X = \frac{R - R_{min}}{R + 1}$$

A correlation between R and R_{min} should be available, if not assume that R= 1.5 R_{min}

3.2.4 Plate efficiency

The O'Connell relationship is used to calculate actual number of stages of the column using the theoretical number of stages which was calculated using the Gilliland correlation. It is most probable, that the actual number of stages required in the tower will be larger than the number of theoretical stages, since mass transfer can't be 100%, which will prevent perfect equilibrium from being obtained on each tray.

$$E_o = 0.542 - 0.285 \cdot \ln(\alpha_{LH} \cdot \mu_L) \qquad \text{.............................. (11)}$$

Where:

E_o = overall stage efficiency ($0 < E_o < 1$, typically between 0.7 and 0.9)

α_{LH} = relative volatility between the key components

μ_L = viscosity (mN.s/m^2 = cP) of the feed at average column condition

Equation (11) has some limitations, which are:

- This equation is inaccurate for distillation trays with a long flow path across the active plate area; the overall efficiency is usually higher than the calculated value.
- The equation should only be used for preliminary design to estimate the actual number of distillation trays. This is since the stage efficiency usually differs with the type of mixtures to be separated, and in order to perform more accurate calculations, information on tray type, geometry, and physical properties of the fluids should be utilized.
- Typically, the number of trays is increased by 5 to 10% to allow for the design uncertainties.

Thereafter by dividing $N_{theoretical}$ by E_o, N_{actual} is obtained:

$$N_{act} = \frac{N}{E_o}$$

$$\dots\dots\dots\dots\dots\dots\dots\dots (12)$$

Where,

N_{act} = actual number of trays

N = theoretical number of trays from Fenske, Underwood, Gilliland Equations

3.2.5 Feed-point location

This equation was taken from (Sinnott, 2005). An empirical equation given by Kirkbride, (1944) can be used to determine the feed-point location:

$$\log\left[\frac{N_r}{N_s}\right] = 0.206\log\left[\left(\frac{B}{D}\right)\left(\frac{x_{f,HK}}{x_{f,LK}}\right)\left(\frac{x_{b,LK}}{x_{d,HK}}\right)^2\right] \quad \dots\dots\dots\dots\dots\dots (13)$$

Where,

N_r = number of stages above the feed, including any partial condenser.

N_s = number of stages below the feed, including the reboiler.

B = molar flow bottom product.

D = molar flow top product.

$x_{f,HK}$ = concentration of the heavy key in the feed.

$x_{f,LK}$ = concentration of the light key in the feed.

$x_{b,LK}$ = concentration of the heavy key in the top product.

$x_{d,HK}$ = concentration of the light key if in the bottom product.

3.2.6 Height of the Column

A general equation to estimate the height of the column is as follows:

Column Height = (Actual number of trays × tray spacing) + 1 or 2 m for top and

bottom liquid and vapor disengagement ....(14)

- Tray spacing is typically taken as 0.45m or as 0.6m.
- There is a maximum height for a column, which is 100m; however it could be smaller for really extreme conditions. If the maximum height is exceeded, then the column must be split into multiple shells. A column must be designed to mechanically withstand the wind loads that it is exposed to. The maximum height decided for the column will depend on the local weather conditions (such as tornados, hurricanes and typhoons).
- For taller columns, to decrease the column height the tray spacing is decreased (practically, the minimum tray spacing 0.35 m).

3.2.7 Diameter of the Column

An operating condition which will influence the diameter of a column is the flood point. The floodpoint is a limit to any distillation operation; therefore it can decrease the separation efficiency. A floodpoint will occur when the liquid can no longer flow down the column in order to allow for the efficient operation of the column due to the relative vapor and liquid flowrates in the column.

Liquid 'entrained' upwards instead of flowing downwards

High vapor velocity
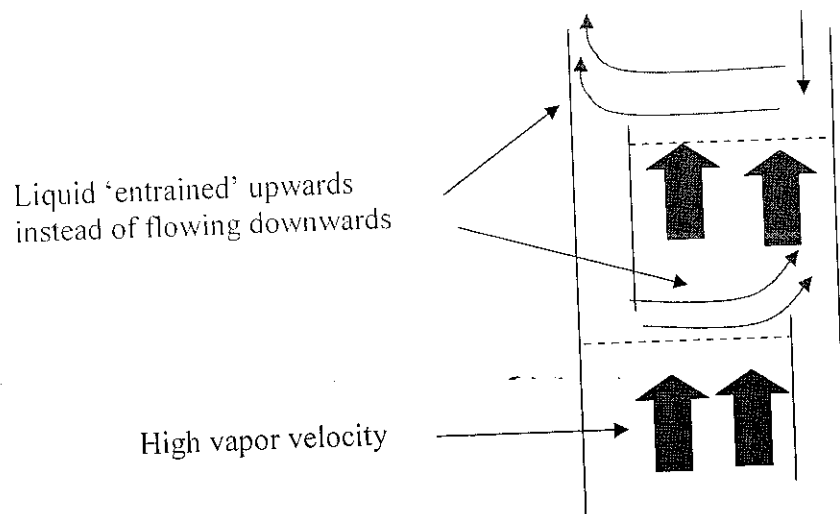
Figure 3. 3: Floodpoint operating condition

A floodpoint can occur due to one the following conditions:

- excessive liquid entrainment (high vapor velocity)
- downcomer unable to allow the liquid to flow at the required flowrate

3.2.7.1 Diameter Calculation Equation

The diameter of a column is calculated from the equation below. The terms below are explained, and the equations on how to obtain these terms will be elaborated on further in the report.

$$D = \left(\frac{4 M_V \cdot V}{0.9 \cdot \pi \cdot \rho_V \cdot 0.8 . v_T} \right)^{0.5} \quad \dots\dots\dots\dots\dots\dots (15)$$

Where,

v_T = vapor flooding velocity (must calculate, see equation 16 below)

0.9 = Due to 10% allowance for downcomer area (an approximation)

0.8 = Vapor velocity is 80% of the flooding velocity (an approximation)

V = Vapor molar flowrate (kmol/s) (Calculate by doing a mass balance, equation (3))

M_V = vapor molar mass (kg/kmol) (Given)

ρ_V = vapor density (kg/m^3) (Given)

3.2.7.2 Vapor flooding velocity

Assuming a 90% foaming factor, the vapor flooding velocity can be determined by Equation (16).

$$v_T = 0.9 \cdot K_T \left(\frac{\rho_L - \rho_V}{\rho_V} \right)^{0.5} \quad \dots\dots\dots\dots\dots\dots (16)$$

Where,

ρ_V = vapor density (kg/m^3) (Given)

ρ_L = liquid density (kg/m^3) (Given)

K_T = parameter for terminal velocity (m/s) (must calculate, see
   equation (17) below)

0.9 = Assuming a 90% foaming factor (an approximation), since the
   system might be exposed to foaming. Typical values of the
   foaming factor are as follows:

   • Distillation involving light gases typically 0.8 to 0.9
   • Crude oil distillation typically 0.85

3.2.7.3 Parameter for terminal velocity

Use the Fair correlation to find the parameter for terminal velocity (m/s)

$$K_T = \left(\frac{\sigma}{20}\right)^{0.2} \exp\left[\begin{array}{l} -2.979 - 0.717\ln F_{LV} - 0.0865(\ln F_{LV})^2 + 0.997\ln H_T \\ -0.07973\ln F_{LV} \cdot \ln H_T + 0.256(\ln H_T)^2 \end{array}\right] \quad (17)$$

Where,

   K_T = Parameter for terminal velocity (m/s)

   σ = surface tension (mN/m= mJ/m^2= dyne/cm)

   H_T = tray spacing (m), typically it is 0.25 m $<$ H_T $<$ 0.6 m, but
      assume 0.45m for preliminary design

   F_{LV} = liquid–vapor flow parameter (dimensionless) (must calculate,
      see equation (18) below)

In some text, the following Fair correlation diagram is used:
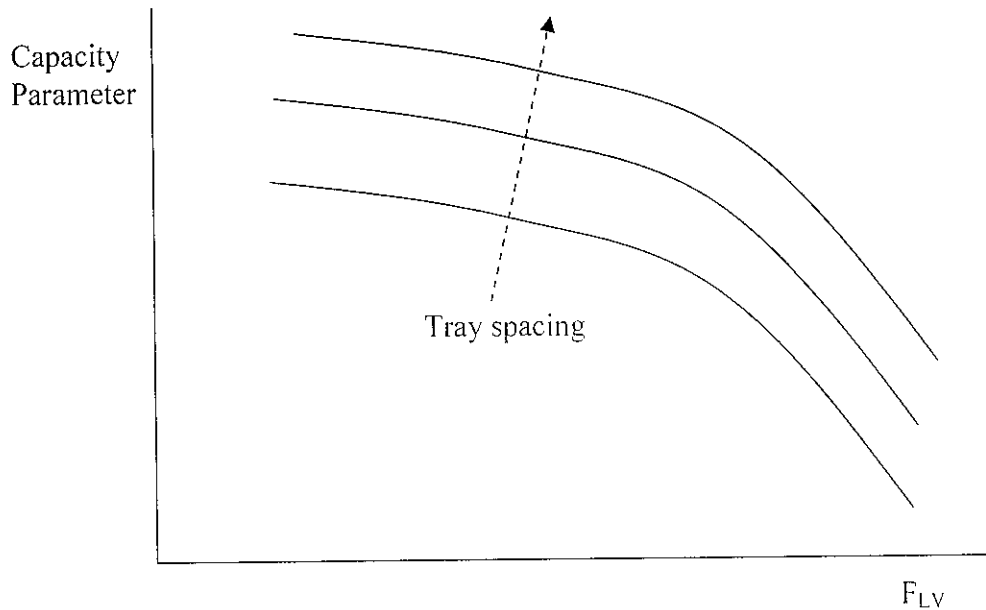
Figure 3. 4: Fair correlation diagram which is used to determine the parameter for terminal velocity

3.2.7.3 Liquid-vapor flow parameter

The liquid-vapor flow parameter is directly correlated with the column's operating pressure. Low values of this parameter are generally due to vacuum distillation, and high values of this parameter indicate a high pressure distillation. This parameter can be used to determine if packing or trays should be used as internals for the column. If the parameter is smaller than 0.1, then packing is preferred, if it is greater than 0.1, then trays are recommended as the internals for the distillation process. The equation of the liquid-vapor flow parameter is given by Equation (18).

$$F_{LV} = \left(\frac{M_L \cdot L}{M_V \cdot V} \right)\left(\frac{\rho_V}{\rho_L} \right)^{0.5} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (18)$$

Where,

L = liquid molar flowrate (kmol/s)

V = vapor molar flowrate (kmol/s)

M_L = liquid molar mass (kg/kmol)

M_V = vapor molar mass (kg/kmol)

ρ_V = vapor density (kg/m^3)

ρ_L = liquid density (kg/m^3)

3.3 Software Design Using Visual Basic

The Multicomponent Distillation Design and Simulation Software (MDDSS) design is divided into two stages. First the product prediction (stage 1) programming was completed and thereafter, the column design programming (stage 2) was done. The input and output variables for each stage will be explained below.

3.3.1 Stage 1 – Product Prediction

The programming for this stage was performed in order to determine the N_{min}, composition of products and R_{min}, by using the Fenske, Underwood and Gilliland equations.

3.3.1.1 Input Variables

The input variables for "Product Prediction" are as follows:

- The feed composition and flowrate.
- The feed condition($0<q<1$)
  -q=1(saturated liquid, recommended)
  -q=0(saturated vapor)

- The components to be separated properties (relative volatilities based on K values (equilibrium constants), therefore operating pressure should be known).
- Select the heavy key (HK) and light key (LK) (check if there any components between the HK and LK based on relative volatility).
- Recovery of the LK in the top product (distillate).
- Recovery of the HK in the bottom product.

3.3.1.2 Output Variables

⚬ The output variables for "Product Prediction" are as follows:

➤ Minimum number of stages.
➤ Composition of overhead and bottom product.
➤ Minimum reflux ratio.

3.3.2 Stage 2 – Column Design

The programming of this stage was done in order to determine the number of stages, feedpoint location, height and diameter of the column.

3.3.2.1 Input Variables

The input variables for "Column Design" are as follows:

o Feed viscosity at average column conditions.
o Enter the R/R_{min} ratio or enter in the reflux (assume R/R_{min} ratio is 1.5 if no data available).
o Tray spacing (typically 0.25m<spacing<0.6m, assume 0.45m if no data available).

o Allowance for downcomer area (typically 5 to 15% of the cross sectional area of the column, assume 10% if no data available).

o Percentage of flooding velocity that is vapor velocity (typically ranges between 70 to 90%, assume 80% if no data available).

o Foaming factor

   • Distillation involving light gases typically 0.8 to 0.9

   (Assume 0.9 if no data available).

   • Crude oil distillation typically 0.85.

o Physical properties of the top and bottoms compositions

   • Molecular Weight of the liquid in the Distillate

   • Molecular Weight of the liquid in the Bottoms

   • Molecular Weight of the vapor in the Distillate

   • Molecular Weight of the vapor in the Bottoms

   • Density of the liquid in the Distillate

   • Density of the liquid in the Bottoms

   • Density of the vapor in the Distillate

   • Density of the vapor in the Bottoms

   • Surface tension of the Distillate

   • Surface tension of the bottoms

3.3.2.2 Output Variables

The output variables for "Column Design" are as follows:

➤ Theoretical number of stages (trays) needed assuming a total condenser.

➤ Stage (Tray) efficiency ($0 < E_o < 1$, typically between 0.7 and 0.9).

➤ Actual number of stages (trays) needed (Value is increased by 5 to 10% to allow for design uncertainties).

➤ Height of the column(Check to see if it is taller than 100m)

- it includes the 2 meters consideration for top and bottom liquid and vapor disengagement, which is 4meters.

➢ Feed point location.

➢ Recommended internals (if F_{LV} < 0.1 then packing, else trays can be used).

➢ Diameter of the column based on conditions at the top and bottom of the column.

- The maximum height of packed bed column is normally taken to be 6 m or 10 column diameters, whichever is smaller.

- A top and bottom diameter will be obtained. In conceptual design, it is reasonable to take the largest value. Diameters valid only if the different sections of a column require diameters that differ by less than 20%.

3.3.3 Program Flow Chart

Examining Figure 3.5, it can be noted that the user can choose to either perform a product prediction calculation, or the user can perform a product prediction and column design calculation. If the user chooses to perform a product prediction calculation, then only the feed input and product prediction fields should be entered. If the user performs the latter, the all the fields (feed input, product prediction and column design fields) in the data input page should be entered. It should be noted that it is not compulsory to enter fields that have an asterix. If the user is not sure of the field value, then a reasonable assumption for that field will be made.

After the results have been generated, the user can either exit, save results or perform another calculation.
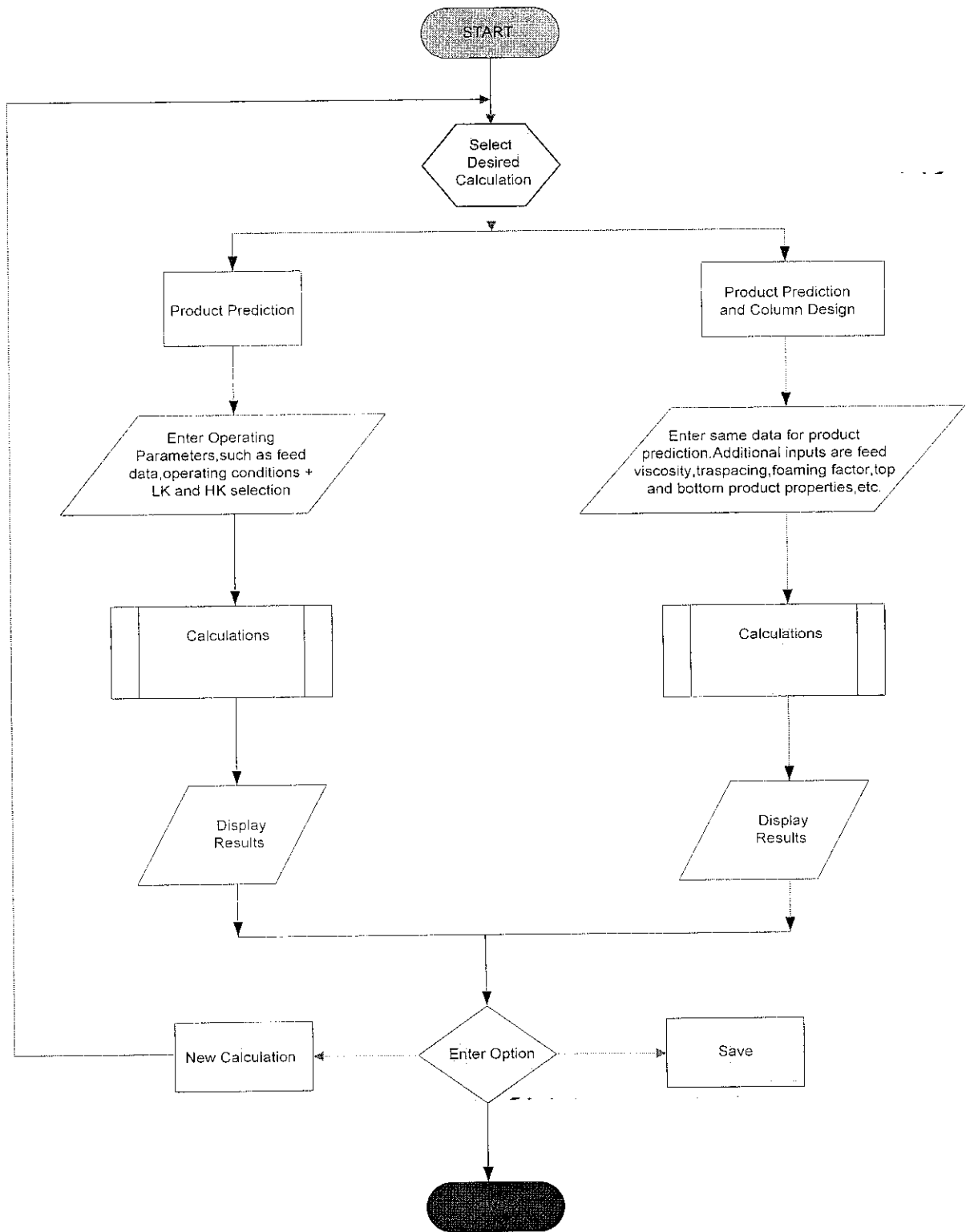
Figure 3. 5: Program Flow Chart

CHAPTER 4

RESULTS AND DISCUSSION

The overall simulation software environment consists of four different interfaces. Two of which are pop up screens. These pop up screens are the introduction (Figure 4.1) and help (Figure 4.5) interfaces. The software then has a menu interface, which contains user options such as File, New, Save, Exit and Run (Figure 4.2 and Figure 4.3). The last and main interface is the software environment interface (Figure 4.8). This interface consists of three pages, where each page is selected by selecting the appropriate tab. The three pages allow the user to input data (Figure 4.6), display the results (Figure 4.7) and graphically display the results by means of a sketch (Figure 4.8). Each of the interfaces will be discussed for the rest of this chapter.

4.1 Software Introduction Interface

This interface appears when the software is opened. By pressing the continue button, the software will proceed to the software environment interface.
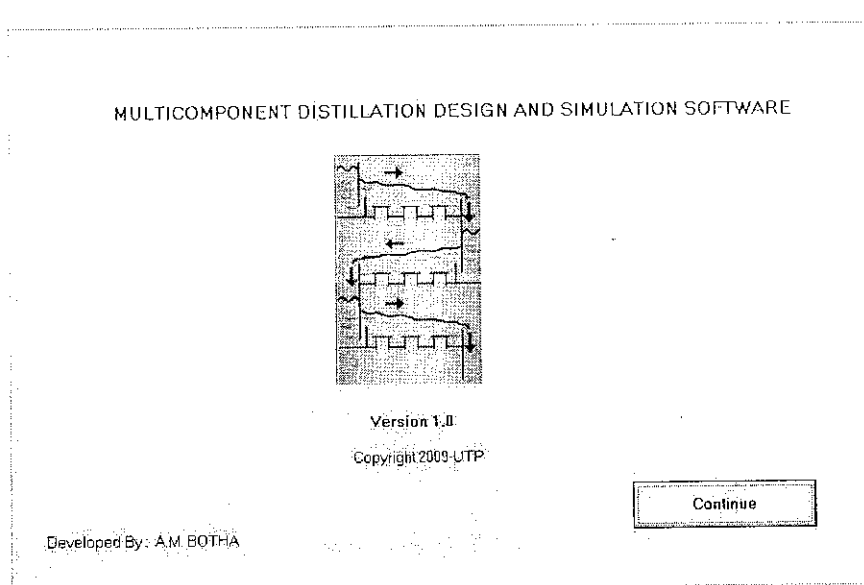
Figure 4. 1: Introduction Interface generated when the software is opened

4.2 Menu Interface

The menu interface is placed above the software environment interface. This interface is used to obtain selections from the user in order to perform the general commands a user will have when in the software simulation environment. The interface shown in Figure 4.2 consists of three menu selection icons namely: file, run and help. These menus consist of more submenus. The commands performed from the menu icons are as follows:

File   Run   Help
  - New   - Calculate   -About Software
  - Save
  - Save As
  - Exit

Furthermore, shortcut icons (New, Save, Run, Close & Help) of the commands most commonly performed are provided for convenience. More menu selection icons can be easily added in the future based on system requirements.

Figure 4. 2: Menu Tool bar of Software Simulation Environment
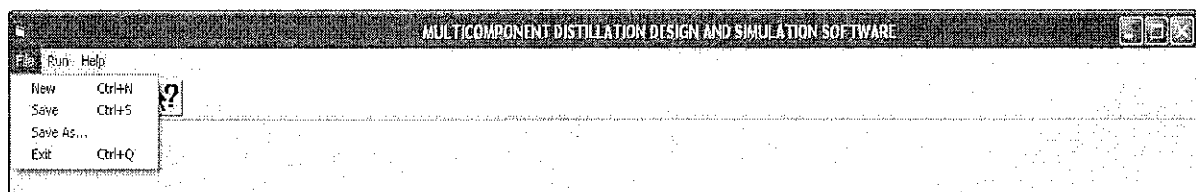
Figure 4. 3: File submenu of the Software Simulation Environment

4.2.1 New Command

The "New" command allows the user to perform another simulation without exiting the simulation environment i.e. the program does not need to be closed and open to perform another simulation. A "New" selection is under the File menu, and a blank page represents the "New" shortcut icon (See first shortcut icon Figure 4.2).

4.2.2 Save Command

The "Save" command allows the user to save the results obtained after each simulation run. A "Save" and "Save As" selection is under the File menu, and a hard disk icon (second shortcut icon in Figure 4.2) represents the "Save" shortcut icon. When a simulation run is saved, it can either be saved as a Text file or Word file. The figure below shows how the data is saved and displayed in Word/Text format.

```
|----------------------------------------------------------------------------------|
| MULTICOMPONENT DISTILLATION DATA SHEET                                           |
|----------------------------------------------------------------------------------|
|                        PRODUCT SPECIFICATIONS                                    |
|----------------------------------------------------------------------------------|
|               |          Top prodct          |       Bottom product            |
| Component     |-------------------------------|---------------------------------|
|               |Flowrate(Kmol/h)| Mole fraction| Flowrate(Kmol/h) | Mole fraction |
|---------------|-------------------------------|---------------------------------|
| 1.Propane     |30.3            |0.109         |0                 |0             |
| 2.i-Butane    |90.624         |0.326         |0.076             |0             |
| 3.n-Butane    |149.688        |0.538         |1.512             |0.002         |
| 4.i-Pentane   |6.045          |0.022         |114.855           |0.159         |
| 5.n-Pentane   |1.554          |0.006         |210.146           |0.291         |
| 6.n-Hexane    |0              |0             |119.3             |0.165         |
| 7.n-Heptane   |0              |0             |156.3             |0.217         |
| 8.n-Octane    |0              |0             |119.6             |0.166         |
| 9.            |0              |0             |0                 |0             |
| 10.           |0              |0             |0                 |0             |
| 11.           |0              |0             |0                 |0             |
| 12.           |0              |0             |0                 |0             |
|---------------|-------------------------------|---------------------------------|
|    TOTAL      |278.211        |721.789       |1                 |1             |
|----------------------------------------------------------------------------------|

|-----------------------------------------------------------|
|                  COLUMN SPECIFICATIONS                    |
|-----------------------------------------------------------|
|   Minimum Reflux               :    2.864                 |
|   Minimum Number of stages     :    17                    |
|   Theoretical Number of stages :    42                    |
|   stage Efficiency             :    0.77                  |
|   Actual Number of stages      :    54                    |
|   Height of Column             :    27.85                 |
|   Feedpoint Location           :    27                    |
|   Recommended Internals        :     Trays                |
|   Topdiameter                  :    2.59                  |
|   Bottom Diameter              :    3.71                  |
|   Recommended Diameter         :    3.71                  |
|-----------------------------------------------------------|
```

Figure 4. 4: Simulation Results saved in Text format

4.2.3 Exit Command

The "Exit" command allows the user to exit the simulation environment. An "Exit" selection is under the File menu, and a black cross represents the "Exit" shortcut icon (See fourth shortcut icon in Figure 4.2).

4.2.4 Run Command

The "Run" command allows the user to perform a simulation. After entering the required fields, clicking on the "Run" command will generate results. A "Calculate" selection is under the Run menu, and a blue arrow head represents the "Run/Calculate" shortcut icon (See third shortcut icon Figure 4.2).

4.2.5 Help Command

When the help command is selected, the help interface will be generated. This interface gives a general overview as to what the MDDSS is used for, and what are the input and output variables of the software. An "About Software" selection is under the Help menu, and a question mark icon represents the "Help/About Software" shortcut icon (See fifth shortcut icon Figure 4.2). Figure 4.5 shows the Help interface generated.
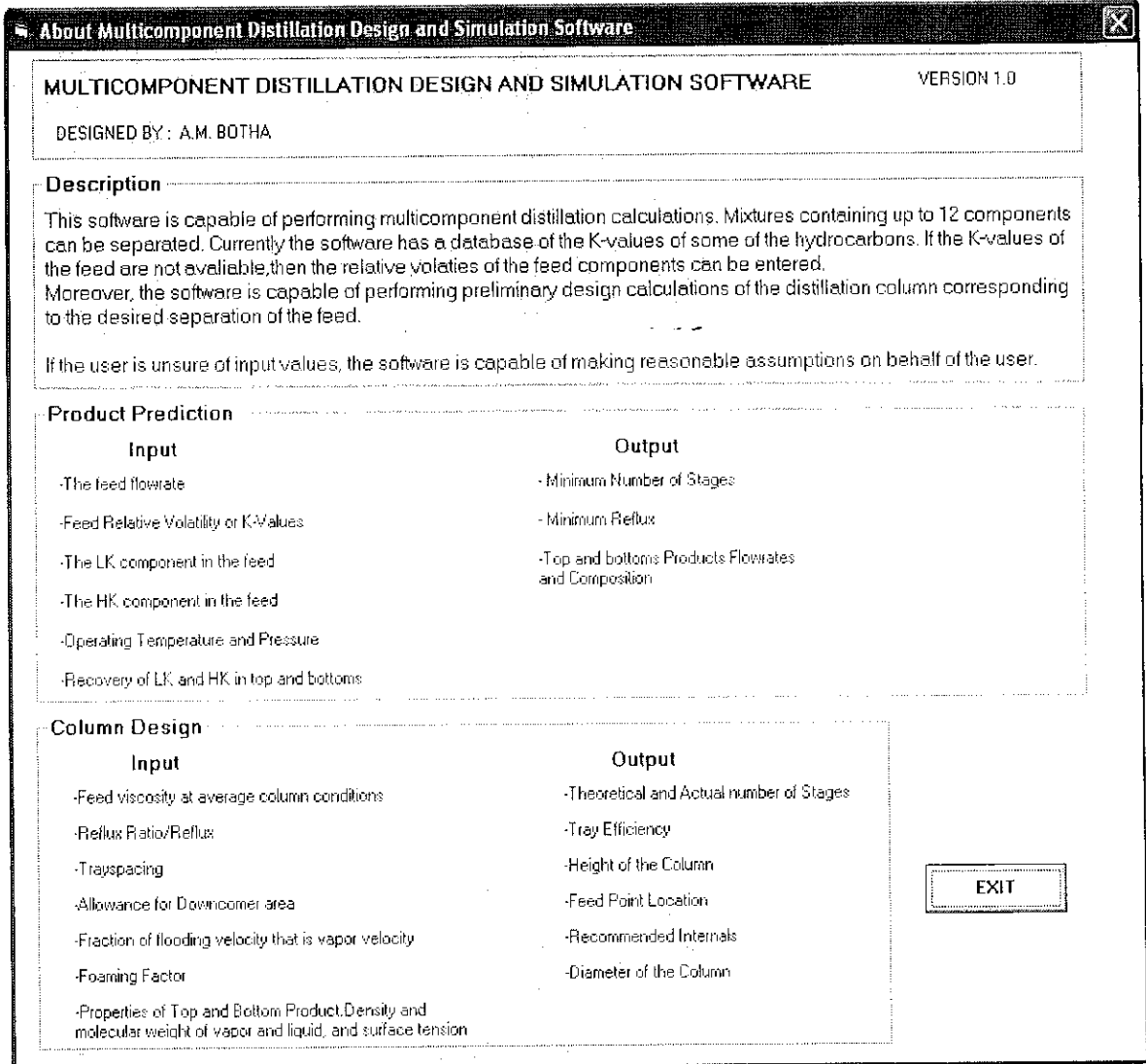
MULTICOMPONENT DISTILLATION DESIGN AND SIMULATION SOFTWARE   VERSION 1.0

DESIGNED BY : A.M. BOTHA

Description

This software is capable of performing multicomponent distillation calculations. Mixtures containing up to 12 components can be separated. Currently the software has a database of the K-values of some of the hydrocarbons. If the K-values of the feed are not available,then the relative volaties of the feed components can be entered.
Moreover, the software is capable of performing preliminary design calculations of the distillation column corresponding to the desired separation of the feed.

If the user is unsure of input values, the software is capable of making reasonable assumptions on behalf of the user.

Product Prediction

Input	Output
-The feed flowrate	- Minimum Number of Stages
-Feed Relative Volatility or K-Values	- Minimum Reflux
-The LK component in the feed	-Top and bottoms Products Flowrates and Composition
-The HK component in the feed	
-Operating Temperature and Pressure	
-Recovery of LK and HK in top and bottoms	

Column Design

Input	Output
-Feed viscosity at average column conditions	-Theoretical and Actual number of Stages
-Reflux Ratio/Reflux	-Tray Efficiency
-Trayspacing	-Height of the Column
-Allowance for Downcomer area	-Feed Point Location
-Fraction of flooding velocity that is vapor velocity	-Recommended Internals
-Foaming Factor	-Diameter of the Column
-Properties of Top and Bottom Product.Density and molecular weight of vapor and liquid, and surface tension	

EXIT

Figure 4. 5: Help Interface generated when the "Help/About Software" icon is selected.

4.3 Software Environment Interface

The software environment interface consists if three pages. Each page is selected by pressing the corresponding tab of the page. The first page is named "Data Input", the second page is named "Results" and the third page is named" Sketch". Figure 4.6 demonstrates the "Data Input" page, Figure 4.7 demonstrates the "Results" Page, and Figure 4.8 demonstrates the "Sketch" Page.

4.3.1 Data Input

This page is divided into four sections, namely: Desired Calculation, Feed Input, Product Prediction and Column Design. The data entered will depend on the Desired Calculation that the user selected. If the user selected "Product prediction" as the Desired Calculation input, the fields in the Feed Input and Product Prediction sections have to be entered. If the user selected "Product Prediction + Column Design" as the Desired Calculation input, the fields in the Feed Input, Product Prediction and Column Design sections have to be entered. It should be noted that not all fields have to be filled in. If a field is marked with an asterix, then the field can be left empty since this implies that the software will make a reasonable assumption for that field.

In the Feed Input section, the feed data should be entered in descending order of volatility. This means that the most volatile material should be listed as the first component when entering the feed data. The user has the option to enter either enter the components relative volatilities or K-values. The software has the ability to calculate K-values of some hydrocarbons. If the user selects the K-value of a hydrocarbon on its database, then it is compulsory to enter the operating temperature and pressure of the system, otherwise the user does not need to enter the operating temperature and pressure of the system.

The product prediction section has 7 fields which can be entered. However, it is compulsory to enter four of the seven fields. It is compulsory to select the HK and LK components and to specify the fraction recover of the HK and LK components in the bottom and products respectively.

The following assumptions are made for the fields with an asterix if they are left empty:
- Feed condition = 1
- Column Operating Temperature: No assumption is made for this field, this field is compulsory to be entered when the K-value from the database is used.
- Column Operating Pressure: No assumption is made for this field, this field is compulsory to be entered when the K-value from the database is used.

The column design section has 18 fields which can be entered. However, it is compulsory to enter 12 of the 18 fields.

It is compulsory to enter the following fields:

- Reflux Data
- Feed viscosity at average column conditions
- Molecular weight of the liquid in the distillate
- Molecular weight of the liquid in the bottoms
- Molecular weight of the vapor in the distillate
- Molecular weight of the vapor in the bottoms
- Density of the liquid in the distillate
- Density of the liquid in the bottoms
- Density of the vapor in the distillate
- Density of the vapor in the bottoms
- Surface tension in the distillate
- Surface tension in the bottoms

The following assumptions are made for the fields with an asterix if they are left empty:

- Minimum Reflux = Value from calculation for product prediction, if the calculated value is negative, a value of 3 is assumed.
- Reflux Input = R/Rmin =1.5
- Tray Spacing = 0.45 meters
- Allowance for downcomer area= 0.1(10%)
- Foaming factor = 0.9 (90%)
- Fraction of flooding velocity that is vapor velocity = 0.8 (80%)

Figure 4. 6: Simulation Software Data input page

4.3.2 Results

The results page is made up of three sections. The sections are as follows: Minimum Number of Stages & Minimum Reflux, Product Specification and Column Specifications. The data displayed will depend on the Desired Calculation selected in the Data Input page. If a "Product prediction" calculation was selected, then the Minimum Number of Stages & Minimum Reflux and Product Specification sections will show results. If a "Product prediction + Column Design" calculation is selected, then the Minimum Number of Stages & Minimum Reflux, Product Specification and Column Specifications sections will show results.
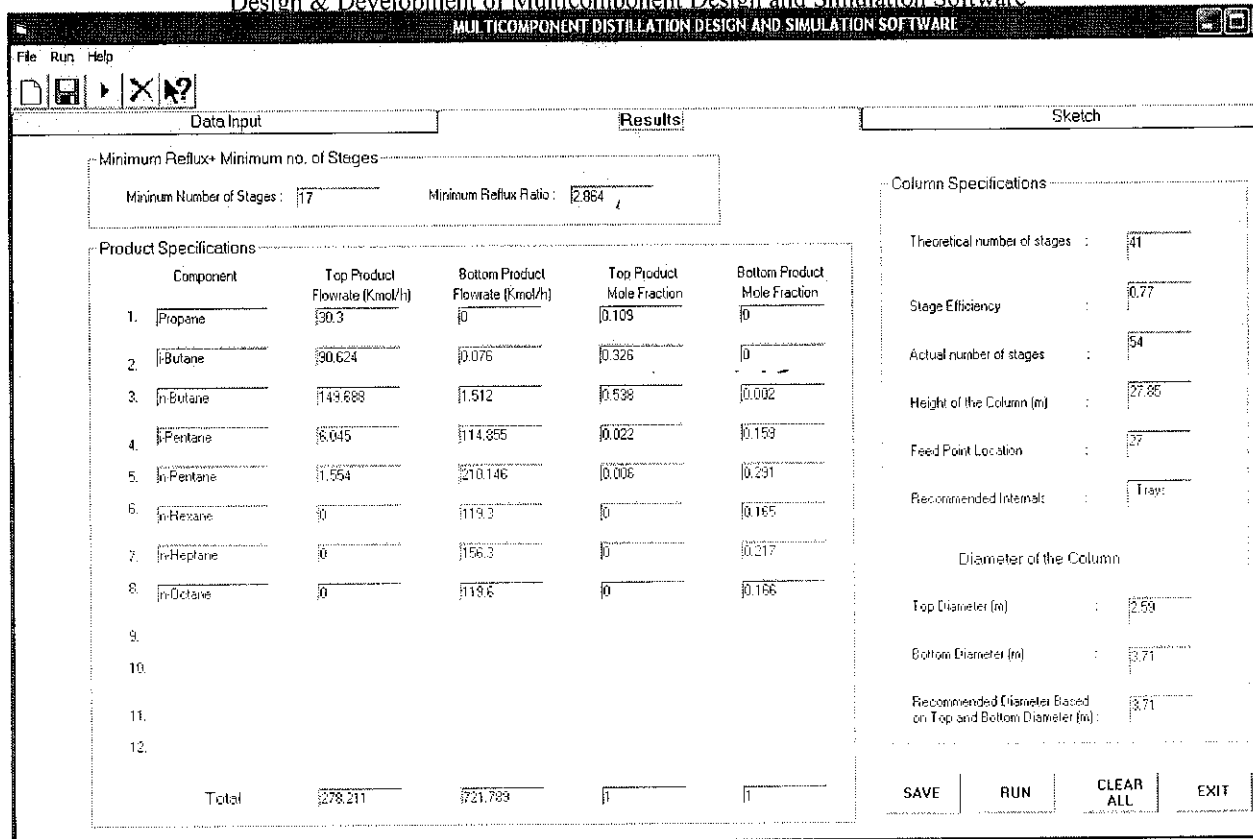
Figure 4. 7: Simulation Software Results page

4.3.3 Sketch

This page is made up of two sections, namely a sketch outlining the column specification data and stream compositions section. If on the Data Input page a "Product Prediction" calculation was selected, then only the stream compositions section will display results. If a "Product Prediction + Column Design" calculation was selected, then the stream compositions section and the sketch will show results.
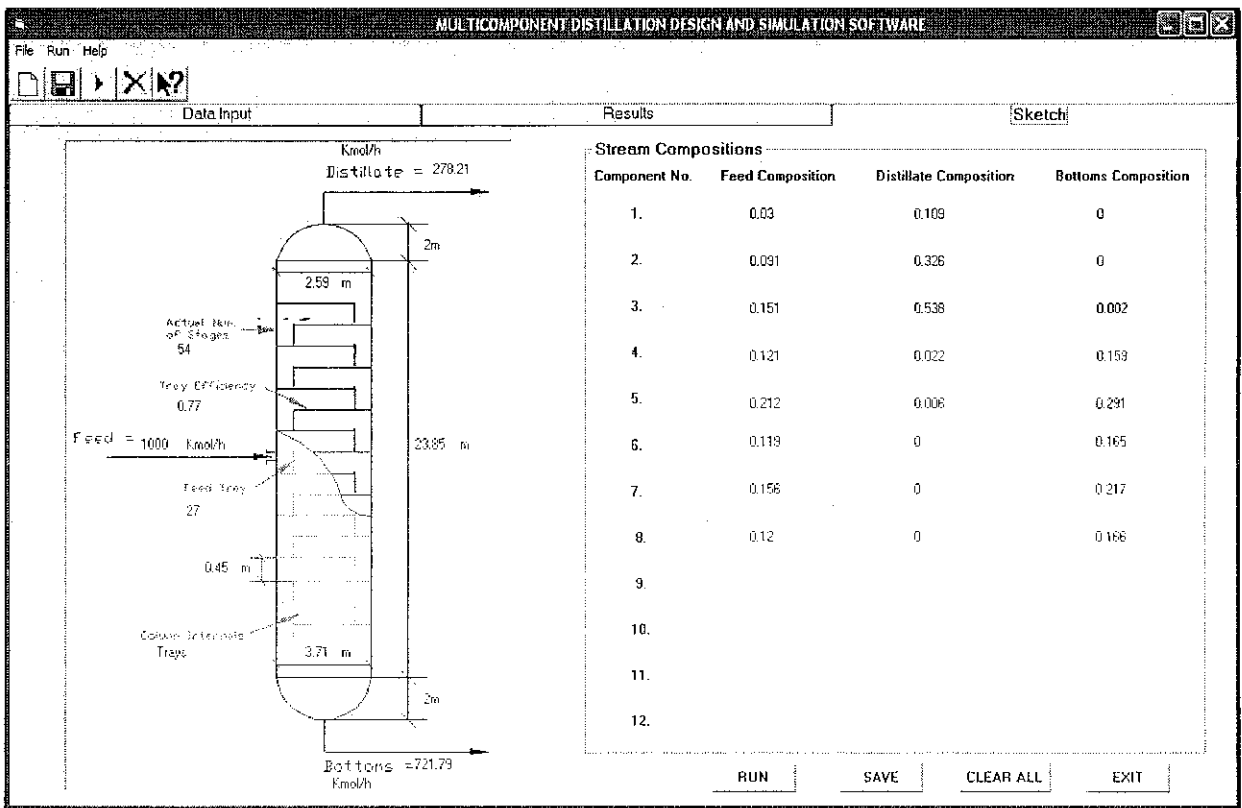
Figure 4. 8: Simulation Software Sketch page

4.4 Validation and Verification

Computer code developers, analysts who use the codes and decision makers who rely on the results of the analyses, share the same concern on the accuracy of modeling and simulation methods. Verification and validation of computational simulations is the main method to build confidence and quantify results. Verification assesses the accuracy of a solution to a computational model. Validation is the assessment of the accuracy of a computational simulation by comparison with experimental data.

The validation process confirms that an efficient and accurate system is being constructed (i.e., the system requirements are correct, complete, consistent, operationally and technically feasible, and verifiable). The Verification process ensures that the design solution has met the systems requirement and that the system is ready for use in the operational environment for which it is intended.

The MDDSS results will be validated and verified by comparing the results to commercialized software and published literature. The results generated by the software were generated in the following ways:

- The generated results in Figure 4.6 and Figure 4.7 was compared to a Mutlicomponent Distillation Example in R. Smith's Chemical Process Design and Integration (See Appendix A for the example).
- The generated results in Figure 4.6 and Figure 4.7 was compared to a HYSYS Simulation (See Appendix B for the HYSYS Simulation results).

The results obtained from the designed simulation software are exactly the same as the results obtained from the calculation in R. Smith's book. Moreover, the results from the designed simulation software are also the same as the results obtained from a distillation column simulation using HYSYS simulation software.

See Tables 4.1, Table 4.2, Table 4.3 for comparison:

Method Used	Minimum No. of Stages	Minimum Reflux
MDDSS	17	2.866
Textbook Example	17	2.866
HYSYS Simulation Software	17	2.808

Table 4. 1: R_{min} and N_{min} Results Comparison between HYSYS, textbook calculation and MDDSS

Examining the Table 4.1 it can be noted that the MDDSS 's R_{min} and N_{min} determination is accurate. This is since its results are within 5% error of the other textbook example and HYSYS Simulation Software.

	Top Product Composition			Bottom Product Composition		
	MDDSS	Textbook Example	HYSYS Simulation Software	MDDSS	Textbook Example	HYSYS Simulation Software
Propane	0.109	0.109	0.109	0	0	0
i-Butane	0.326	0.326	0.325	0	0	0
n-Butane	0.538	0.538	0.538	0.002	0.002	0.002
i-Pentane	0.022	0.022	0.022	0.159	0.159	0.159
n-Pentane	0.006	0.006	0.007	0.291	0.291	0.291
n- Hexane	0	0	0	0.165	0.165	0.165
n- Heptane	0	0	0	0.217	0.217	0.217
n-Ocane	0	0	0	0.166	0.166	0.166
Total flowrate	278.2	278.2	278.5	721.8	721.8	721.5

Table 4. 2: Product Comparison between HYSYS, textbook calculation and MDDSS

Examining the Table 4.2 it can be noted that the MDDSS 's product determination is accurate. This is since its results are within 5% error of the other textbook example and HYSYS Simulation Software.

	MDDSS	Textbook Example	HYSYS Simulation Software
$N_{theoretical}$	41	41	40
Stage efficiency	0.77	0.77	-
N_{actual}	54	54	-
Height of Column	27.85	27.85	-
Feed Location	27	-	13
Recommended Internals	Tray	Tray	-
Top Diameter	2.59	2.59	-
Bottom Diameter	2.71	2.71	-

Table 4. 3 : Column Specification Comparison between HYSYS, textbook calculation and MDDSS

Examining Table 4.3 it can be noted that the MDDSS's variable determination is exactly the same as the Textbook example's values. Only two of Table 4.3's variables can be obtained from HYSYS, the theoretical number of stages and the feedpoint location. The only variable where there is a noticeable difference, is with the

feedpoint location. The feed point location is not calculated in R. Smiths Example, hence the value is blank. The HYSYS feedpoint location is very low compared to that obtained by the MDDSS because the feed point location calculated by HYSYS is for the theoretical number of stages in the column. MDDSS calculated the feedpoint location for the actual number of stages in the column.

4.5 Data Input and Output Validation

MDDSS has the capability to ensure that the correct data type is entered into fields. If the data type is not the correct format (i.e. text or numerical) or not in the correct range (e.g. the feedcondition range should be $0 <$ feedcondition < 1), then an error message will appear and afterwards the field where the error occurred will be highlighted in red, see Figure 4.9.

Data output validation applies mainly to the minimum reflux output. The minimum reflux is calculated by trial and error using the Underwood equation, hence at times the minimum reflux value calculated by the MDDSS could be negative or slightly inaccurate. If a negative R_{min} value is calculated when performing a "Product Prediction" calculation, then the minimum reflux value won't be displayed. If performing a "Product Prediction + Column Design" calculation and the minimum reflux calculated is negative, a minimum reflux value will be set as 3 by default. The user has the option of entering a minimum reflux value, if he leaves the field blank, then the default minimum reflux of 3 will remain.
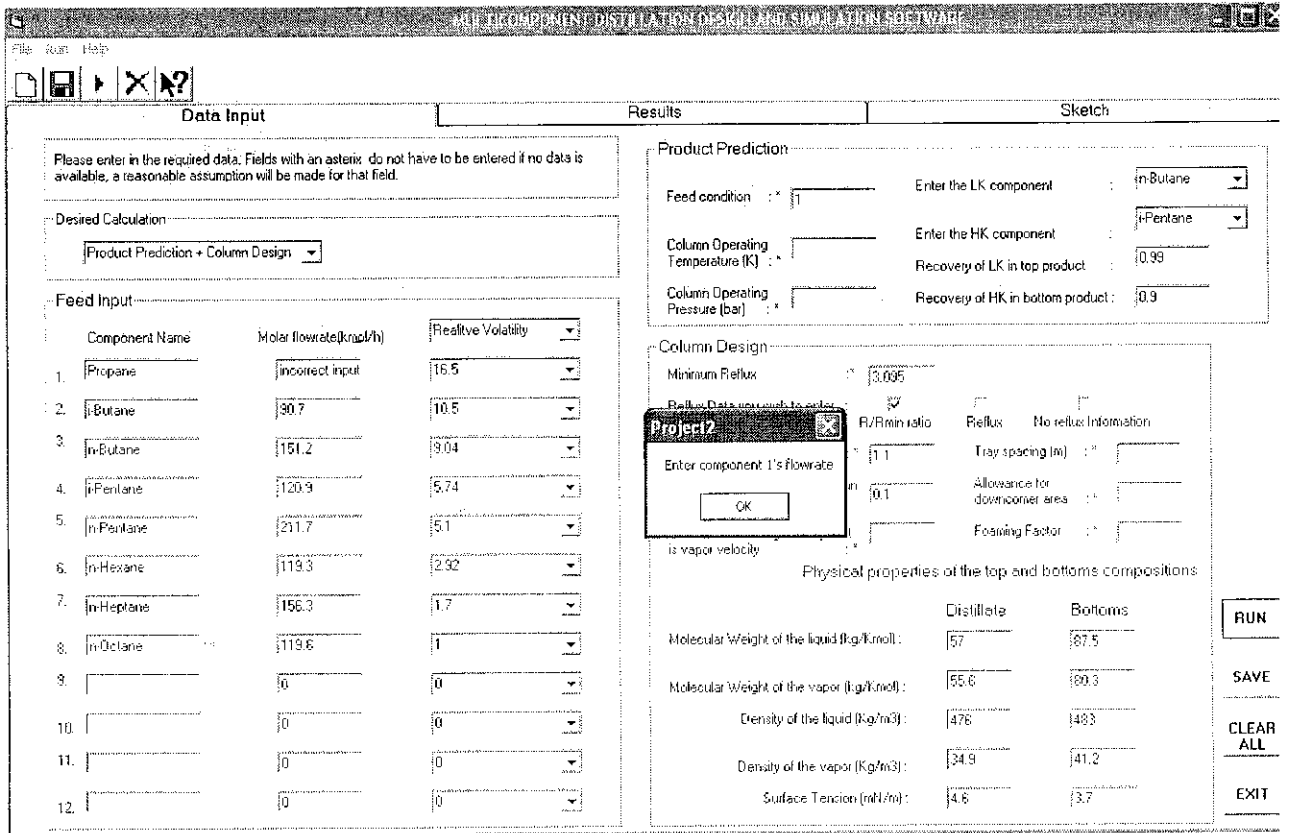
Figure 4. 9: MDDSS validates input data

4.6 MDDSS Benefits

If performed correctly, the application and use of the simulation software can have the following benefits:

- Accurate design information.

- Software-produced mass balances.

- Multiple design cases at a fraction of the cost.

- Process optimization, finding the process' maximum performance point.

- Sensitivity analyses, determining the process' key control variables and degree of operating stability.

CHAPTER 5

CONCLUSION

The MDDSS will be useful due to the following reasons:

- The software will be capable to work as a stand alone application.
- The cost of developing the software is fairly cheap.
- The size of the software is small, which enables users to run the application instantly.
- The software is compatible with all windows operating systems.

The software is designed to help and train people in the operation of the distillation unit. Moreover, the software can be used to optimise and design multicomponent distillation towers by avoiding tedious manual calculations where the probability of making mistakes is high.

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APPENDIX A

Multicomponent Distillation Sample Calculation

(Main Reference: Chemical Process Design and Integration, Robin Smith, 2005, Choice of Separator for Homogeneous Fluid Mixtures I – Distillation, Page 168)

Example 9.1 A distillation column operating at 14 bar with a saturated liquid feed of 1000 kmol·h^{-1} with composition given in Table 9.1 is to be separated into an overhead product that recovers 99% of the n-butane overhead and 95% of the i-pentane in the bottoms. Relative volatilities are also given in Table 9.1.

Table 9.1 Distillation column feed and relative volatilities.

Component	f_i (kmol·h^{-1})	α_{ij}
Propane	30.3	16.5
i-Butane	90.7	10.5
n-Butane (LK)	151.2	9.04
i-Pentane (HK)	120.9	5.74
n-Pentane	211.7	5.10
n-Hexane	119.3	2.92
n-Heptane	156.3	1.70
n-Octane	119.6	1.00

a. Calculate the minimum number of stages using the Fenske Equation.
b. Estimate the compositions of the overhead and bottoms products using the Fenske Equation.
c. Calculate the minimum reflux ratio using the Underwood Equations.

Solution

a. Substitute $r_{L,D} = 0.99$, $r_{H,B} = 0.95$, $\alpha_{LH} = 1.5749$ in Equation 9.39:

$$N_{min} = \frac{\log\left[\frac{0.99}{(1-0.99)} \cdot \frac{0.95}{1-0.95}\right]}{\log 1.5749}$$

$$= 16.6$$

b. Using the heavy key component as the reference:

$$\frac{d_H}{b_H} = \frac{f_H(1 - r_{H,B})}{f_H r_{H,B}} = \frac{1 - r_{H,B}}{r_{H,B}} = \frac{1 - 0.95}{0.95} = 0.05263$$

Substitute N_{min}, $\alpha_{i,H}$, f_i and (d_H/b_H) in Equation 9.43 to obtain d_i and determine b_i by mass balance. For the first component

(propane):

$$d_i = \frac{2.875^{16.6} \times 30.3 \times 0.05263}{1 + 2.875^{16.6} \times 0.05263}$$

$$= 30.30 \text{ kmol·h}^{-1}$$

$$b_i = f_i - d_i$$

$$= 30.30 - 30.30$$

$$= 0 \text{ kmol·h}^{-1}$$

and so on, for the other components to obtain the results in Table 9.2.

Table 9.2 Distribution of components for Example 9.1.

Component	d_i	b_i	$x_{i,D}$	$x_{i,B}$
Propane	30.30	0.0	0.1089	0.0
i-Butane	90.62	0.08	0.3257	0.0001
n-Butane	149.69	1.51	0.5380	0.0021
i-Pentane	6.05	114.86	0.0217	0.1591
n-Pentane	1.55	210.15	0.0056	0.2911
n-Hexane	0.0	119.30	0.0	0.1653
n-Heptane	0.0	156.30	0.0	0.2165
n-Octane	0.0	119.60	0.0	0.1657
Total	278.21	721.80	0.9999	0.9999

c. To calculate minimum reflux ratio, first solve Equation 9.50. A search must be carried out for the root θ that satisfies Equation 9.50. Since there are no components between the key components, there is only one root, and the root will have a value between α_L and α_H. This involves trial and error to satisfy the summation to be equal to zero, as summarized in Table 9.3.

Table 9.3 Solution for the root of the Underwood Equation.

$x_{F,i}$	$\alpha_{i,j}$	$\alpha_{i,j}x_{i,F}$	$\frac{\alpha_{i,j}x_{i,F}}{\alpha_{i,j}-\theta}$			
			$\theta=7.0$	$\theta=7.3$	$\theta=7.2$	$\theta=7.2487$
0.0303	16.5	0.5000	0.0526	0.0543	0.0538	0.0540
0.0907	10.5	0.9525	0.3721	0.2796	0.2886	0.2923
0.1512	9.04	1.3668	0.6709	0.7855	0.7429	0.7630
0.1208	5.74	0.6940	−0.5508	−0.4449	−0.4753	−0.4600
0.2117	5.10	1.0797	−0.5682	−0.4598	−0.5141	−0.5025
0.1193	2.92	0.3484	−0.0854	−0.0795	−0.0814	−0.0805
0.1563	1.70	0.2657	−0.0501	−0.0474	−0.0483	−0.0479
0.1106	1.00	0.1106	−0.0199	−0.0190	−0.0193	−0.0191
			−0.2797	0.0559	−0.0532	0.0000

Now substitute $\theta = 7.2487$ in Equation 9.51, as summarized in Table 9.4.

$$R_{min} + 1 = 3.866$$

$$R_{min} = 2.866$$

The calculation in this example can be conveniently carried out in spreadsheet software. However, many implementations are available in commercial flowsheet simulation software.

Table 9.4 Solution of the second Underwood Equation.

$x_{D,i}$	α_{ij}	$\alpha_{ij} x_{i,D}$	$\dfrac{\alpha_{ij} x_{i,D}}{\alpha_{ij} - \theta}$
0.1089	16.5	1.7970	0.1942
0.3257	10.5	3.4202	1.0520
0.5380	9.04	4.8639	2.7153
0.0217	5.74	0.1247	−0.0827
0.0056	5.10	0.0285	−0.0133
0.0	2.92	0.0	0.0
0.0	1.70	0.0	0.0
0.0	1.00	0.0	0.0
			3.8655

Example 9.3

Assuming a total condenser, calculate the number of theoretical stages required if $R/R_{min} = 1$ for the value of obtained in the previous example.

Solution

$$R_{min} = 2.866$$

Given $R/R_{min} = 1.1$

$$R = 3.153$$

From Equation 9.59

$$X = \frac{R - R_{min}}{R + 1}$$

$$= \frac{3.153 - 2.866}{3.153 + 1}$$

$$= 0.0691$$

Substitute $X = 0.0691$ in Equation 9.60

$$Y = 0.2788 - 1.3154 \times 0.0691 + 0.4114 \times 0.0691^{0.2910}$$

$$+ 0.8268 \ln 0.0691 + 0.9020 \ln \left[0.0691 + \frac{1}{0.0691} \right]$$

$$= 0.5822$$

Substitute $Y = 0.5822$ in Equation 9.59

$$0.5822 = \frac{N - 16.6}{N + 1}$$

$$N = 41.1$$

Thus, 42 theoretical stages are needed.
Repeat the calculation for $R_{min} = 3.095$

$$R = 3.405$$

$$X = 0.0703$$

$$Y = 0.5805$$

$$N = 41.0$$

53

Example 9.4 For the distillation column from Examples 9.1, 9.2 and 9.3, assuming $R_{min} = 3.095$ and $R/R_{min} = 1.1$, estimate:

a. The actual number of trays
b. Height of the column
c. Diameter of the column based on conditions at the top and bottom of the column. The system can be assumed to be susceptible to moderate foaming with a foaming factor of 0.9.

The relative volatility between the key components is 1.57 and the viscosity of the feed is 0.1 mN·s·m^{-2}. The physical properties for the distillate and bottoms compositions are given in Table 9.7.

Table 9.7 Physical properties of distillation and bottoms compositions.

	Distillate	Bottoms
M_L (kg·kmol^{-1})	57.0	87.5
M_V (kg·kmol^{-1})	55.6	80.3
ρ_L (kg·m^{-3})	476	483
ρ_V (kg·m^{-3})	34.9	41.2
σ (mN·m^{-1})	4.6	3.7

Solution

a. From Example 9.3, for $R_{min} = 3.095$, the number of theoretical stages $N = 41.0$. The overall plate efficiency can be estimated from Equation 9.61:

$$E_O = 0.542 - 0.285 \, \log(\alpha_{LK} \mu_L)$$

$$= 0.542 - 0.285 \, \log(1.57 \times 0.1)$$

$$= 0.77$$

Number of real trays

$$= \frac{41.0}{0.77}$$

$$= 53.2$$

say 54

b. Assuming a plate spacing of 0.45 m and 4 m allowance at the top of the column for vapor–liquid disengagement and the bottom for a sump:

$$\text{Height} = 0.45(54 - 1) + 4$$

$$= 27.85 \text{ m}$$

c. The diameter of the column will be based on the flooding velocity, which is correlated in terms of the liquid–vapor flow parameter F_{LV}. F_{LV} requires the liquid and vapor rates, which change through the column. Here, the assessment will be based on the flow at the top and bottom of the column assuming constant molar overflow. From Example 9.1, the

distillate flow is:

$$D = 278.21 \ \mathrm{kmol \cdot h^{-1}}$$

A mass balance around the top of the column gives:

$$V = D + L$$

$$= D(R + 1)$$

where V and L are the vapor and liquid molar flowrates at the top of the column.

$$V = 278.21(3.095 \times 1.1 + 1)$$

$$= 1225.4 \ \mathrm{kmol \cdot h^{-1}}$$

$$L = RD$$

$$= 3.095 \times 1.1 \times 278.21$$

$$= 947.2 \ \mathrm{kmol \cdot h^{-1}}$$

The feed of 1000 kmol·h^{-1} is saturated liquid. Thus the liquid flowrate below the feed is:

$$L' = 947.2 + 1000$$

$$= 1947.2 \ \mathrm{kmol \cdot h^{-1}}$$

From Example 9.1, the bottoms flowrate is:

$$B = 721.8 \ \mathrm{kmol \cdot h^{-1}}$$

The vapor flowrate below the feed is:

$$V' = 1947.2 - 721.8$$

$$= 1225.4 \ \mathrm{kmol \cdot h^{-1}}$$

The liquid–vapor flow parameter is given by Equation 9.62:

$$F_{LV} = \left(\frac{M_L L}{M_V V}\right)\left(\frac{\rho_V}{\rho_L}\right)^{0.5}$$

At the top of the column:

$$F_{LV} = \left(\frac{57.0 \times 947.2}{55.6 \times 1225.4}\right)\left(\frac{34.9}{476}\right)^{0.5}$$

$$= 0.2146$$

At the bottom of the column:

$$F'_{LV} = \left(\frac{87.5 \times 1947.2}{80.3 \times 1225.4}\right)\left(\frac{41.2}{483}\right)^{0.5}$$

$$= 0.5057$$

The terminal velocity parameter K_T is given by Equation 9.63:

$$K_T = \left(\frac{\sigma}{20}\right)^{0.2} \exp(-2.979 - 0.717 \ln F_{LV} - 0.0865(\ln F_{LV})^2$$

$$+ 0.997 \ln H_T - 0.07973 \ln F_{LV} \ln H_T + 0.256(\ln H_T)^2$$

At the top of the column:

$$\sigma = 4.6 \ \mathrm{mN \cdot m^{-1}}$$

$$F_{LV} = 0.2146$$

$$H_T = 0.45 \ \mathrm{m}$$

Substituting in Equation 9.63:

$$K_T = 0.0448 \text{ m·s}^{-1}$$

At the bottom of the column:

$$\sigma = 3.7 \text{ mN·m}^{-1}$$

$$F_{LV} = 0.5057$$

$$H_T = 0.45 \text{ m}$$

Substituting in Equation 9.63:

$$K_T^1 = 0.0289 \text{ m·s}^{-1}$$

The vapor flooding velocity can now be calculated from Equation 8.3 assuming a foaming factor of 0.9:

$$v_T = 0.9 K_T \left(\frac{\rho_L - \rho_V}{\rho_V} \right)^{0.5}$$

At the top of the column:

$$v_T = 0.9 \times 0.0448 \left(\frac{476 - 34.9}{34.9} \right)^{0.5}$$

$$= 0.143 \text{ m·s}^{-1}$$

At the bottom of the column:

$$v_T = 0.9 \times 0.0289 \left(\frac{483 - 41.2}{41.2} \right)^{0.5}$$

$$= 0.0852 \text{ m·s}^{-1}$$

To obtain the column diameter, an allowance must be made for downcomer area (say 10%), and the vapor velocity should be some fraction (say 80%) of the flooding velocity.

$$\text{Diameter} = \left(\frac{4 M_V V}{0.9 \times 0.8 \times \pi \rho_V v_T} \right)^{0.5}$$

At the top of the column:

$$\text{Diameter} = \left(\frac{4 \times 55.6 \times 1225.4/3600}{0.9 \times 0.8 \times \pi \times 34.9 \times 0.143} \right)^{0.5}$$

$$= 2.59 \text{ m}$$

At the bottom of the column:

$$\text{Diameter} = \left(\frac{4 \times 80.3 \times 1225.4/3600}{0.9 \times 0.8 \times \pi \times 41.2 \times 0.0852} \right)^{0.5}$$

$$= 3.71 \text{ m}$$

APPENDIX B

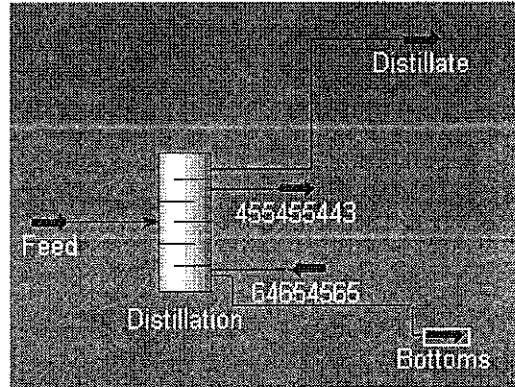# Distillation Column Simulation Using HYSIS Simulation Software

Figure B. 1: Distillation Simulation using HYSYS Simulation Software

Results Generated

The results obtained from a HYSYS simulation are as follows:

Name	Feed	Distillate	Bottoms
Vapour	0.0000	1.0000	0.0000
Temperature [C]	143.1	88.70	174.6
Pressure [kPa]	1500	1400	1400
Molar Flow [kgmole/h]	1000	278.5	721.5
Mass Flow [kg/h]	7.900e+004	1.587e+004	6.313e+004
Std Ideal Liq Vol Flow [m3/h]	123.0	27.84	95.18
Molar Enthalpy [kJ/kgmole]	-1.625e+005	-1.229e+005	-1.873e+005
Molar Entropy [kJ/kgmole-C]	151.3	145.2	173.8
Heat Flow [kJ/h]	-1.625e+008	-3.421e+007	-1.207e+008
Name	455455443		
Vapour	<empty>		
Temperature [C]	<empty>		
Pressure [kPa]	<empty>		
Molar Flow [kgmole/h]	<empty>		
Mass Flow [kg/h]	<empty>		

Figure B. 2: Distillation Simulation Results using HYSYS Simulation Software

Figure B. 3: HYSYS composition of feed and product streams

Distillation			Feed	Distillate	Bottoms
Worksheet					
	Propane		0.0303	0.1088	0.0000
Conditions	i-Butane		0.0907	0.3254	0.0001
Properties	n-Butane		0.1512	0.5375	0.0021
	i-Pentane		0.1209	0.0217	0.1592
Composition	n-Pentane		0.2117	0.0066	0.2909
	n-Hexane		0.1193	0.0000	0.1653
	n-Heptane		0.1563	0.0000	0.2166
	n-Octane		0.1196	0.0000	0.1658

Design | Rating | **Worksheet** | Performance | Dynamics

Delete   □ Ignored

Figure B. 4: HYSYS Column Design Specifications

Distillation	
Performance	Trays
	Minimum Number of Trays 16.216
	Actual Number of Trays 39.139
	Optimal Feed Stage 12.033
	Temperatures
	Condenser [C] 88.70
	Reboiler [C] 174.6
	Flows
	Rectify Vapour [kgmole/h] 1156.545
	Rectify Liquid [kgmole/h] 878.061
	Stripping Vapour [kgmole/h] 1156.545
	Stripping Liquid [kgmole/h] 1878.061
	Condenser Duty [kJ/h] -13950792.092
	Reboiler Duty [kJ/h] 21563591.744

Design | Rating | Worksheet | **Performance** | Dynamics

Delete   □ Ignored