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COMPUTER AIDED DESIGN MODULE FOR MULTI-COMPONENT DISTILLATION COLUMN

(FUG – LINEAR ALGEBRA METHOD)

A THESIS

BY

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MINNA.

MARCH, 2001

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PRESENTED TO

The Chemical Engineering Department
Federal University of Technology, Minna.

In partial fulfillment of the requirements for the award of Master of Engineering (Chemical Engineering) Degree

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CERTIFICATION

This is to certify that this thesis entitled ***Computer Aided Design For Multi-component Distillation Column*** was carried out by Abdullah B. Makama and submitted to the Chemical Engineering Department, Federal University of Technology, Minna in partial fulfillment of the requirements for the award of Master of Engineering (M.Eng) degree in Chemical Engineering.

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External Examiner
Signature and Date

DECLARATION

I hereby declare that this project is my original work and has never to my knowledge been submitted elsewhere.

Abdullah B. Makama
PGS/M.Eng/SEET/1999/2000/343

DEDICATION

This thesis is dedicated to my mother Sa'adatu Umar Makama.

ACKNOWLEDGEMENT

‘O Allah, what blessing I or any of Your creation have risen upon, is from You alone, without partner, so for You is all praise and unto You all thanks.

I give praise unto You Allah for that which You have given and bestowed, for inspiring rectitude and guiding to it, for imparting understanding and making wisdom manifest. May Your blessing be on Muhammad (S.A.W), Your beloved among prophets and messengers.

My thanks and immense gratitude goes to my project supervisor **Dr. K. R. Onifade** for his invaluable contributions and guidance towards the success of this thesis. May Allah bless and continue to guide him towards the supreme success .

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NOMENCLATURE

A = Antoine constant A. mmHg

a = Thomas parameter mol/hr

B = Antoine constant B. K

b_n = Thomas parameter mol/hr

b_i = componential flowrate in bottoms mol/hr

CAD = Computer Aided Design

C = Thomas parameter mol/hr

D = Distillate flowrate mol/hr

d_i = componential flowrate in distillate mol/hr

F = Feed flowrate mol/hr

FUG = Fenske, Underwood Gilliland

f_i = Componential feed flowrate mol/hr

H = vapour phase enthalpy kJ/mol

h = liquid phase enthalpy kJ/mol

I = denoting component

K = Equilibrium distribution constant

L = liquid phase flowrate mol/hr

l = componential liquid phase flowrate mol/hr

N = Total number of stage

N_m = minimum number of stage

n = state number

P = total pressure mmHg

P^o = vapour pressure of pure component mmHg

ρ = partial pressure of component mmHg

Q = heat added/removed kJ/mol

q = ratio of

R = reflux ratio

R_m = minimum ratio

Strip = stripping section

T = Temperature K

TDM = Tridiagonal matrix

V = vapour flow rate mol/hr

v = componential vapour flow rate mol/hr.

ABSTRACT

A computer Aided Design module was developed for a multi-component distillation column involving single, narrow boiling feeds Fenske, Underwood and Gilliland shortcut methods were combined to obtain the initial estimates of the design parameters.

The actual parameters were then calculated using the Linear – Algebra (via the Thomas algorithms) rigorous solution.

The module can be run with many feed specifications for optimum design.

There is a good match between the shortcut result and the rigorous result.

Product purity of 3 wt% maximum iC_5 and 1wt% maximum C_4 in distillate and bottoms respectively was achieved in the shortcut method but not in the rigorous method.

CHAPTER ONE

INTRODUCTION

The separation of liquid mixtures into their several components is one of the major processes of chemical and petroleum industries, and distillation is the most widely used method of achieving this end. It is the key operation of the oil refinery. Throughout the chemical industry, the demand for purer products, coupled with a relentless pursuit of greater efficiency, has necessitated continued research into the techniques of distillation. The separation of liquid mixtures by distillation depends on differences in volatility (or boiling points) between the components. The greater the relative volatilities, the easier the separation. (Coulson and Richardson 1977).

The feed in a distillation column can be binary – or multi-component. The former involves two while the latter involves many components. The basic process of vapourization and condensation holds in both types. However, the analysis of the latter is more complicated, especially where many columns are needed. Furthermore, multiple feeds may be introduced, making the analysis more difficult (Philips 1979).

The design of multi-component distillation column involves many steps, but the principal steps on which the others resolve are the determination of stages and reflux requirements. Determination of these basic requirements for multi-component distillation is much more complex than for binary mixture. With a multi-component mixture, fixing one component composition does not uniquely determine the other component composition and stage temperature. Also when the feed contains more than two components, it is not possible to specify the complete composition of the top and bottom products independently.

Chemical engineering design revolves around calculation of physical and thermodynamic properties as more than 80% of design time is used on this process, especially in distillation (Raznjevic 1976; Perry and Green 1984).

In multi-component distillation design, two methods are combined (Coulson and Richardson 1977; Treybal 1981). The shortcut methods (or loop) used to calculate such values as k-values and enthalpies. These calculations by approximations are accurate over a limited range of pressure, temperature and composition. The method is employed to reduce the overall rigorous calculations and therefore save computer time and cost. Some of the shortcut methods have also been adopted for state-to-stage calculations and reflux requirements in separation columns especially for hydrocarbon systems in petroleum and petrochemical industries. But caution must be exercised in using them. The second method, the rigorous method, calculates thermodynamic properties using equations of state and activity coefficient methods (Kern 1990). It is used to establish optimum design conditions.

The computer has infiltrated all aspects of our working lives. We are accustomed to its prominence in the world of business and finance where it has assumed many of the book-keeping and communications functions of most organizations and companies. It has become a key tool for engineering design.

CAD is a catch phrase for a large variety of technological innovations and application of computer-based technology. It represents a set of methods, procedures, equipment (hardware), and programs (software) involved in the design of physical objects and assemblies. It brings advanced computer technology into engineering and production.

CAD is a utility that enables speedy processing of design procedures with the resultant benefits of :

- increased productivity.
- improved product quality.

- new concept of what is possible.

In searching for innovative concepts or creative solutions to problems, the designer needs a means of representing concepts rapidly, changing them readily, and analyzing their properties. Design Engineers are not always seeking completely new innovative concepts, but are often involved in redesigning existing objects or part of an object or assembly – often to conform to new situations, criteria, regulations, or standards. CAD systems allow the designer to retrieve previous designs, try changes and elaborations, and observe the results.

There are basically two methods of developing CAD flow-sheeting in chemical processing industries. These are namely the equation – oriented method and the modular methods. In equation oriented method, the process or system is regarded as a unit and the equations, correlations e.t.c. that describe the process are collected together and solved. The modular method regards the design process or system as a collection of subsystems or modules.

Although the modular approach has its own drawbacks it is usually preferred because of its inherent advantages of individuality and portability. It employs databank, or modules to store the process data such as properties, thermodynamic data e.t.c; and modules for processing algorithms, equations and optimization needed by design. A master program synchronizes the passing of information between the data bank and the modules (Onifade 1999, Westerberg 1979).

Each module can be developed, tested and debugged on its own and incorporated into the overall design or flow-sheeting. Furthermore, many plants or processes consist of the same or similar units that require the same kind of calculations. The modular option therefore allows a module used in the design of one plant to be "imported" into the design of another plant in which it has a similar function.

1.2 Aims and Objectives

The objective of this work is therefore to develop a module that uses Fenske – Underwood – Gilliland (FUG) shortcut method and the Linear – Algebra tridiagonal matrix (TDM) rigorous method for handling the calculations involved in the design of a multi-component distillation column.

The FUG shortcut method for multi-component distillation column uses the Fenske equations for minimum stages, the Underwood equations for minimum reflux and the Gilliland correlation for the number of stages for a given reflux.

The TDM is an equation – tearing method which computes liquid – phase mole fractions by developing linear matrix equations in a manner shown by Amundson and Pontinen (1958). To this type of sparse matrix equation, the highly efficient version of the Gaussian elimination procedure called the Thomas algorithm (Perry and Green, 1984) is applied to solve for the liquid – phase mole fractions.

CHAPTER TWO

2.10 PRINCIPLES OF MULTI-COMPONENT DISTILLATION DESIGN

Multi-component distillation is more difficult than binary distillation in that graphical techniques are not really useful, except in special cases. The computations require much more labour as well as the knowledge of the necessary approximation methods. Even before high speed, large electronic computers can be used, one must do a great deal of hard calculation in order to develop necessary input data for an existing computer program. For multi-component distillation calculations we use the following :

- Material balances
- Energy balances
- Vapour – liquid equilibrium
- Estimation procedures
- Facilities limitation (cooling/heating restrictions)
- A well organized approach.

Multi-component systems cannot be separated into the individual components through use of one single column tower. Instead, the separation occurs between two of the components which are concentrated – one overhead in the distillate and one below in the bottoms. The basic ideas of binary distillation still apply but, necessarily, are adapted or extended to fit the new and more complex situation.

The two components upon which we focus our attention are called the "key components". The design aims at separating the "keys" to the extent desired in the product specifications. In other words, while we can specify the split of the keys, top and bottom, we cannot as well specify the distribution of the nonkey components. The latter distribution depends primarily on vapour – liquid equilibrium, the number of contact units, and to a lesser extent enthalpy considerations. The more volatile of the keys is called the "light key" (LK) and the less volatile is called the "heavy key" (HK).

The computational approach used is based on the idea of binary distillation, with the "keys" being akin to the binary components. Even though we use shortcut or approximate method for the initial calculations, the preliminary work has many steps. The overall approach is as follows :

1. Establish preliminary compositions for the top and bottom products using available specifications for the keys and assuming a distribution for the nonkey components.
2. Determine column separating conditions (temperature and pressure) at the top and bottom, using appropriate vapour – liquid equilibrium data and limitations imposed by the facilities available.
3. Select and verify the keys.
4. Estimate the minimum number of equilibrium contact stages required for the desired separation.
5. Make sure there is consistency between the column operating conditions, product compositions (both top and bottom), and equilibrium data for the system.
6. Estimate the minimum reflux ratio for the required separation. Inherent in the estimate is the need to establish the thermal conditions of the feed (or what is the degree of vapourization).
7. Using available stage reflux correlations, obtain the number of equilibrium stages and the reflux ratio required to each product specifications.
8. Estimate the feed tray location within the column.

9. Estimate tray efficiency, column diameter, and height, and overall column pressure drop. When column pressure drop is established, it should be compared with the assumed pressure drop.

Note that the procedure is not necessarily - a single – pass calculation. In step 1 product compositions were assumed. In step 5 we require consistency, at which point we may have to revise the initial estimates used in step 1 and repeat the calculations. Similar comments apply to step 9.

2.1.1 BASIC DATA

It is obvious that good design requires good data – especially so with multi-component calculations. In this section we consider some basic relations and sources of data. The reason for such a limited treatment, quite simply, is that the estimation/prediction/extrapolation/ interpolation of equilibrium data is an immense problem with no clear-cut unequivocal method of solution. Entire textbooks have been written on this subject alone – and doubtless more will be printed.

2.1.2 Vapour Pressure

Vapour pressure is the most important of the basic thermodynamic properties affecting liquids and vapours. The vapour pressure is the pressure exerted by a pure component at equilibrium at any temperature when both liquid and vapour phases exit and thus extends from a minimum at the triple point temperature to a maximum at the critical temperature, and critical pressure. Except at very high total pressures (above about 10Mpa), there is no effect of total pressure on vapour pressure. If such an effect is present, a correction, the pouting correction, can be applied (Perry and Green 1984).

If the system is ideal, Raoult's and Dalton's law apply and vapour-liquid equilibria can be calculated from vapour pressure alone. For nonideal system the vapour pressure still is very important .

Vapour pressure is correlated as a function of temperature by numerous methods mainly derived from the Clapeyron equation. The classic simple equation used for correlation of low to moderate vapour pressures is the Antoine equation (Perry and Green, 1984) .

$$\text{In } P^{o} = A - \frac{B}{T + C} \qquad (2.1)$$

Antoine constants A, B, and C for many compounds are tabulated in (Coulson & Richardson 1977). P^{o} is vapour pressure (mmHg), T is absolute temperature (K).

2.1.3 Relative Volatilities

If the multi-component system is ideal (low pressure, not near critical temperature and pressure, and chemically similar components), we can use vapour – pressure data to get relative volatilities from Raoult's and Dalton's laws :

$$x_i P^o_i = p_i = Py_i \quad \text{or} \quad \frac{y_i}{x_i} = \frac{P^o_i}{P} \qquad (2.2)$$

which holds for any component(i).

x_i, y_i = mole fractions of component i in the liquid and vapour phases respectively.

P^o_i = vapour pressure of pure component(i) (mmHg)

p_i = partial pressure of component i in mixture (mmHg)

P = total pressure of the system. (mmHg)

Relative volatility is defined as

$$\alpha_{1\text{-}2} = \frac{y_1/x_1}{Y_2/x_2} = \frac{y_1}{x_1} \cdot \frac{x_2}{y_2} \qquad (2.3)$$

If $\alpha > 1$, substance 1 is the more volatile. The greater the value of α, the easier the separation. The relative volatility does not remain constant even in ideal systems because vapour pressure does not change proportionally between two components. Often the change in ratio is small and average relative volatilities are used.

We combine the Raoult – Dalton expression with the definition of relative volatility to get

$$\alpha_{1\text{-}2} = \frac{y_1}{x_1} \cdot \frac{x_2}{y_2} = \frac{P^o_1}{P} \cdot \frac{P}{P^o_2} = \frac{P^o_1}{P^o_2} \qquad (2.4)$$

Relative volatilities can be calculated between any pair of components; however, one substance is usually chosen as a reference to which all other components are referred.

$$\alpha_{ir} = \frac{y_i}{x_i} \cdot \frac{x_r}{y_r} = \frac{P^o_i}{P^o_r} \qquad (2.5)$$

The subscript r denotes reference component.

2.1.4 Equilibrium Ratios

For many systems the equilibrium ratio k can be used. This is especially so for mixtures of hydrocarbons because the non-ideality effects due to structural differences are minimized. By definition :

$$K_i = \frac{y_i}{x_i} \qquad (2.6)$$

We observe that

$$\alpha_{ir} = \frac{K_i}{K_r} \qquad (2.7)$$

Hence equilibrium ratios are easily converted into relative volatilities.

2.2.0 PROCEDURES OF MULTI-COMPONENT DISTILLATION DESIGN

A few techniques and ideas are used time and time again. All that is important are the ideas of equilibrium on a stage, mass balances, and energy (enthalpy) balances. Bubble and dew points are used frequently as well.

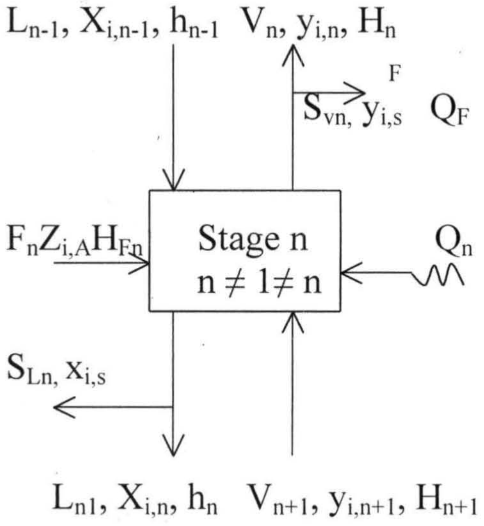
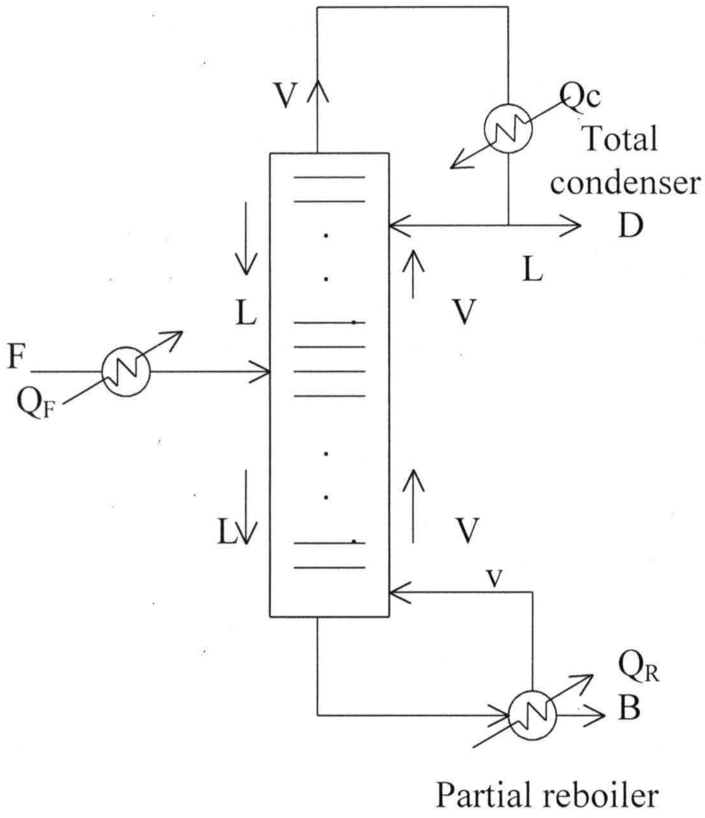


Figure.2.1 The general equilibrium stage



L = Reflux
R = L/D = external reflux ratio
L/V = internal reflux ration
V/B = boiling ratio

Figure 2.2 Typical distillation tower.

2.2.1 The equilibrium stage

Figure 2.1 is a general equilibrium stage n, with components i. By convention, streams leaving a stage are identified with the stage number. Streams L_n and V_n are in equilibrium. P_n and T_n are constant.

Streams F, L_{n-1} and V_{n+1} enter the stage. Sidestreams S_{Ln} and S_{vn} may be withdrawn. These are total streams in quantities such as moles per hour.

Mole fractions in the streams are identified as, say $y_{i,n}$ in the V_n stream and $x_{i,n}$ in the L_n stream.

Componential flowrates are sometimes used. The notation is

$$V_n y_{i,n} = v_{i,n} \qquad (2.8)$$

Q_n is enthalpy added or removed. The total vapour enthalpy is H_n and the liquid stream enthalpy is h_n.

2.2.2 The Mass Balance

Referring to Figure 2.1, the total moles (or mass) entering the stage must equal the total moles leaving the stage. Naturally this applies to each component as well. Ignoring the sidestreams, for simplicity, the overall balance is

$$L_n + V_n = F + L_{n-1} + V_{n+1} \qquad (2.9)$$

And for each component :

$$L_n x_{i,n} + V_n y_{i,n} = F_{zi,F} + L_{n-1} x_{i,n-1} + V_{n+1} y_{i,n+1} \qquad (2.10)$$

2.33 The Enthalpy Balance

Referring to Figure 2.1, the corresponding enthalpy balances are

$$h_n + H_n = h_F + h_{n-1} + H_{n+1} + Q_n$$

or

$$L_n h_n + V_n H_n = F_{hF} + L_{n-1} h_{n-1} + V_{n+1} h_{n+1} + Q_n \qquad (2.11)$$

2.2.4 Extension of the Basic Equilibrium Stage.

The use of multiple equilibrium stages to make the desired separation is an obvious extension. The arrangement of the equilibrium stage units can result in parallel, cross-, or countercurrent flow.

For the distillation process the most efficient configuration is that of a countercurrent arrangement (vapour and liquid in opposite directions). A schematic representation is given in Figure 2.2.

2.2.5 Bubble Points

By definition, a saturated-liquid stream is at the boiling (or bubble) point. The first and tiniest of bubbles formed has a composition different from the liquid, but the amount of material in the bubble is too small to change the composition of the liquid. Obviously, the liquid and bubble are in equilibrium - a restriction that enables us to determine vapour composition and pressure (or composition and temperature if the liquid is at a pre-chosen pressure).

One of the components is chosen as a reference substance. Often this is the heavy key. In general the reference component is the dominant component in the mixture or that component having the greatest contribution to the design equation. In arriving at the bubble-point relationship, the following definitions are used, recall equations (2.6) and (2.7).

$$\frac{y_i}{x_i} = K_i \qquad - \qquad (2.12)$$

We observe that

$$\alpha_{ir} = \frac{K_i}{K_r} \qquad (2.13)$$

Mathematically, the design equation bubble-point calculation is

$$\Sigma y_i = \Sigma K_i x_i = 1.0 \qquad (2.14)$$

Using the relative volatility α_{ir}, the design equation becomes

$$\Sigma y_i = K_r \Sigma \alpha_{ir} x_i = 1.0 \qquad (2.15)$$

From which $K_r = {}^1/\Sigma\, \alpha_{ir} x_i$ (2.16)

These formulae (2.14) and (2.15) are used for calculation of bubble point even though these are trial – and – error operations. Part of the computational procedure when using eqn (2.15) is the comparison of K_r and ${}^1/\Sigma\, \alpha_{ir} x_i$. If K_r and the reciprocal of the summation $\Sigma\alpha_{ir} x_i$ are equal (within the accuracy of the data),

We can calculate y_i :

$$y_i = \frac{\alpha_{ir} x_i}{\Sigma\alpha_{ir} x_i} \qquad (2.17)$$

If $K_r \neq {}^1/\Sigma\, \alpha_{ir}\, x_i$, we use the reciprocal summation as the new estimate of K_r and thus find the new estimated temperature (if the pressure is fixed), since the reference components vapour – liquid equilibrium constant is functionally dependent on temperature. If the temperature is preset, the reused/new pressure is obtained using

$$P_{new} = \frac{P_{assumed}\ K_{r,\,assumed}}{K_{r\ cal}} \qquad (2.18)$$

Where

$$K_{r,\,cal} = {}^1/\Sigma\, \alpha_{ir}\, x_i \qquad (2.19)$$

2.2.6 Dew Points

For dew-point calculation we have vapour composition available and desire to obtain the pressure or temperature at which the first drop (dew) of liquid is formed. Using the basic equations presented in the development of the bubble-point design equation, an analogous design equation for dew – point calculation can be obtained:

$$\Sigma x_i = \Sigma y_i/K_i = 1.0 \qquad (2.20)$$

Again using relative – volatility data the dew – point design equation becomes

$$\Sigma x_i = 1/K_r\, \Sigma y_i/K_i = 1.0 \qquad (2.21)$$

From \which $K_r = y_i/\alpha_{ir}$ (2.22)

Again, we compare K_r and $\Sigma(y_i/\alpha_{ir})$ and correct the temperature or the pressure as in the bubble – point format. When the assumed and calculated values of K_r agree,

$$x_i = \frac{y_i/\alpha_{ir}}{\Sigma(y_i/\alpha_{ir})} \qquad (2.23)$$

Like the bubble – point calculation, the dew – point calculation is also a trial - and – error calculation.

2.2.7 Minimum Stages At Total Reflux – The Fenske Equation

The Fenske (or Fenske – Underwood) equation estimates the minimum number of theoretical stages at total or infinite reflux. This equation uses the desired separation between two components in a binary system and assumes that the relative volatility remains constant throughout the column.

If the equilibrium data have some interaction between components, it is desirable to determine a third set of equilibrium data. The third set of data can be obtained by using the arithmetic average of the conditions (temperature and pressure) obtained for the equilibrium stages at the top and bottom of the column.

Then

$$\alpha_{Lk,av} = \sqrt[3]{\left(\frac{K_{Lk}}{K_{Hk}}\right)_{top} \left(\frac{K_{Lk}}{K_{Hk}}\right)_{middle} \left(\frac{K_{Lk}}{K_{Hk}}\right)_{Bottom}} \qquad (2.24)$$

Otherwise, the average relative volatility can be obtained using a two point geometric mean :

$$\alpha_{Lk,av} = \sqrt[3]{\left(\frac{K_{Lk}}{K_{Hk}}\right)_{top} \left(\frac{K_{Lk}}{K_{Hk}}\right)_{Bottom}} \qquad (2.25)$$

It should be noted that by definition the value $\alpha_{Hk,av} = 1.0$.

The Fenske equation yields the minimum number of theoretical equilibrium stages via the equation.

$$N_{min} = \frac{\log[\,(x_{Lk}/x_{Hk})_{dist}\,(x_{Hk}/x_{Lk})]}{\mathrm{Log}\,(\alpha_{Lk,av} \,/\, \alpha_{Hk,av}\,)} \qquad (2.26)$$

The Fenske equation has a weakness. As the relative – volatility difference between column top and column bottom increases, the estimated minimum stages get increasingly too small (i.e. the number of equilibrium stages is underestimated). In these circumstances, a better estimate can be made by calculating the number of stages in the rectifying and stripping sections separately; taking the feed concentration as the base concentration for the stripping section, and estimating the relative volatilities separately for each section. This procedure will also give an estimate of feed point location.

2.2.8 Distribution of Nonkey Components.

By combining the Fenske equation with a component material balance, the fractionation of the nonkey components can be predicted. The relationship to be used are the component material balance.

$$f_i = d_i + b_i \qquad (2.27)$$

where f_i, d_i and b_i are component i initial flowrates in feed, distillate and bottoms respectively and the original form of the Fenske equation written in terms of an arbitrary component i and a reference component r :

$$\left(\frac{d}{b}\right)_i = \left(\frac{\alpha_{i,av}}{\alpha_{r,av}}\right)^{Nmin} \left(\frac{d}{b}\right)_r \qquad (2.28)$$

In determining the product composition values using the combination of equations 2.27 and 2.28, one takes advantage of whether a component is very volatile or not very volatile. This decision as to the degree of volatility is aided by defining, arbitrary, a mean α value

$$\alpha_{mean,av} = \frac{\alpha_{Lk,av} + \alpha_{Hk,av}}{2} \qquad (2.29)$$

The following set of equations can be used to revise the estimate of the distillate and bottoms product.

Light components ($d_i > b_i$).

$$\alpha_{i,av} > \alpha_{mean,av} \tag{2.30}$$

Reference component r is the heavy key (Hk).

$$b_i = \frac{f_i}{1 + \left(\frac{d}{b}\right)_{Hk} \left(\frac{\alpha_{i,\,av}}{\alpha_{Hk,\,av}}\right)^{Nmin}} \tag{2.31}$$

$$d_i = f_i - b_i \tag{2.32}$$

Heavy components ($b_i > d_i$):

$$\alpha_{i,av} < \alpha_{mean,\,av} \tag{2.33}$$

Reference component r is the light key (Lk)

$$d_i = \frac{f_i}{1 + \left(\frac{b}{d}\right)_{Lk} \left(\frac{\alpha_{Lk,\,av}}{\alpha_{i,\,av}}\right)^{Nmin}} \tag{2.34}$$

$$b_i = f_i - d_i \tag{2.35}$$

Using the revised product distribution, the appropriate specifications can be verified. If necessary the distillate and bottoms products are adjusted, and the equilibrium data/column operating conditions are verified. The resulting cyclic computational procedure is repeated until the minimum number of theoretical stages for two trials agree to within ~ 5%.

2.2.9 Calculation of Minimum Reflux - The Underwood Equation.

For conditions where the relative volatilities remain constant, Underwood has developed the following equations from which the minimum reflux ratio R_m may be calculated.

Based on the degree of feed vapourization, the value of θ is solved for using the equation.

$$\Sigma\left(\frac{(\alpha_{i,\,av})\,(x_{i,f}\ )}{(\alpha_{i,\,av})\ -\ \theta}\right) = 1 - q \qquad (2.36)$$

For the case of adjacent key components θ is bounded by $\alpha_{Hk} < \theta < \alpha_{Lk}$. The $x_{i,f}$ and mol fractions of components in the feed.

The value of $1 - q$ is the fraction of the feed that is vapour and is defined as

$$1 - q = \frac{H_{f\,(dew\ point)} - h_{f\,(feed\ condition)}}{H_{f\,(dew\ point)} - h_{f\,(bubble\ point)}} \qquad (2.37)$$

where q is the ratio of the heat required to vapourize 1 mol of the feed to the molar latent heat of the feed and

θ is the common root for the top section and bottom section equations developed by Underwood for a column at minimum reflux with separate zones of constant compositions in each section (Perry and Green,1984)

Evaluating θ in equation (2.36) is a trial and error procedure. Newton's method of approximation can be used to determine θ starting with, an assumed θ midway between α_{Hk} and α_{Lk}

Use the θ so found in the equation

$$R_{min} + 1 = \Sigma\left(\frac{(\alpha_{i,av})\,x_{i,n}}{(\alpha_{i,av}) - \theta}\right) \tag{2.38}$$

to solve for R_{min}

2.3.0 Gilliland Stage Reflux Correlation

Gilliland (1940) has given an empirical relation between the reflux ratio R and the number of plates N, in which only the minimum reflux ratio R_m and the number of plates at total reflux N_{min} are required. $(R - R_{min})/(R + 1)$ is plotted against the group $(N - N_{min})/(N + 1)$.

Molokanov (1972) has developed an equation which satisfies the end points and fits the Gilliland curve reasonably well. This is given by:

$$\frac{N - N_{min}}{N + 1} = 1 - \exp\left\{\left(\frac{1 + 54.4\,\Psi}{11 + 117.2\Psi}\right)\left(\frac{\Psi - 1}{\Psi^{0.5}}\right)\right\} \tag{2.39}$$

where $\Psi = (R - R_{min})/(R + 1)$ (2.40)

2.3.1 Feed Location

The Fenske equation can be used to estimate the minimum number of theoretical stages in the rectifying and stripping sections. The basis of the analysis is the separation of the distillate and the feed, and the feed and bottoms. The necessary equations are :

$$(N_{min})_{rect} = \frac{\log\left\{\left(\frac{x_{Lk}}{x_{Hk}}\right)_{dist}\left(\frac{x_{Hk}}{x_{Lk}}\right)_{feed}\right\}}{\log\left(\frac{(\alpha_{Lk})_{av\,(rect)}}{(\alpha_{Hk})_{av,\,(rect)}}\right)} \qquad (2.41)$$

$$(N_{min})_{strp} = \frac{\log\left\{\left(\frac{x_{Lk}}{x_{Hk}}\right)_{feed}\left(\frac{x_{Hk}}{x_{Lk}}\right)_{bottom}\right\}}{\log\left(\frac{(\alpha_{Lk})_{av\,(strp)}}{(\alpha_{Hk})_{av,\,(strp)}}\right)} \qquad (2.42)$$

The relative – volatility values that should be used are those representatives of the rectifying and stripping sections and may have to be specifically calculated. If a two-point geometric average was used to determine the minimum number of theoretical stages in the column, there exists only a single relative – volatility describing the rectifying section and the stripping section.

$$(\alpha_i)_{av(rect)} = (\alpha_i)_{av(top)}$$

$$(\alpha_i)_{av(strp)} = (\alpha_i)_{av(bottom)}$$

For the case of a three-point geometric average being used for the column's minimum number of theoretical stages, there is an additional relative – volatility value representative of the conditions in the middle of the column, and thus :

$$(\alpha_i)_{av(rect)} = \sqrt{[(\alpha_i)_{av(top)}][(\alpha_i)_{av(middle)}]} \quad (2.43)$$

$$(\alpha_i)_{av(strp)} = \sqrt{[(\alpha_i)_{av(middle)}][(\alpha_i)_{av(bottom)}]} \quad (2.44)$$

It should be noted that the minimum number of theoretical stages in the respective column rectifying and stripping sections do not sum to the minimum number of theoretical stages for the desired separation because of variations in the relative - volatility data within the column. In general

$$(N_{min})_{rect} + (N_{min})_{strp} \geq N_{min} \quad (2.45)$$

The procedures up to this point are what constitute the shortcut design procedures (for new columns). These methods are used to develop preliminary column estimates before going to a computer or for screening studies.

2.4.0 Rigorous – Solution Methods

The rigorous analysis of a multi-component fractionating column requires the simultaneous solution of the basis relationships associated with each stage. From a computational point of view each stage is considered to be an equilibrium stage – the vapour and liquid streams leaving the stage being in equilibrium with each other. The equations associated with each stage are the MESH equations: (1) material balance, (2) equilibrium relationships, (3) sum relations, and (4) energy (heat) balances. To minimize the number of variables with each stage, the stage pressure normally is preset via the results of the preliminary calculations.

Each equilibrium stage can be represented by Figure 2.1. This figure incorporates all the features of a general stage: entering and leaving liquid and vapour streams, vapour and liquid sidestreams, an external feed, and provisions for external heat input/output. Exchanging the sidestreams draw off (to make the development somewhat more simple), the restricting equations involved in the equilibrium stage model are

1. Component material balances around stage n,

$$l_{I,n-1} - l_{i,n} - v_{i,n} + v_{i,n+1} + f_{i,n} = 0 \quad (2.46)$$

where $l_i, = Ly_{i,vi} = V = V_{yi}$ (2.47)

and $f_i = Fx_{Fi}$ (2.48)

2. Equilibrium relationship

$$y_{i,n} = K_{i,n}x_{i,n} \quad (2.49)$$

3. Sum relations on the mole fractions,

$$\sum_i x_{i,n} = 1.0 \text{ and } \sum_i y_{i,n} = 1.0 \quad (2.50)$$

4. Energy balance around stage n,

$$L_{n-1} h_{n-1} - L_n h_n - V_n H_n + V_{n+1} H_{n+1} + F_n h_{fn} + Q_n = 0 \quad (2.51)$$

Where h and H are the liquid – and vapour – phase enthalpies and Q_n is the energy input to stage n.

Historically, the solution of the set of stage equations have been governed by the level of sophistication of the computational aids available to the process engineer. The methods used initially involved the reduction of a multi-component system into a binary system. The binary solution was then adjusted for the presence of the ignored components. In the early 1930s, Lewis and Matheson (1932) as well as Thiele and Geddes (1933) published methods for solving the set of equations. Both methods required that constant molar overflow be assumed (thus neglecting enthalpy balance) and that the equations be solved in a decoupled form (that is , stage by stage). Because desk-top mechanical calculators and slide rule were the only machines available, the procedures were time consuming and repetitious. It was not until the advent of digital computers in the late 1950s that these methods were fully implemented.

With the coming of the large-digital computer and the Fortran language alternative methods were developed for solving the complete set of equations. The emphasis was on using more advanced mathematical techniques and simultaneously extending the capabilities of the various steady-state programs that have been prepared. Chronologically, the development started with the use of linear – algebra techniques to solve the equations in a decoupled form as before. The question of convergence soon arose, that is, what methods are best used so that final solution is developed. In the study of convergence methods applied to the solution of the decoupled set of column equations it was noted that many cases experienced convergence problems even though the algorithm was satisfactory for a large number of problems. In the late 1960s, the Newton Raphson algorithm was used successfully to solve all the column equations simultaneously. At the same time there were significant advances in the size of the computer core and in associated hardware and software.

Several different approaches has been taken to develop program that are efficient in the use of computer time and suitable for the full range of multi-component separation process that are used in the process industries. A design group will use those methods that are best suited to the processes that it normally handles.

It is convenient to consider the methods available under the following four headings:

1. Lewis – Matheson method
2. Thiele - Geddes method
3. Relaxation methods
4. Linear algebra methods.

With the exception of the Lewis-Matheson method, all the methods listed above require the specification of the number of stages below and above the feed point. They are therefore not directly applicable to design: where the designer wants to determine the number of stages required for a specified separation. They are strictly what are referred to as "rating methods"; used to determine the performance of existing, or given the number of stages they can be used to determine product composition. Iterative procedures are necessary to apply rating methods to the design of new columns. An initial estimate of the number of stages can be made using shortcut methods and the programs used to calculate the product compositions, repeating the calculations with revised estimates till a satisfactory design is obtained.

2.4.1 Simple Procedure (constant pressure and constant molar overflow).

From the shortcut methods we have an estimate of the compositions of distillate D and bottom B and the external reflux ratio R. At the top of the tower the mass balance are

Overall mass : $V_2 = L_1 + D = D(R + 1)$ (2.52)

Component : $V_2 y_{i,2} = D(R + 1)x_{i,D}$ (2.53)

Since we assume a total condenser, all streams must have the same composition. Because the reflux ratio R is known along with D, we can calculate the masses of streams L and V_2. We now know the flowrates (both total and componential) and compositions of the vapour stream leaving and the liquid stream entering the top stage in the tower (refer to Figure 2.3 below with $V_1 = 0$ and $D_L = D$ or to Figure 2.4).

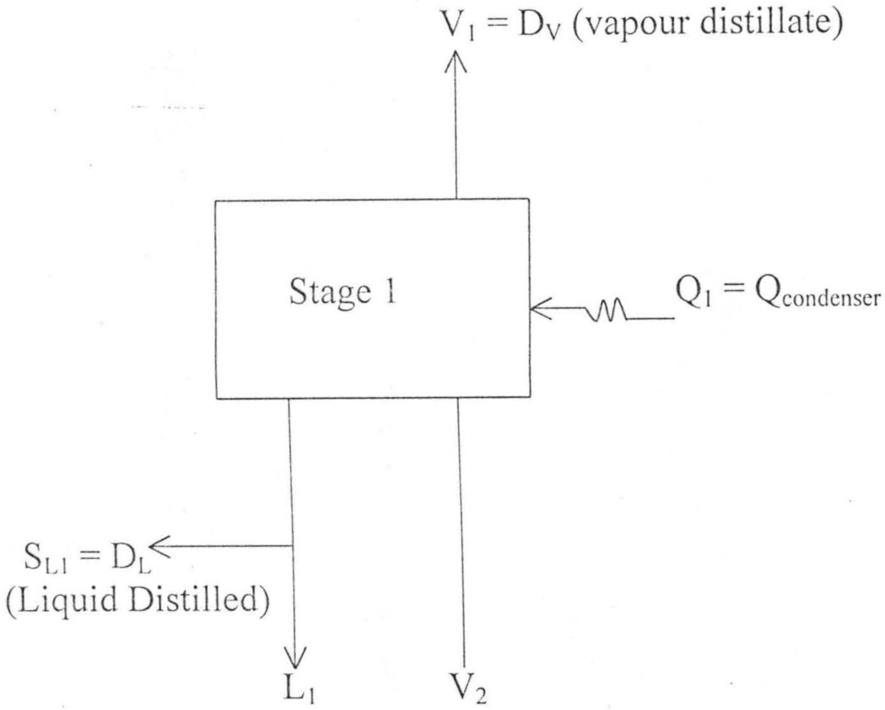


Figure 2.3 : Stage 1 condenser – reflux separator.

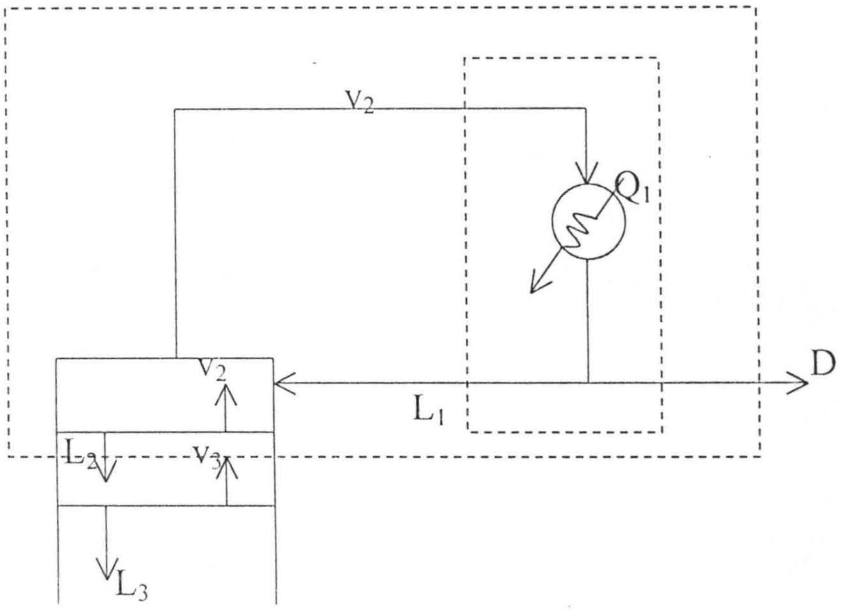


Figure 2.4. Relationship at the top of column with total condenser.

Now using the outmost envelope on Figure. 2.4, write a new material balance:

$$V_3y_{i,3} = L_2x_{i,2} + Dx_{i,D} \tag{2.54}$$

Or $$y_{i,3} = \frac{L_2}{V_3} x_{i,2} + \frac{D}{V_3} x_{i,D} \tag{2.55}$$

There is one such equation for each component. This set of equations applies above the feed stage. For simplification, constant molar overflow is assumed so that :

$$L_1 = L_2 = L_3 = \dots\dots\dots = L, \text{ to the feed stage} \tag{2.56}$$

$$V_2 = V_3 = V_4 = \dots\dots\dots = V, \text{ to the feed stage} \tag{2.57}$$

The general form for these equations is

$$Y_{i,n+1} = \frac{L}{V} x_{i,n} + \frac{D}{V} x_{i,D} \tag{2.58}$$

In the reboiler, we again have a full set of (assumed) componential flowrates for stream B which leaves the tower. From an overall mass balance :

$$F = D + B \tag{2.59}$$

or $$B = F - D \tag{2.60}$$

and around feed stage

$$F + V_{F+1} + L_{F-1} = V_F + L_F \tag{2.61}$$

But $L_{F-1} = L$ (2.62)

and $V_{F+1} = V$ (2.63)

then $F + L_{F-1} - V_F = L_F - V_{F+1} = L - V$ (2.64)

where L and V are constant molar flowrates below the feed stage.

Thus we how B, L and V, and the composition of B.

(Referring to Figure 2.5.)

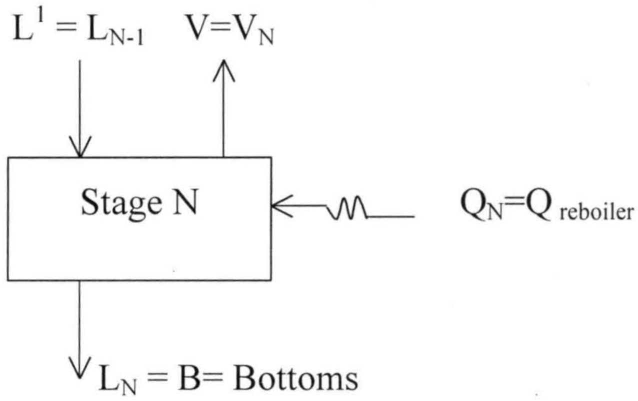


Figure 2.5 Equilibrium - Stage reboiler

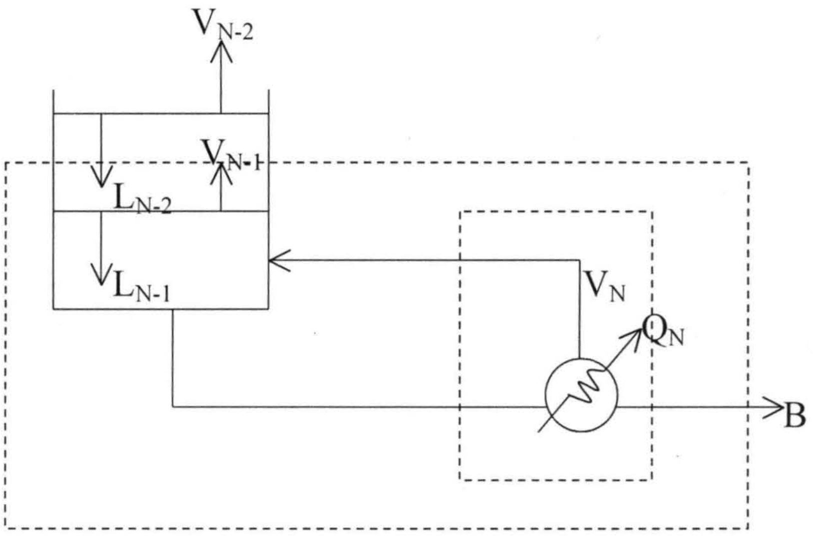


Figure 2.6. : Relationship at bottom of column with equilibrium stage reboiler.

The material balance around the first stage up from the reboiler is :

$$Bx_{i,B} + V_{n-1}\, y_{i,n-1} = L_{n-2}x_{i,n-2} \qquad (2.65)$$

Or

$$x_{i,n-2} = \frac{V_{n-1}}{L_{n-2}}\, y_{i,n-1} + \frac{B}{L_{n-2}}\, x_{i,B} \qquad (2.66)$$

For constant molar overflow

$$L_{n-1} = L_{n-2} = \ldots\ldots\ldots = L, \text{ to the feed stage} \qquad (2.67)$$

$$V_n = V_{n-1} = \ldots\ldots\ldots = V, \text{ to the feed stage} \qquad (2.68)$$

The general form of these equations is

$$X_{i,m-1} = \frac{V}{L}\, y_{i,m} + \frac{B}{L}\, x_{i.B} \qquad (2.69)$$

Where m is any stage between the reboiler and the feed stage.

2.4.2 LINEAR – ALGEBRA METHOD

The application of linear – algebra to the solution of problems in multi-component distillation was proposed by Amundson and Pontinen in 1958. In 1966, Wang and Henke applied the linear – algebra method only to the material – balance equations associated with the equilibrium relationships but clearly illustrated how to handle multiple feeds and multiple side stream draw off. Within this paper they called this technique the "tridiagonal" method.

For the sake of clarity, the following presentation will ignore intermediate sidestreams and will have a single feed stage. The computations with the short-cut procedures developed earlier provide the necessary input data, especially the number of stages, the feed-stage, location, and the external reflux ratio. The actual computation procedure starts with the development of the internal flow map (vapour and liquid flowrates) and a temperature map. The easiest flow map assumes constant liquid overflow or constant stripping flow. The actual flowrates are functions of the distillate and bottoms flowrates, the feed rate, and the external reflux ratio. The simplest temperature map assumes a linear temperature distribution between overhead and reboiler temperature.

The application of linear – algebra is confined to the solution of the mass and energy – balance equations for the respective compositions (liquid and mole fractions) and internal stream flowrates (vapour – phase flowrates). The key to the tridiagonal method is development of standard forms. The stages are counted from the top downward with the condenser – reflux separator (figure 2.1) being stage 1. Neglecting sidestreams for simplicity, the material balance for any stage is written

$$L_n x_{i,n} + V_n y_{i,n} = L_{n-1} x_{i,n-1} + V_{n+1} y_{i,n+1} + F_n x_{i,nF}. \qquad (2.70)$$

The vapour-phase compositions are eliminated using $y_i = K_i x_i$, and the equation is regrouped into standard patterns:

$$L_{n-1}x_{i,n-1} - (L_n + K_{i,n}V_n)x_{i,n} + V_{n+1}K_{i,n+1}x_{i,n+1} = -F_n x_{i,nF}. \qquad (2.71)$$

Most stages will not have an F_n term and the right side of equation (2.71) will be zero.

Stage 1, the condenser - reflux separator, is a special stage with no external feed and can be written as

$$-(L_1 + D_L + K_{i,1}D_v)x_{i,1} + K_{i,2}V_2x_{i,2} = 0.0 \qquad (2.72)$$

Stage N, the reboiler is also special and is

$$L_{N-1}x_{i,N-1} - (B + K_{i,N}V_N)x_{i,N} = 0.0 \qquad (2.73)$$

The equations maintain a definite order in the subscript for x_i only three groupings occur, and for ease in presentation these are defined as

$$a_n = L_{n-1} \qquad (2.74)$$

$$b_n = -(L_n + V_nK_{i,n}) \qquad (2.75)$$

$$c_n = V_{n+1}K_{i,n+1} \qquad (2.76)$$

For stages 1 and N

$$a_1 = 0.0 \qquad (2.77)$$

$$b_1 = -(L_1 + D_L + D_{Vi,1}) \qquad (2.78)$$

$$c_1 = V_2K_{i,2} \qquad (2.79)$$

$$a_N = L_{N-1} \qquad (2.80)$$

$$b_N = -(B + V_N K_{i,N}) \qquad (2.81)$$

$$c_N = 0.0 \qquad (2.82)$$

For each component a matrix can be written in the form.

$$\begin{pmatrix} b_1 & c_1 & \cdot & \cdot & \cdot & & & \\ a_2 & b_2 & c_2 & \cdot & \cdot & & & \\ \cdot & a_3 & b_3 & c_3 & \cdot & & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & & & \\ & & & a_n & b_n & c_n & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & a_{N-1} & b_{N-1} & c_{N-1} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & a_N & b_N \end{pmatrix} \cdot \begin{pmatrix} x_{i,1} \\ x_{i,2} \\ x_{i,3} \\ \cdot \\ x_{i,n} \\ \cdot \\ \cdot \\ x_{i,N-1} \\ x_{i,N} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \cdot \\ F_n x_{i,nF} \\ \cdot \\ \cdot \\ 0 \\ 0 \end{pmatrix} \qquad (2.83)$$

This matrix is written for a tower with a single feed.

The N x N matrix is tridiagonal in form, and there is one of such matrix for each component. All these matrix relations must hold true simultaneously, for they are stylized material balance. In each matrix, the values of the x terms are those of interest.

Each matrix is solved for the vector ($x_{i,n}$) in which the $x_{i,n}$ are composition values for component I on each plate. Each component has its own tridiagonal matrix which must be solved. If there are j components, there are j set of matrix equations.

After all the material balances are solved, the sum of the x_i values is found for each stage. If the flow streams and the temperature map are not correct, the sum of the mole fractions will not equal 1.0. In fact, any given stage may have a sum less than zero or greater than unity, and individual x_i values may show the same extremes.

The temperature map is corrected by determining bubble – point temperatures on each stage using the estimated compositions, but first these compositions must be corrected. When x_i values as calculated are less than zero or more than unity, they must be corrected to the normal range. An arbitrary but workable correction is

$$\text{If } x_i \geq 1.0 \qquad x_i = \frac{x_{i,old} + 1.0}{2} \tag{2.84}$$

$$\text{If } x_i \leq 0.0 \qquad x_i = \frac{x_{i,old} + 0.0}{2} \tag{2.85}$$

The compositions on each stage are then normalized so that $zx_i = 1.0$.

$$x_{i,new} = \frac{x_{i,old}}{\Sigma x_{i,old}} \tag{2.86}$$

Bubble – points are computed for each stage, as are the corresponding vapour compositions.

“A procedure for making new temperature estimate “.

Consider the function

$$\alpha_n = \sum_i K_{i,n} x_{i,n} \tag{2.87}$$

Where α_n depends upon temperature alone. Expanding α_n in a Taylor series taking only the linear terms.

$$\alpha_{n(tn)} = \alpha_{n(tn)} + \left(\frac{\delta\,\alpha_n}{\delta t_n}\right)_{t_n^1} (t_n - t_n^1) \tag{2.88}$$

If t_n is the correct temperature then $\alpha_n = 1.0$, thus

$$t_n = t_n^1 + [1 - \alpha_n(t_n^1)] \left.\frac{\delta\,\alpha_n}{\delta t_n}\right._{t_n^1}^{-1} \tag{2.89}$$

Equation (2.89) is the Newton approximation for the corrected temperature.

Where $$\frac{\delta\alpha_n}{\delta t_n} = \sum_i x_{i,n} \frac{\delta k_{i,n}}{\delta t_n} \tag{2.90}$$

Equation (2.89) can be used if a relationship between k_i and temperature can be found to fit the column operating conditions perfectly otherwise the normal bubble – point calculations is carried out using k_i values from Depriester’s charts.

The internal flow map (of L values) is revised using a set of energy balances with the temperature map. This requires molar enthalpies if the systems are relatively ideal (petroleum mixtures) or partial molar enthalpies if the system is rather non-ideal. Enthalpies of both liquid and vapour are required. If the solutions are ideal, the stage enthalpies are

$$H_n = \sum_i H_i(T_n)y_{i,n} \qquad (2.91)$$

$$h_n = \sum_i h_i(T_n)x_{i,n} \qquad (2.92)$$

Combining the energy balance with the overall material balance around each stage leads to the following set of relations :

Stage 1, condenser

$$-V_1(H_1 - h_1) + V_2(H_2 - h_1) = -Q_i \qquad (2.93)$$

Stage n, rectifying section

$$-V_n(H_n - h_{n-1}) + V_{n+1}(H_{n+1} - h_n) = -D(h_n - h_{n-1}) \qquad (2.94)$$

Stage F, the feed stage (h_F is the molar feed enthalpies).

$$-V_F(H_F - h_{F-1}) + V_{F+1}(H_{F+1} - h_F) = -D(h_F - h_{F-1}) - B(h_F - h_F) \qquad (2.95)$$

Stage m, stripping section

$$-V_n(H_m - h_{m-1}) + V_{m+1}(H_{m+1} - h_m) = B(h_m - h_{m-1}) \qquad (2.96)$$

Stage N, the reboiler

$$-V_N(H_N - h_{N-1}) = Q_R + B(h_N - h_{N-1}) \quad (2.97)$$

This set of equations is biadiagonal in form.

$$\begin{pmatrix} b_1 & c_1 & \cdot & \cdot & & & & \\ \cdot & \cdot & \cdot & \cdot & & & & \\ \cdot & \cdot & b_n & c_n & & & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & & & \\ & & & & b_F & c_F & & \\ & & & & \cdot & \cdot & \cdot & \\ & & & & & b_m & c_m & \\ & & & & & \cdot & \cdot & \\ & & & & & & \cdot & b_N \end{pmatrix} \begin{bmatrix} \\ \cdot \\ \\ \\ \cdot \\ \\ \\ \\ \\ \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \\ V_n \\ \cdot \\ V_F \\ \cdot \\ V_m \\ \cdot \\ V_N \end{bmatrix} = \begin{bmatrix} d_1 \\ \cdot \\ d_n \\ \cdot \\ d_F \\ \cdot \\ d_m \\ \cdot \\ d_N \end{bmatrix} \quad (2.98)$$

Stage 1:

$$b_1 = -(H_1 - h_1) \quad (2.99)$$

$$c_1 = H_2 - h_1 \quad (2.100)$$

$$d_1 = -Q_c \quad (2.101)$$

Stage n:

$$b_n = -(H_n - h_{n-1}) \quad (2.102)$$

$$c_n = H_{n+1} - h_n \quad (2.103)$$

$$d_n = -D(h_n - h_{n-1}) \tag{2.104}$$

Stage F:

$$b_F = -(H_F - h_{F-1}) \tag{2.105}$$

$$c_F = H_{F+1} - h_F \tag{2.106}$$

$$d_F = -D(h_F - h_{F-1}) - B(h_F - h_F). \tag{2.107}$$

Stage m:

$$b_m = -(H_m - h_{m-1}) \tag{2.108}$$

$$c_m = H_{m+1} - h_m \tag{2.109}$$

$$d_m = B(h_m - h_{m-1}). \tag{2.110}$$

Stage N:

$$b_N = -(H_N - h_{N-1}) \tag{2.111}$$

$$d_N = -Q_R + B(h_N - h_{N-1}). \tag{2.112}$$

If the first stage is a total condenser, $V_1 = 0.0$. This matrix equation is solved as before and yields values of V_n. This new vapour – flow map is combined with the overall material balance to obtain a new liquid – flow map (L_n), and the first iteration is complete.

Similar trials are repeated until the computed Σx_i through out the column differ from unity by a specified tolerance.

The problem is not yet solved at this point – a particular case has converged. The printout from the computer is studied for inconsistencies and to see if satisfactory results have been obtained. The distillate and bottoms compositions must be compared with the desired specifications. If the results are not satisfactory, additional computation (trials) are made in which the following parameters are altered.

- Total number of stages
- Number of stages in the rectifying section
- Number of stages in the stripping section
- Reflux
- Feed preheat.

2.4.3 Thomas Algorithm

The Thomas algorithm begins by a forward elimination, row by row starting from the top row (n = 1, the condenser stage), to get for row 1 (condenser)

$$J_1 = c_1/b_1 \qquad (2.113)$$

$$E_n = c_1/b_1 \qquad (2.114)$$

For all subsequent rows

$J_n = C_n/(b_n - a_nJ_{n-1})$ (2.115)

$E_n = (F_n - a_nE_{n-1})/(b_n - a_nJ_{n-1})$ (2.116)

a_n is replaced by 0

b_n is replaced by 1

c_n is replaced by J_n

f_n is replaced by E_n.

at the bottom row for component i, $x_N = E_n$. (2.117)

The remaining values of x_i for species are computed recursively by backward substitution.

$X_{n-1} = E_{n-1} - J_{n-1}x_n$ (2.118)

2.4.4 The Lewis-Matheson Method

The first really successful method for multi-component distillation was developed by Lewis and Matheson. Before the advent of computers, this method was the most widely used approach, and a number of useful procedures were developed.

The method is a stage-by-stage calculation using equilibrium calculations and material balances alternately. The method (in its simplest form) depends on two facts:

1. If we know the composition of one stream leaving an equilibrium stage, we can calculate the composition of the other stream leaving the stage.
2. For any given stage, if we have all molar flowrates except for one stream, we can calculate the flowrates for that stream by a material balance.
3. For any given stage, if we can calculate the enthalpy for all stream except one, we can calculate the enthalpy of that stream by an enthalpy balance.

The calculations start with a series of assumptions and specifications. As usual, start with the keys and split of the keys required between the distillate and the bottoms. Also needed are the overhead and bottoms compositions, which are estimated using the shortcut methods given previously. The shortcut methods also yield estimates of the external reflux ratio, total stages required, and feed-tray location. We must use the reflux ratio directly in the calculations, but the number of stages and the feed-stage location will be used only as check points or indicators. The shortcut procedures set the pressure in the condenser, and in the usual simple application this pressure is considered constant throughout the tower.

2.4.5 Thiele-Geddes Method

Thiele and Geddes proposed a method for multi-component distillation that was significantly different from the Lewis-Matheson procedure in that the temperature profile of the tower was assumed first. This choice of independent variable implies that the number of stages in the tower is preset and hence that the shortcut procedures have been used. The usual other assumptions are column pressure, feed-plate location, feed condition, the external reflux ratio, and the internal reflux ratio L/V and L/V.

The method proper usually employs composition ratios and not compositions. In the stripping section, the compositions are expressed as ratios to the bottoms composition, while in the rectifying section the distillate composition is used. The numerical values of the streams are not determined until the end of the calculation procedure. The method starts at either top or bottom and uses equilibrium relations and material balances alternately (as does Lewis-Matheson).

2.4.6 θ Method of Convergence

The θ method of convergence was developed by Lyster (1959) as a convergence procedure for the Thiele-Geddes type of calculation. The method has been expanded in scope over the years primarily by Halland

(1963).This method is a way of adjusting distillate and bottoms compositions so as to satisfy the initial specifications on the tower. However, material balances, enthalpy balances, and equilibrium relations all are used to develop the calculated molar flowrates which are adjusted by the correction factor θ. In addition, liquid and vapour flowrates and temperatures throughout the column are generated by the computer program. The procedure is iterative and may include forcing procedures although often these forcing producers are not absolutely necessary.

CHAPTER THREE

3.1.0 DESIGN MODULE PROGRAM

The design program was developed using QBasic Language because of the language's inherent advanced features, which makes it adaptable for modular programming structure (Echinoids 1983).

The popular shortcut method of Fenske, Underwood and Gilliland and the rigorous method of Linear-Algebra method (solved via Thomas – algorithm) were used in developing the source code of this design work.

Two files are present in the program disk, these are

a. CADMCDC2.BAS

b. Data.fil

CADMCDC2.BAS

This is the main program file. Other files like data/output files may be created by the user. There is no restriction to the number of files to be created.

Data.Fil

The various physical properties and constants needed by the CAD program are stored in this file. It is a sequential file that stores compound name, molecular weight, Antoine constants.

3.1.1 ASSUMPTIONS

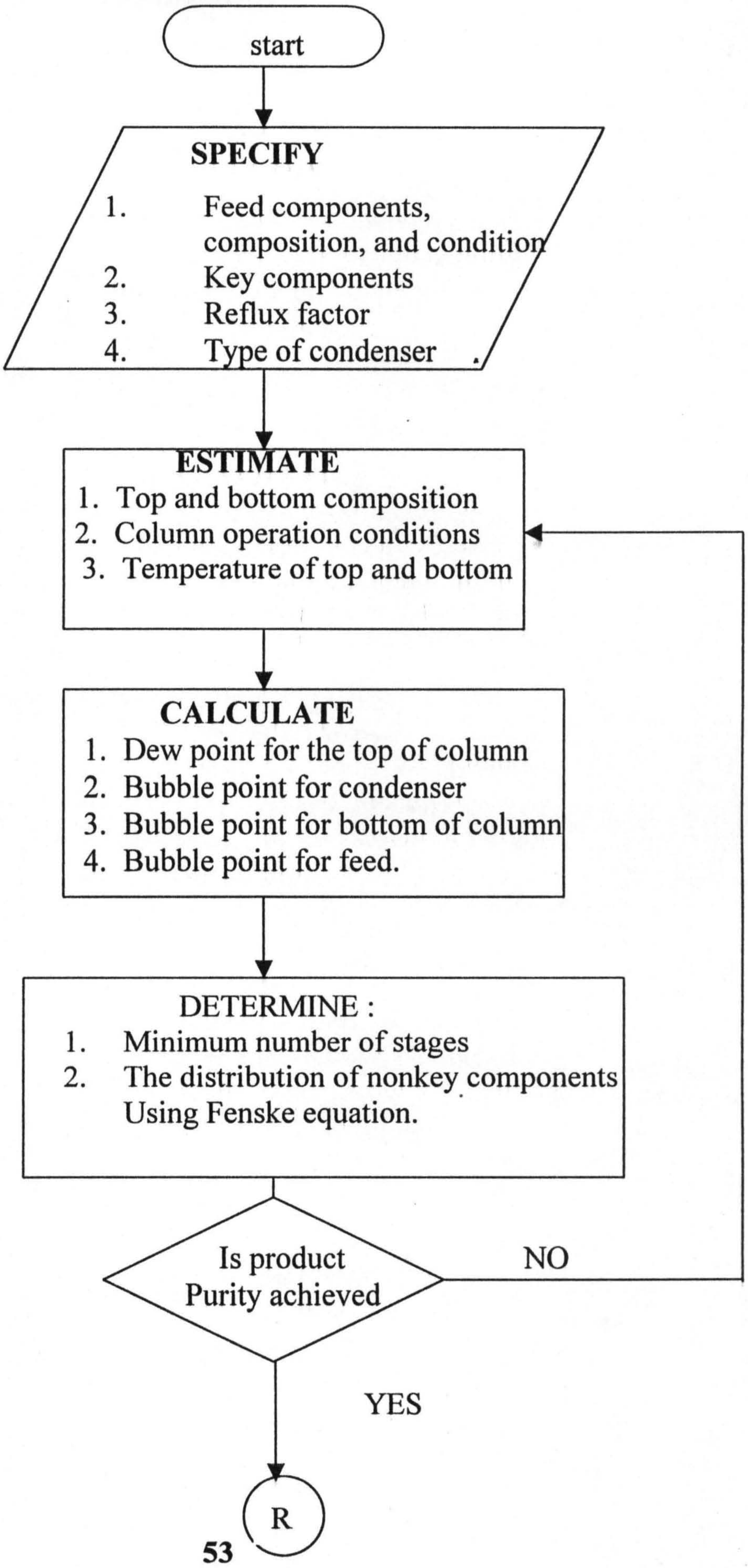
The following assumptions were made to simplify the calculation and minimize the computer time and cost.

1. Single narrow – boiling mixture.
2. Constant molar overflow.
3. Phase equilibrium between an existing vapour and a single existing liquid phase is achieved at each stage.
4. Neither of the existing phases entrains the other phase.
5. No chemical reaction occurs
6. No sub-cooling of reflux
7. Single feed point
8. The nominal pressure drop through the column is in the range of 103.40 to 760 mmHg.
9. The pressure drop due to condenser and associated piping is in the range of 51.70 to 517.00 mmHg.
10. Total condenser.
11. The temperature and pressure are normal and “reasonable”.
12. Adjacent key components.
13. Constant relative volatilities.

14. Constant column operating pressure (in the case of rigorous solution method).

3.1.2 FLOWCHART

A flowchart was designed to give a pictorial representation of route taken in solving the design problem and arriving at a solution. The flowchart is shown below.


start
SPECIFY
1. Feed components, composition, and condition
2. Key components
3. Reflux factor
4. Type of condenser .
ESTIMATE
1. Top and bottom composition
2. Column operation conditions
3. Temperature of top and bottom
CALCULATE
1. Dew point for the top of column
2. Bubble point for condenser
3. Bubble point for bottom of column
4. Bubble point for feed.
DETERMINE :
1. Minimum number of stages
2. The distribution of nonkey components Using Fenske equation.
Is product Purity achieved
NO
YES
R

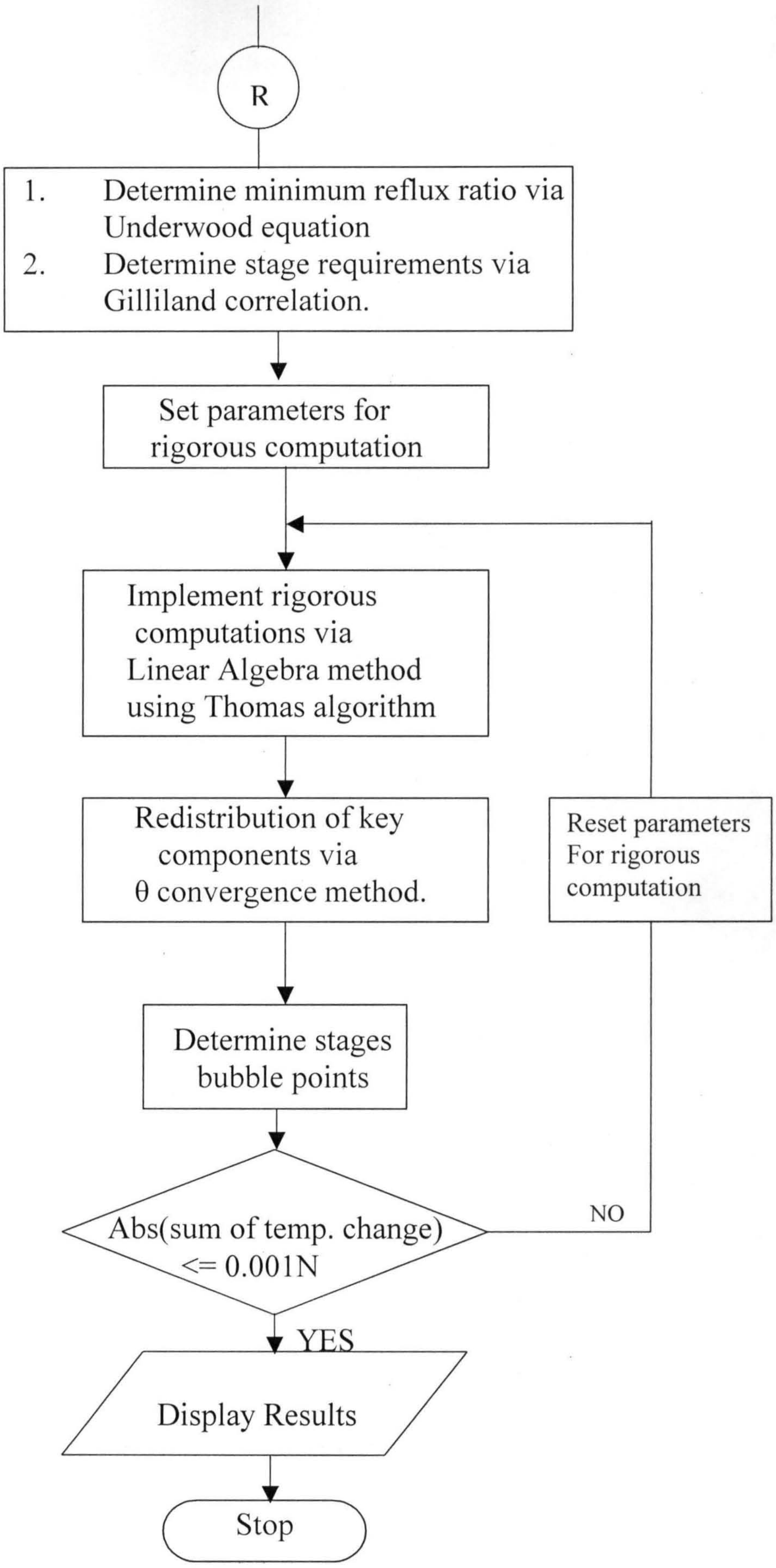


Figure 3.1 CADCMDC2 Program Flowchart

3.1.3 Source code

```
DECLARE SUB GETDATA ()
COMMON Tcon, Ttop
COMMON C$(), AntA(), AntB(), AntC(), Wt(),
summolf()
DIM C$(24), AntA(24), AntB(24), AntC(24), Wt(24)
DIM CN$(24), PWt(24), COMP(24), T(500),
oldT(500), DT(500)
GOTO menu
99
CLS
LOCATE 6, 20: PRINT "1. Use Components In Data
Bank"
LOCATE 8, 20: PRINT "2. Use New Data From My
File"
LOCATE 10, 20: PRINT "3. Enter New Data"
LOCATE 12, 20: PRINT "4. Quit"
LOCATE 14, 20: INPUT "Enter selection (1,2,3 or
4) "; sel%
    IF sel% < 1 AND sel% > 4 THEN GOTO 99
    IF sel% = 4 THEN GOTO menu
    IF sel% = 2 THEN
       LOCATE 20, 20: INPUT "Enter filename : ";
filnm$
       filnm$ = "a:\" + filnm$
       OPEN filnm$ FOR INPUT AS #3: j = 0
22     IF EOF(3) THEN GOTO 11
        j = j + 1
       INPUT #3, C$(j), AntA(j), AntB(j),
AntC(j), Wt(j), PWt(j)
       GOTO 22
11
       CLOSE #3

GOTO 100
       END IF

    IF sel% = 3 THEN
```

```
        CLS
        LOCATE 8, 20: INPUT "Number of
components in feed : "; j
        FOR x = 1 TO j
        CLS : COMP(x) = x
        LOCATE 8, 20: PRINT "No. "; x
        LOCATE 9, 20: INPUT "Component Name ";
C$(x)
        LOCATE 10, 20: INPUT "Antoine A ";
AntA(x)
        LOCATE 11, 20: INPUT "antoine B ";
AntB(x)
        LOCATE 12, 20: INPUT "Antoine C ";
AntC(x)
        LOCATE 13, 20: INPUT "Molecular Weight
"; Wt(x)
        LOCATE 14, 20: INPUT "Weight % in Feed
"; PWt(x)
       NEXT x
       LOCATE 18, 20: INPUT "Do you want to
write these data to file ? (Y/N)"; yn$
       IF UCASE$(yn$) = "Y" THEN
       LOCATE 20, 20: INPUT "Enter filename : ";
filnm$
       filnm$ = "a:\" + filnm$
       OPEN filnm$ FOR OUTPUT AS #3
       FOR x = 1 TO j
       WRITE #3, C$(x), AntA(x), AntB(x),
AntC(x), Wt(x), PWt(x)
       NEXT x
       CLOSE #3
       END IF
GOTO 100
END IF

CLS
row = 7
    LOCATE 5, 10: PRINT "COMPONENTS IN DATA
BANK"
CALL GETDATA
```

```
cl = 10
FOR K1 = 1 TO 24
        LOCATE row, cl: PRINT K1; C$(K1)
        row = row + 1
        IF row = 21 THEN
           cl = 30
           row = 7
        END IF

NEXT K1
    LOCATE row, cl: PRINT "0"; " QUIT"
j = 1
5
    LOCATE 22, 10: INPUT "Select components : ";
COMP(j)
    LOCATE 22, 10: PRINT SPC(40);
FOR Z = 1 TO j - 1
    IF COMP(Z) = COMP(j) THEN
    LOCATE 22, 20: PRINT "Component already
selected"
SLEEP 3
    LOCATE 22, 20: PRINT SPC(50);
   GOTO 5
    END IF
NEXT Z
    IF COMP(j) <> 0 THEN
    j = j + 1
GOTO 5
    END IF
    j = j - 1

10
SORTED = 1
FOR C = 1 TO j - 1
    IF COMP(C) > COMP(C + 1) THEN
        SWAP COMP(C), COMP(C + 1)
        SORTED = 0
    END IF
NEXT C
    IF SORTED = 0 THEN 10
```

```
    LOCATE 22, 10: PRINT "Total number of
components : "; j
FOR x = 1 TO j
        C$(x) = C$(COMP(x))
NEXT x

100
DIM feed(24), DISTL(24), BOTTM(24)
DIM TEMPFEED(j), TEMPDISTL(j), TEMPBOTTM(j)
DIM XF(j), XD(j), XB(j)
DIM Kcon(j), dum1(j) AS DOUBLE

    IF sel% = 3 OR sel% = 2 THEN GOTO 101

12
CLS
    LOCATE 7, 10: PRINT "COMPONENT"
    LOCATE 7, 35: PRINT "Wt%"

FOR I = 1 TO j
    FOR K1 = 1 TO 24
        IF COMP(I) = K1 THEN
          Wt(I) = Wt(K1)
          AntA(I) = AntA(K1)
          AntB(I) = AntB(K1)
          AntC(I) = AntC(K1)
        END IF
   NEXT K1
NEXT I

 row = 9
  FOR I = 1 TO j
      LOCATE row, 10: PRINT I; C$(I)
      row = row + 1
  NEXT I

66
     TOTWt = 0
     row = 9
FOR I = 1 TO j
        LOCATE row, 35: INPUT PWt(I)
```

```
        TOTWt = TOTWt + PWt(I)
        row = row + 1
NEXT
  IF TOTWt > 100 AND TOTWt < 100 THEN
         PRINT "Error -  Total percent cannot be
    less or greater than 100%"
     SLEEP 2
     GOTO 66
  END IF

15
    LOCATE 22, 10
    INPUT " Any error in your (Wt%) entries ?
(Y/N)"; er$
    IF UCASE$(er$) <> "Y" AND UCASE$(er$) <> "N"
    THEN 15
    IF UCASE$(er$) = "Y" THEN 12
    LOCATE 22, 10: PRINT SPC(50);

101
CLS
    LOCATE 10, 20: INPUT "Enter heavy key number
    "; hkey
    lkey = hkey - 1
CLS
    LOCATE 12, 10
    INPUT "Maximum Wt% of Heavy key Component in
    distillate "; mhk
    LOCATE 14, 10
    INPUT "Maximum Wt% of Light key Component in
    bottoms "; mlk
    LOCATE 16, 10: INPUT "Feed flow rate (Kg/hr)
    "; Cfr

CLS
    LOCATE 8, 20: PRINT "Feed degree of
    Vapourization"
    LOCATE 10, 20: PRINT "1.  Saturated Feed"
    LOCATE 12, 20: PRINT "2.  Saturated Vapour"
    LOCATE 14, 20: PRINT "3.  Partial vapour"
```

```
    LOCATE 16, 20: INPUT "Enter 1, 2 or 3 "; f%
    IF f% = 1 THEN
        q = 1
END IF
CLS
    IF f% = 2 THEN
    LOCATE 10, 10: PRINT " Note. Reflux Factor
    Must Be >= 1.30 For Water Condenser"
SLEEP 3
        q = 0
END IF
    IF f% = 3 THEN
77
    LOCATE 10, 30: INPUT "Enter value of q "; q
        IF q <= 0 OR q >= 1 THEN
            LOCATE 22, 20: PRINT "Error - q
    cannot be less then zero or  greater than
    one"
SLEEP 3
GOTO 77
END IF

END IF


    RESP$ = ""
    sel% = 0
CLS
    LOCATE 12, 15: INPUT "DO YOU WISH TO ASSIGN
    REFLUX FACTOR (Y/N) "; RESP$
    IF UCASE$(RESP$) = "Y" THEN
CLS
7
    LOCATE 10, 20: PRINT "Choose type of total
    Condenser"
    LOCATE 11, 20: PRINT "1.   Water condenser "
    LOCATE 12, 20: PRINT "2.   Air fin
    condenser"
    LOCATE 13, 20: INPUT "Select condenser type
    "; sel%
    IF sel% < 1 OR sel% > 2 THEN GOTO 7
```

```
    IF sel% = 1 THEN
9
    LOCATE 16, 20: PRINT "Economic range of
    Reflux factor 1.2  -  1.5"
    LOCATE 18, 20: INPUT "Enter reflux factor";
    Rfactor
    IF Rfactor < 1.2 OR Rfactor > 1.5 THEN
        LOCATE 20, 20: PRINT "Reflux factor out
    of range"
SLEEP 3: GOTO 9
    END IF
                Tcon = 330.37
    END IF
    IF sel% = 2 THEN
8
    LOCATE 16, 20: PRINT "Economic range of
    Reflux factor 1.4  -  1.5"
    LOCATE 18, 20: INPUT "Enter reflux factor";
    Rfactor
    IF Rfactor < 1.4 OR Rfactor > 1.5 THEN
    LOCATE 20, 20: PRINT "Reflux factor out of
    range"
SLEEP 3: GOTO 8
    END IF
                Tcon = 327.57
    END IF
CLS
    END IF
    IF UCASE$(RESP$) = "N" THEN
    LOCATE 12, 12: PRINT "Computations  carried
    out with reflux factor of 1.30 and"
    LOCATE 13, 12: PRINT "condenser temperature
    set at 327.59 K"
        Rfactor = 1.3
        Tcon = 327.59
    END IF
SLEEP 3: GOTO menu

999
CLS
```

```
    LOCATE 12, 20: INPUT "Enter Output filename:
    "; op$
    op$ = op$ + ".out"
    OPEN "a:\" + op$ FOR OUTPUT AS #2
CLS
    LOCATE 12, 20: PRINT "COMPUTATION IN
    PROGRESS, PLS. WAIT..."


 FOR x = 1 TO j
    MFR(x) = PWt(x) / 100 * Cfr
 NEXT
MFD = 0
MFB = 0
FOR x = 1 TO j
     IF x <= lkey THEN MFD = MFD + MFR(x)
     IF x > lkey THEN MFB = MFB + MFR(x)
NEXT x

ASSUMEDMASS:

mA = (mhk * MFD) / (100 - mhk)
mB = (mhk * mlk * MFB) / ((100 - mlk) * (100 -
mhk))
mC = (mhk * mlk) / ((100 - mhk) * (100 - mlk))
mD = 1 - mC
MHD = (mA - mB) / mD
MLB = ((mlk * MFB) / (100 - mlk) - (mlk * MHD) /
(100 - mlk))

 FSUM = 0
 DSUM = 0
 BSUM = 0

 FOR x = 1 TO j
    MFEED(x) = MFR(x)
    FSUM = FSUM + MFEED(x)
        IF x = lkey THEN
             MFR(x) = MFR(x) - MLB
             MDISTL(x) = MFR(x)
```

```
                MFB = MLB
                MBOTTM(x) = MFB
                DSUM = DSUM + MFR(x)
           END IF
           IF x < lkey THEN
                MDISTL(x) = MFR(x)
                DSUM = DSUM + MFR(x)
                MBOTTM(x) = 0
           END IF
           IF x = hkey THEN

                MDISTL(x) = MHD
                MFR(x) = MFR(x) - MHD
                MBOTTM(x) = MFR(x)
                SUM = BSUM + MFR(x)
           END IF
           IF x > hkey THEN
           MDISTL(x) = 0
                 MBOTTM(x) = MFR(x)
                 BSUM = BSUM + MFR(x)
            END IF
            TEMPFEED(x) = MFEED(x)
            TEMPDISTL(x) = MDISTL(x)
            TEMPBOTTM(x) = MBOTTM(x)
 NEXT x
            DSUM = DSUM + MHD
            BSUM = BSUM + MLB



OLDNmin = 0

CONVERSION:
FOR x = 1 TO j
     feed(x) = MFEED(x) / Wt(x)
     DISTL(x) = MDISTL(x) / Wt(x)
     BOTTM(x) = MBOTTM(x) / Wt(x)
NEXT

FEEDSUM = 0
DISTLSUM = 0
```

```
BOTTMSUM = 0

FOR x = 1 TO j
     FEEDSUM = FEEDSUM + feed(x)
     DISTLSUM = DISTLSUM + DISTL(x)
     BOTTMSUM = BOTTMSUM + BOTTM(x)
NEXT

FOR x = 1 TO j
     XF(x) = feed(x) / FEEDSUM
     XD(x) = DISTL(x) / DISTLSUM
     XB(x) = BOTTM(x) / BOTTMSUM
     XDSUM = XDSUM + XD(x)
     XFSUM = XFSUM + XF(x)
     XBSUM = XBSUM + XB(x)
NEXT

FOR x = 1 TO j
     p0(x) = EXP(AntA(x) - AntB(x) / (Tcon +
     AntC(x)))
NEXT x
     dump = p0(lkey)
ehh:

FOR x = 1 TO j
     Kcon(x) = p0(x) / dump
NEXT x
FOR x = 1 TO j
     FP(x) = Kcon(x) * XD(x)
NEXT x

sumfp = 0
FOR x = 1 TO j
     sumfp = sumfp + FP(x)
NEXT x
      IF ABS(sumfp - 1) <= .02 THEN GOTO ebb
      dump = p0(3) * sumfp
GOTO ehh
ebb:

      PCtop = dump + 130
```

```
     TEST = (AntB(lkey) / (AntA(lkey) -
LOG(PCtop))) - AntC(lkey)
     TCtop = TEST
dcont:
FOR x = 1 TO j
     dum3(x) = AntA(x) - (AntB(x) / (TCtop +
AntC(x)))
     dum1(x) = EXP(dum3(x))
NEXT x
FOR x = 1 TO j
     Ktop(x) = dum1(x) / PCtop
NEXT x
FOR x = 1 TO j
     ytop(x) = XD(x)
NEXT x
divsum = 0
FOR x = 1 TO j
     divsum = divsum + (ytop(x) / Ktop(x))
NEXT x

     IF ABS(divsum - 1) <= .02 GOTO ALST

     IF divsum > 0 THEN
     TCtop = TCtop - 1.5
     FLAGP = 1
     END IF
     IF divsum < 0 THEN
     TCtop = TCtop + 2
     FLAGM = 2
     END IF
GOTO dcont

ALST:

     PCbott = PCtop + 258.5
    TEST2 = (AntB(hkey) / (AntA(hkey) -
    LOG(PCbott))) - AntC(hkey)
    TCbott = TEST2
ACONT:
FOR x = 1 TO j
```

```
    dum3(x) = AntA(x) - (AntB(x) / (TCbott +
AntC(x)))
    dum1(x) = EXP(dum3(x))
NEXT x
FOR x = 1 TO j
    Kbott(x) = dum1(x) / PCbott
NEXT x
psum = 0
FOR x = 1 TO j
    psum = psum + (XB(x) * Kbott(x))
NEXT x
    IF ABS(psum - 1) <= .02 GOTO BLST

    IF psum > 0 THEN
    TCbott = TCbott + 2
    FLAGP = 1
    END IF
    IF psum < 0 THEN
    TCbott = TCbott - 2
    FLAGM = 2
    END IF
GOTO ACONT

BLST:

    PCmid = (PCtop + PCbott) / 2
    T = (AntB(lkey) / (AntA(lkey) - LOG(PCmid)))
    - AntC(lkey)

FNrepeat:
FOR x = 1 TO j
    Kf(x) = EXP(AntA(x) - AntB(x) / (T +
    AntC(x))) / Pcmid
NEXT x
FOR x = 1 TO j
    Ff(x) = Kf(x) * XF(x)
NEXT x

sumFf = 0
FOR x = 1 TO j
    sumFf = sumFf + Ff(x)
```

```
        NEXT x
    IF ABS(sumFf - 1) <= .02 THEN GOTO Egg

FOR x = 1 TO j
    Ff1(x) = Ff(x) * AntB(x) / (T + AntC(x)) ^ 2
NEXT x
sumFf1 = 0
FOR x = 1 TO j
     sumFf1 = sumFf1 + Ff1(x)
NEXT x
     T = T - (sumFf - 1) / (sumFf1)
     Tfeed = T
GOTO FNrepeat
Egg:
FOR x = 1 TO j
     alphatop(x) = Ktop(x) / Ktop(hkey)
NEXT x
    TCmid = (TCtop + TCbott) / 2
FOR x = 1 TO j
    dum3(x) = AntA(x) - (AntB(x) / (TCmid +
    AntC(x)))
    dum1(x) = EXP(dum3(x))
    Kmid(x) = dum1(x) / PCmid
NEXT x
FOR x = 1 TO j
        ALPHAmid(x) = Kmid(x) / Kmid(hkey)
NEXT x
FOR x = 1 TO j
        ALPHAbott(x) = Kbott(x) / Kbott(hkey)
NEXT x
FOR x = 1 TO j
NEXT x

FOR x = 1 TO j

    AveAlpha(x) = (alphatop(x) * ALPHAmid(x) *
    ALPHAbott(x)) ^ (1 / 3)

NEXT x
    meanAlpha = (AveAlpha(lkey) + 1) / 2
```

```
    AveALPHArect = (alphatop(lkey) *
    ALPHAmid(lkey)) ^ (1 / 2)

    AveALPHAstrp = (ALPHAmid(lkey) *
    ALPHAbott(lkey)) ^ (1 / 2)

    SPCUT1 = LOG((XD(lkey) / XD(hkey)) *
    (XF(hkey) / XF(lkey)))

     Nmin1 = SPCUT1 / LOG(AveALPHArect)

     SPCUT2 = LOG((XF(lkey) / XF(hkey)) *
     (XB(hkey) / XB(lkey)))

     Nmin2 = SPCUT2 / LOG(AveALPHAstrp)

     Nmin = CINT(Nmin1 + Nmin2)

     IF ABS(Nmin - OLDNmin) <= .01 GOTO
     UNDERWOOD

         OLDNmin = Nmin

sumnewbottm = 0
sumnewdistl = 0
sumfeed = 0

FOR x = 1 TO j
     IF (x <> lkey AND x <> hkey) THEN
     IF AveAlpha(x) > meanAlpha THEN
     RBOTTM(x) = feed(x) / ((1 + (DISTL(hkey)
     /(BOTTM(hkey)) * (AveAlpha(x)) ^
     Nmin))DISTL(x) = feed(x) - RBOTTM(x)
END IF
     IF AveAlpha(x) < meanAlpha THEN
     RDISTL(x) = feed(x) / ((1 + (BOTTM(lkey) /
     DISTL(lkey)) * (AveAlpha(lkey) /
     AveAlpha(x)) ^ Nmin))
    BOTTM(x) = feed(x) - RDISTL(x)
END IF
```

```
END IF
    MRBOTTM(x) = RBOTTM(x) * Wt(x)
    MRDISTL(x) = RDISTL(x) * Wt(x)
    MBOTTM(x) = BOTTM(x) * Wt(x)
    MDISTL(x) = DISTL(x) * Wt(x)
    sumnewbottm = sumnewbottm + (RBOTTM(x) +
    BOTTM(x))
    sumnewdistl = sumnewdistl + (RDISTL(x) +
    DISTL(x))
    sumfeed = sumfeed + feed(x)

    IF x < lkey THEN
    TEMPBOTTM(x) = MRBOTTM(x)
    TEMPDISTL(x) = MDISTL(x)
    END IF
    IF x = lkey THEN
    TEMPDISTL(x) = TEMPFEED(x)
    TEMPBOTTM(x) = 0
    END IF
    IF x = hkey THEN
    TEMPDISTL(x) = 0
    TEMPBOTTM(x) = TEMPFEED(x)
    END IF
    IF x > hkey THEN
    TEMPDISTL(x) = MRDISTL(x)
    TEMPBOTTM(x) = MBOTTM(x)

    END IF
NEXT x

SUMTEMPDISTL = 0
SUMTEMPBOTTM = 0
FOR x = 1 TO j
    SUMTEMPDISTL = SUMTEMPDISTL + TEMPDISTL(x)
    SUMTEMPBOTTM = SUMTEMPBOTTM + TEMPBOTTM(x)
NEXT x

        MFB = SUMTEMPBOTTM
        MFD = SUMTEMPDISTL
mA = (mhk * MFD) / (100 - mhk)
```

```
mB = (mhk * mlk * MFB) / ((100 - mlk) * (100 -
mhk))
mC = (mhk * mlk) / ((100 - mhk) * (100 - mlk))
mD = 1 - mC
MHD = (mA - mB) / mD
MLB = ((mlk * MFB) / (100 - mlk) - (mlk * MHD) /
(100 - mlk))

FSUM = 0
DSUM = 0
BSUM = 0

FOR x = 1 TO j
     FSUM = FSUM + MFEED(x)
         IF x < lkey THEN
                 LOCATE r, 40
                    DSUM = DSUM + MDISTL(x)
                 LOCATE r, 55
                 MBOTTM(x) = MRBOTTM(x)
                 BSUM = BSUM + MBOTTM(x)
            END IF

         IF x = lkey THEN
                    MDISTL(x) = MFEED(x) - MLB
                    LOCATE r, 55
                 MBOTTM(x) = MLB
                    DSUM = DSUM + MDISTL(x)
         END IF
         IF x = hkey THEN
                    MDISTL(x) = MHD
                    MBOTTM(x) = MFEED(x) - MHD
                    BSUM = BSUM + MBOTTM(x)
                 END IF
         IF x > hkey THEN
                    MDISTL(x) = MRDISTL(x)
              MBOTTM(x) = MFEED(x) - MDISTL(x)
                    DSUM = DSUM + MDISTL(x)
                 BSUM = BSUM + MBOTTM(x)
                 END IF
NEXT x
         DSUM = DSUM + MHD
```

```
        BSUM = BSUM + MLB
GOTO CONVERSION
UNDERWOOD:
theta = meanAlpha
55 :
FOR x = 1 TO j
   FG(x) = AveAlpha(x) * XF(x) / (AveAlpha(x) -
theta)
NEXT x

SUMFG = 0
FOR x = 1 TO j
   SUMFG = SUMFG + FG(x)
NEXT x
  Vapfac = 1 - q
   IF ABS(SUMFG - Vapfac) <= .0001 THEN GOTO
minimumreflux

FOR x = 1 TO 5
        FG1(x) = FG(x) / (AveAlpha(x) - theta)
NEXT x
SUMFG1 = 0
FOR x = 1 TO j
        SUMFG1 = SUMFG1 + FG1(x)
NEXT x
       theta = theta - (SUMFG - Vapfac) /
(SUMFG1)

GOTO 55
minimumreflux:

    rgard = 0
FOR x = 1 TO j

        rgard = rgard + (XD(x) * alphatop(x)) /
(alphatop(x) - theta)
NEXT x
        refluxmin = rgard - 1
        Reflux = refluxmin * Rfactor
```

```
    Rfunct = (Reflux - refluxmin) / (Reflux + 1)
        Sfunct = (1 + 54.4 * Rfunct) / (11 +
117.2 * Rfunct)
        Sfunct1 = (Rfunct - 1) / (Rfunct) ^ .5
        Sfunct2 = EXP(Sfunct * Sfunct1)
        Sfunct3 = 1 - Sfunct2
        stage = CINT((Sfunct3 + Nmin) / (1 -
Sfunct3))

     Rectsec = stage * Nmin1 / Nmin
     Stripsec = stage * Nmin2 / Nmin
     Feedpoint = CINT(Rectsec) + 1

PRINT #2, "FEED SPECIFICATION"
PRINT #2, "Degree of vapourization (q):"; q
PRINT #2, "Feed Temperature (K) : "; : PRINT #2,
USING "###.##"; Tfeed
PRINT #2, "  "; "Component", "X-Feed"
FOR x = 1 TO j
        PRINT #2, x; C$(x), ; : PRINT #2, USING
"#.####                             "; XF(x)
        NEXT x
PRINT #2, ""
PRINT #2, "COLUMN SPECIFICATION (Short-cut
result)"
PRINT #2, ""
PRINT #2, "Minimum number of stages : "; Nmin
PRINT #2, "Minimum reflux ratio : "; : PRINT #2,
USING "#.##"; refluxmin
PRINT #2, "Reflux factor : "; Rfactor
PRINT #2, "Reflux ratio : "; : PRINT #2, USING
"#.##"; Reflux
PRINT #2, "Feed point : "; Feedpoint
PRINT #2, "Total number of stages : "; stage
PRINT #2, ""
PRINT #2, "", "Pressure (mmHg)", "Temperature
(K)"
PRINT #2, "Condenser :       "; : PRINT #2, USING
"#####.##                "; dump; Tcon
PRINT #2, "Column Top :      "; : PRINT #2, USING
"#####.##                "; PCtop; TCtop
```

```
PRINT #2, "Column Bottom :  "; : PRINT #2, USING
"#####.##                   "; PCbott; TCbott
PRINT #2, ""

PRINT #2, ""
PRINT #2, "Overall column Pressure (mmHg) :"; :
PRINT #2, USING "####.##"; PCmid
PRINT #2, ""
PRINT #2, "  "; "Component", "X-distillate", "X-
bottom"
FOR x = 1 TO j
        PRINT #2, x; C$(x), ; : PRINT #2, USING
"#.####          "; XD(x); XB(x)
NEXT x
PRINT #2, ""
PRINT #2, "Distillate product molar flowrate
(mols/hr) :"; : PRINT #2, USING "###.###";
sumnewdistl
PRINT #2, ""
PRINT #2, "Bottom product molar flowrate
(mols/hr) :"; : PRINT #2, USING "###.###";
sumnewbottm
PRINT #2, ""
        Vrect = sumnewdistl * (Reflux + 1)
        Lrect = sumnewdistl * Reflux
        Vstrip = Vrect - Vapfac * sumfeed
        Lstrip = Lrect + q * sumfeed
N = CINT(stage)
TempGrad = (TCbott - TCtop) / (N - 1)

FOR s = 1 TO N
   T(s) = TCtop + (s - 1) * TempGrad
NEXT s

DIM Ks(j, N), molf(j, N), p(j, N), G(j, N), W(j,
N)
DIM A(j, N), B(j, N), C(j, N), summolf(N),
molfR(j, N), molfS(j, N)
DIM RmolfRatio(j, N), SmolfRatio(j, N),
rmolfnew(j, N), smolfnew(j, N), sumr(N), sums(N)
DIM FK(j, N), FK1(j, N)
```

```
DIM sumFK(N), sumFK1(N)

FOR x = 1 TO j
     FOR s = 1 TO N
     Ks(x, s) = EXP(AntA(x) - (AntB(x) / (T(s) +
AntC(x)))) / PCmid
        NEXT s
NEXT x
oldT = 0
Thomasvar:

FOR x = 1 TO j
   FOR s = 1 TO N

        IF s = 1 THEN
        s = 1
        A(x, s) = 0
        B(x, s) = -(Lrect + sumnewdistl)
        C(x, s) = Vrect * Ks(x, s + 1)
     END IF

     IF s > 1 AND s < Feedpoint THEN
        A(x, s) = Lrect
        B(x, s) = -(Lrect + Vrect * Ks(x, s))
        C(x, s) = Vrect * Ks(x, s + 1)
      END IF

     IF s = Feedpoint THEN
        A(x, s) = Lstrip
        B(x, s) = -(Lstrip + Vstrip * Ks(x, s))
        C(x, s) = Vstrip * Ks(x, s + 1)
      END IF

     IF s > Feedpoint AND s < N THEN
        A(x, s) = Lstrip
        B(x, s) = -(Lstrip + Vstrip * Ks(x, s))
        C(x, s) = Vstrip * Ks(x, s + 1)
      END IF

        IF s = N THEN
        A(x, s) = Lstrip
```

```
        B(x, s) = -(sumnewbottm + Vstrip * Ks(x,
N))
        C(x, s) = 0
        END IF
NEXT s
NEXT x
FOR x = 1 TO j
    FOR s = 1 TO N
       W(x, s) = B(x, s) - A(x, s) * p(x, s - 1)
       p(x, s) = C(x, s) / (B(x, s) - A(x, s) *
p(x, s - 1))

        IF s < Feedpoint THEN
        G(x, s) = 0
        END IF

        IF s = Feedpoint THEN
        G(x, s) = -feed(x) / (B(x, s) - A(x, s)
* p(x, s - 1))
        END IF

      IF s > Feedpoint THEN
       G(x, s) = (-A(x, s) * G(x, s - 1)) /
(B(x, s) - A(x, s) * p(x, s - 1))
      END IF

    NEXT s
        FOR s = N TO 1 STEP -1
        IF s = N THEN
                molf(x, s) = G(x, s)
           ELSE
           molf(x, s) = G(x, s) - p(x, s) *
molf(x, s + 1)
        END IF
       NEXT s
NEXT x

FOR s = 1 TO Feedpoint
FOR x = 1 TO j
      molfR(x, s) = molf(x, s) / molf(x, 1)
    NEXT x
```

```
NEXT s
FOR s = Feedpoint + 1 TO N
    FOR x = 1 TO j
      molfS(x, s) = molf(x, s) / molf(x, N)
    NEXT x
NEXT s

FOR x = 1 TO j
        molfbd(x) = molf(x, N) / molf(x, 1)
NEXT x

oldp = 0
p = 1
repeat:
FOR x = 1 TO j
        ft(x) = feed(x) / (sumnewdistl +
sumnewbottm * p * molfbd(x))
        ft2(x) = (sumnewbottm * molfbd(x) *
feed(x)) / (sumnewdistl + sumnewbottm * p *
molfbd(x)) ^ 2

NEXT x
        IF ABS(p - oldp) <= .0001 THEN GOTO ep
       oldp = p
sumft = 0
sumft2 = 0
FOR x = 1 TO j
        sumft = sumft + ft(x)
        sumft2 = sumft2 + ft2(x)
NEXT x
        p = p - (sumft - 1) / (-sumft2)
GOTO repeat
ep:
FOR x = 1 TO j
        molf(x, 1) = feed(x) / (sumnewdistl +
sumnewbottm * p * molfbd(x))
        molf(x, N) = p * molfbd(x) * molf(x, 1)
NEXT x
FOR s = 1 TO Feedpoint
      FOR x = 1 TO j
```

```
      RmolfRatio(x, s) = molfR(x, s) *
molf(x, 1)
   NEXT x
NEXT s
FOR s = Feedpoint + 1 TO N
   FOR x = 1 TO j
      SmolfRatio(x, s) = molfS(x, s) *
molf(x, N)
   NEXT x
NEXT s

FOR s = 1 TO Feedpoint
sumr(s) = 0
  FOR x = 1 TO j
    sumr(s) = sumr(s) + RmolfRatio(x, s)
  NEXT x
NEXT s

FOR s = Feedpoint + 1 TO N
sums(s) = 0
  FOR x = 1 TO j
     sums(s) = sums(s) + SmolfRatio(x, s)
  NEXT x
NEXT s

FOR s = 1 TO Feedpoint
  FOR x = 1 TO j
     rmolfnew(x, s) = RmolfRatio(x, s) /
sumr(s)
     molf(x, s) = rmolfnew(x, s)
    NEXT x
NEXT s

FOR s = Feedpoint + 1 TO N
  FOR x = 1 TO j
    smolfnew(x, s) = SmolfRatio(x, s) /
sums(s)
    molf(x, s) = smolfnew(x, s)
    NEXT x
NEXT s
```

```
FOR s = 1 TO N

        DT(s) = T(s) - oldT(s)
NEXT s
sumDT = 0
FOR s = 1 TO N
  oldT(s) = T(s)
  sumDT = sumDT + DT(s)
NEXT s
      IF ABS(sumDT) <= .01 * N THEN GOTO finish

Nrepeat:

FOR s = 1 TO N
        FOR x = 1 TO j
            Ks(x, s) = EXP(AntA(x) - AntB(x) /
(T(s) + AntC(x))) / PCmid
        NEXT x
        FOR x = 1 TO j
            FK(x, s) = Ks(x, s) * molf(x, s)
        NEXT x

sumFK(s) = 0
        FOR x = 1 TO j
            sumFK(s) = sumFK(s) + FK(x, s)
        NEXT x
   IF ABS(sumFK(s) - 1) <= .02 THEN GOTO EN

        FOR x = 1 TO j
            FK1(x, s) = FK(x, s) * AntB(x) /
(T(s) + AntC(x)) ^ 2
        NEXT x
sumFK1(s) = 0
        FOR x = 1 TO j
           sumFK1(s) = sumFK1(s) + FK1(x, s)
        NEXT x

       T(s) = T(s) - (sumFK(s) - 1) /
(sumFK1(s))

GOTO Nrepeat
```

```
EN:
'PRINT " T="; T(s), sumFK(s), sumFK1(s)
NEXT s
GOTO Thomasvar
finish:

PRINT #2, "Rectification Vapour flowrate
(mols/hr) :"; : PRINT #2, USING "###.###"; Vrect
PRINT #2, ""
PRINT #2, "Stripping Vapour flowrate (mols/hr)
:"; : PRINT #2, USING "###.###"; Vstrip
PRINT #2, ""
PRINT #2, "Rectification Overflow (mols/hr) :";
: PRINT #2, USING "###.###"; Lrect
PRINT #2, ""
PRINT #2, "Stripping Overflow (mols/hr) :"; :
PRINT #2, USING "###.###"; Lstrip

PRINT #2, "RIGOROUS METHOD RESULT"
FOR s = 1 TO N
    PRINT #2, ""
    PRINT #2, "Stage Number : "; s
    PRINT #2, "Stage Temperature : "; : PRINT
#2, USING "###.##"; T(s)
    FOR x = 1 TO j
    PRINT #2, x; C$(x), ; : PRINT #2, USING
"#.#### "; molf(x, s)
    NEXT x
NEXT s
CLOSE #1
CLOSE #2
CLS
ERASE feed, DISTL, BOTTM
ERASE TEMPFEED, TEMPDISTL, TEMPBOTTM
ERASE XF, XD, XB
ERASE Kcon, dum1
ERASE Ks, molf, p, G, W
ERASE A, B, C, summolf, molfR, molfS
ERASE RmolfRatio, SmolfRatio, rmolfnew,
smolfnew, sumr, sums
ERASE FK, FK1
```

```
ERASE sumFK, sumFK1

LOCATE 10, 25: PRINT "COMPUTATION IS SUCCESSFUL"
SLEEP 3
GOTO menu
44
CLS
LOCATE 8, 20: PRINT "CHECK THE OUTPUT FILE (i.e
" + op$ + ") FOR RESULTS"
LOCATE 10, 15: PRINT "HINT:    TO OPEN OUTPUT
FILE "
LOCATE 12, 20: PRINT "1.  PRESS Alt+F "
LOCATE 13, 20: PRINT "2.  PRESS 'O' "
LOCATE 14, 20: PRINT "3.  TYPE OUTPUT FILENAME
WITH EXTENSION AND PRESS ENTER "
LOCATE 17, 20: PRINT "PRESS ANY KEY WHEN
READY..."
SLEEP

menu:
CLS
LOCATE 6, 30: PRINT "COMPUTER AIDED DESIGN
MODULE FOR A"
LOCATE 7, 30: PRINT "MULTI-COMPONENT DISTILLTION
COLUMN"
LOCATE 10, 30: PRINT "1.  INPUT SPECIFICATIONS"
LOCATE 12, 30: PRINT "2.  DESIGN"
LOCATE 14, 30: PRINT "3.  VIEW RESULT"
LOCATE 16, 30: PRINT "4.  QUIT PROGRAM"
LOCATE 5, 15: FOR x = 1 TO 60: PRINT CHR$(220);
: NEXT x
LOCATE 18, 15: FOR x = 1 TO 60: PRINT CHR$(220);
: NEXT x
LOCATE 9, 15: FOR x = 1 TO 60: PRINT CHR$(196);
: NEXT x
LOCATE 8, 40: PRINT "Version 2.0"
LOCATE 20, 30: INPUT "ENTER CHOICE (1,2,3 OR
4)"; CH%
IF CH% = 1 THEN GOTO 99
IF CH% = 3 THEN GOTO 44
IF CH% = 2 THEN
```

```
  IF AntA(3) <> 0 AND AntB(3) <> 0 AND AntC(3)
<> 0 THEN GOTO 999
  LOCATE 22, 20: BEEP: PRINT "No Data in Memory,
Pls. Select Option '1' First"
  SLEEP 3
  GOTO menu
END IF
CLS
END

SUB GETDATA
SHARED C$(), AntA(), AntB(), AntC(), Wt()
OPEN "a:\Data.fil" FOR INPUT AS #1
FOR j = 1 TO 24
INPUT #1, C$(j), AntA(j), AntB(j), AntC(j),
Wt(j)
NEXT j
CLOSE #1
'
'OPEN "xdata.fil" FOR INPUT AS #2
'FOR J = 1 TO 5
'INPUT #2, X(J)
'NEXT J
'CLOSE #2
END SUB
```

3.1.4 Program Run

Step 1. LOAD

Step 2. RUN

This brings out the options:

1 Input Specification
2 Design
3 View Result
4 Quit Program

Enter choice: ? Enter 1

Step 3.

Another option comes out

1 Use components in data bank
2 Use data from my file
3 Enter new data
4 Quit

If option 1 is selected (Enter 1), component in databank would be displayed ($C_1 - C_{20}$). To select components enter their corresponding serial number one at a time.e.g

Propane	5,enter
Isobutene	6,enter
Butane	7,enter
Isopentane	8,enter
Pentane	9,enter

When all the components have been selected enter 0.

The program will ask for weight % of the components. Input the following:

1.Propane	5,enter
2.Isobutene	15,enter
3.Butane	25,enter
4.Isopentane	20,enter (hk)
5.Pentane	35,enter

The program will ask if the entries are correct. If they are press N. If there is an error, press Y to re-enter the values.

If option 2 is selected the program will ask for a file name (i.e. file created using option 3 of Step 3). Input the file name and proceed.

A file called TEST was created for the sample problem.

If option 3 is selected this can be inputted if this option is chosen. This option gives the user the option of bypassing the databank. The program will ask for the total number of components in feed and all the relevant data needed. This data include:

1.Compound name ?

2.Antoine constant A ?

3.Antoine constant B ?

4. Antoine constant C ?

5.Molecular wt. of component ?

6.Weight % component in feed ?

The data required is repeated for all the components in the feed.

The program then asks whether the user wants to store the data for future use. If Yes is chosen the user will be required to provide a name.

This filename can then be used in option 2 of step 3. If No is chosen the program will design.

If option 4 is selected the program takes the user to the main menu (i.e. Step 2).

Step 4.The program asks for the serial number of the heavy key. Enter 4

Step 5. The program asks for the maximum wt% of heavy key in distillate. Enter 3

Step 6. The program asks for the maximum wt% of light key in bottoms. Enter 1

Step 7. The program asks for the feed flow rate. Enter 4200

Step 8. The program asks for feed degree of vapourization using the following options:

1.Saturated feed

2.Saturated vapour

3.Partial vapour

Enter choice ? Enter 1

If options 3 is selected then, input the q factor ($0 < q < 1.0$). Enter 0.5

For options 1 and 2, $q = 1.0$ and $q = 0$ respectively.

Step 9. The program asks whether the user wants to assign reflux factor. Enter Y.

Option 1.Water condenser
2.Air condenser

Enter choice ? Enter1

Enter the value of the reflux factor within the range displayed on the screen. E.g for water condenser enter a value between 1.2 and 1.5. For saturated vapour where Reflux factor must be 1.3 or above for saturated vapour. Enter 1.2

If you do not want to assign reflux factor then Enter N. Computation will proceeds with reflux factor of 1.3 and temperature of condenser set at 327.59 K

On successful completion of computation the program takes you back to main menu.

Step 10. Select option 2 (that is enter 2). The program will ask you for output filename. Enter RESULT or any other name you want.

The program returns to main menu

after computation.

Step 11.Select View result by entering 3.

Follow the instructions given to view the design output.

CHAPTER FOUR

RESULTS AND DISCUSSION

4.1.0 THE TEST PROBLEM

The following problem is used to test the module.

A butane-pentane splitter is to be designed to process 4200 kg/hr of C_3-C_5 feed subject to the specifications of:

1. A maximum of 3 wt % i C_5 in the distillate product.
2. A maximum of 1 wt % C_4 in the bottom product.

The heat sink will be water (process design temperature to be 330.37K) and 5170.07 mmHg steam will be used as heat source in the re-boiler. The feed composition is given in Table 4.1

Table 4.1: Feed composition

Component		*wt %*
Propane	C_3	5
Iso-butane	iC_4	15
Butane	C_4	25
Iso-pentane	iC_5	20
Pentane	iC_5	35

Manual calculations of the short cut and rigorous methods are presented in appendix A and B respectively. Appendix C shows complete printout of computer solution while appendix D shows schematic diagram for the designed multi-component distillation column.

4.1.1 RESULTS AND DISCUSSION

The CAD module results obtained are presented in a file.

The module's results file consists of a summary of feed specification and results for shortcut and rigorous methods. These are shown in Tables 4.2, 4.3 and 4.4 respectively.

Table4.2: Feed Specification

```
Degree of vapourization (q): 1
Feed Temperature (K) : 351.76

 Component       Weight %

 1 Propane        5
 2 Iso-butane     15
 3 Butane         25
 4 Iso-pentane    20
 5 Pentane        35
```

Table4.3: Shortcut Result

```
Minimum number of stages:  9
Minimum reflux ratio: 0.85
Reflux factor:  1.24
Reflux ratio: 1.05
Feed point:  9
Total number of stages:  21

             Pressure (mmHg) Temperature (K)
Condenser:       6271.94        330.37
Column Top:      6401.94        340.10
Column Bottom:   6660.40        387.93

Overall column Pressure (mmHg): 6531.19

  Component   X-distillate      X-bottom
 1 Propane       0.1391          0.0000
 2 Iso-butane    0.3162          0.0005
 3 Butane        0.5164          0.0124
 4 Iso-pentane   0.0235          0.3446
 5 Pentane       0.0048          0.6426

Distillate product flow rate (mols/hr): 34.236

Bottom product  flowrate (mols/hr) : 31.480

Rectification Vapour flowrate (mols/hr): 70.317

Stripping Vapour flowrate (mols/hr): 70.317

Rectification Overflow (mols/hr): 36.081

Stripping Overflow (mols/hr):101.797
```

The short cut method results table 4.3 above show the minimum number of stages at total reflux, minimum reflux ratio, reflux factor selected, the reflux ratio required to achieve the separation, feed point location and the stage requirements. These are followed by the pressure and temperature profiles of the condenser, top and bottom of column, overall column pressure and molar flow rates of products distillate and bottoms, vapour and liquid overflow in the rectifying and stripping sections of the column.

Table 4.4 Rigorous Results As Shown In CAD Result File.

```
Stage Number :  1
Stage Temperature : 332.74

  Component      composition
 1 Propane        0.1391
 2 Iso-butane     0.3162
 3 Butane         0.5093
 4 Iso-pentane    0.0243
 5 Pentane        0.0111
```

In module's result file the rigorous method result is presented for each stage as shown in table 4.4 above.

The complete rigorous method result for easy discussion is shown in table 4.5. The first stage (1) is the condenser "stage" while the last stage (21) is the reboiler.

Table 4.5: Condensed Rigorous Method Results

Stage	temp(K)	C_3	iC_4	C_4	iC_5	C_5
1	332.74	0.1391	0.3162	0.5093	0.0243	0.0111
2	341.12	0.0503	0.2707	0.5802	0.0627	0.0360
3	344.88	0.0313	0.2299	0.5669	0.1026	0.0693
4	348.22	0.0265	0.2004	0.5235	0.1396	0.1100
5	350.89	0.0245	0.1790	0.4729	0.1689	0.1547
6	353.51	0.0232	0.1632	0.4264	0.1880	0.1992
7	355.70	0.0223	0.1519	0.3891	0.1967	0.2400
8	356.84	0.0216	0.1440	0.3616	0.1973	0.2755
9	358.03	0.0210	0.1381	0.3416	0.1929	0.3064
10	361.62	0.0077	0.1137	0.3577	0.2032	0.3177
11	364.02	0.0027	0.0902	0.3600	0.2159	0.3312
12	365.31	0.0009	0.0691	0.3498	0.2324	0.3478
13	367.72	0.0003	0.0508	0.3250	0.2539	0.3700
14	370.16	0.0001	0.0355	0.2866	0.2800	0.3978
15	373.58	0.0000	0.0235	0.2379	0.3082	0.4302
16	375.97	0.0000	0.0147	0.1855	0.3350	0.4647
17	379.67	0.0000	0.0087	0.1356	0.3563	0.4994
18	382.19	0.0000	0.0049	0.0934	0.3691	0.5327
19	384.24	0.0000	0.0026	0.0606	0.3718	0.5651
20	385.54	0.0000	0.0013	0.0367	0.3635	0.5985
21	387.93	0.0000	0.0006	0.0202	0.3437	0.6356

The trend in the values of mole fraction from the condenser (stage 1) to the re-boiler (stage 21) follows expectation. The values for the more volatile decreases while those for less volatile components increases.

To show this trend graphically a plot of column stage number and component composition was done and presented in figure 4.1.Figure 4.1 shows the concentration profiles from the final computer solution table 4.5.Note the discontinuities at the feed stage and the fact that feed stage composition differs considerably from the feed stream composition. It can also be seen from the figure that separation between the keys improves rapidly upward toward the condenser. This is as expected from literature (Perry and Green, 1973).

Table 4.6 Mole Fractions Obtained Using Manual, Shortcut and Rigorous Methods.

	X – Distillate			X- Bottoms		
Component	Manual	FUG	Rigorous	Manual	FUG	Rigorous
Propane	0.1386	0.1391	0.1391	0.0000	0.0000	0.0000
Iso- butane	0.3149	0.3162	0.3162	0.0007	0.0005	0.0006
Butane	0.5145	0.5164	0.5093	0.0124	0.0124	0.0202
Iso- pentane	0.0235	0.0235	0.0243	0.3459	0.3446	0.3437
Pentane	0.0085	0.0048	0.0111	0.6411	0.6426	0.6356

Table 4.7 Correlation analysis results of computed mole fractions

Distillate			
	Manual	*FUG*	*Rigorous*
Manual	1		
FUG	0.999978	1	
Rigorous	0.999969	0.999943	1
Bottoms			
	Manual	*FUG*	*Rigorous*
Manual	1		
FUG	0.999995	1	
Rigorous	0.999934	0.999932	1

Table 4.6 extracts the bottom and distillate compositions (stage 1 and 21 respectively) obtained using shortcut and rigorous methods and compared them with those obtained in manual calculation. The correlation coefficient between two set of result is shown in table 4.7. These correlation coefficients show that there is a good agreement between the values. The small differences between these three sets of computed mole fractions (table 4.6) is due to existence of components (especially the key components) having k-values < 1 in one section and k-values > 1 in another section of the cascade. This situation usually leads to computer truncation error (King, 1980).

This difference may also spring from the assumption of constant overall column pressure (6531.19 mmHg). This was different from the condenser and column bottom pressures (6271.94 and 6660.40 mmHg respectively). This difference will cause the computed k-values used in calculations of the rigorous method to vary from those used in the shortcut method.

Table 4.8 Design parameters Calculated

PARAMETER	MANUAL	CAD
N_{Min}	9	9
R_{Min}	0.91	0.85
R	1.13	1.05
Feed point	9	9
N	21	21
D mol/hr	34.369	34.236
B mol/hr	31.347	31.480

The sets of parameters calculated using manual and FUG shortcut calculations are presented in table 4.8.Correlation analysis of the two set of result gave a correlation coefficient of 0.999982. This correlation coefficient (0.999982) shows that there was good agreement between these results.

Product purity is achieved in the FUG method but not in the rigorous method due to approximations in CAD computation as shown below in table 4.9

Table 4.9 : Confirmation of Products Purity

ponent	*Distillate* D =34.236 mol/hr						*Bottoms* B = 31.480 mol / hr					
	FUG			*RIG*			*FUG*			*RIG*		
	XD	Kg/hr	Wt%	XD	Kg/hr	Wt%	XB	Kg/hr	Wt%	XB	Kg/hr	Wt%
ane	0.1391	210.0		0.1391	210.0		0.0000	0.0		0.0000	0.0	
Butane	0.3162	629.0		0.3162	629.0		0.0005	0.9		0.0006	1.1	
ne (LK)	0.5164	1027.2		0.5093	1013.0		0.0124	22.7	**1.00**	0.0202	37.0	**1.60**
entane(HK)	0.0235	58.0	**3.00**	0.0243	60.0	**3.09**	0.3446	782.1		0.3437	780.2	
ane	0.0048	11.9		0.0111	27.4		0.6426	1458.5		0.6356	1442.3	
		1936.1			1939.4			2264.2			2260.6	

To investigate the effects of reflux ratio and degree of vapourization of feed (q) on the number of stages required to achieve a given product purity, a number of program runs were carried out for a fixed product purity (as stated in the test problem) and using water condenser as the heat sink.

The effect of reflux ratio on the number of stages required is shown in Table 4.10. As can be seen as the reflux ratio increases the number of stages required decreases.

Table 4.10 : Effect of reflux ratio on number of stage required for a saturated feed using a water condenser.

Reflux Ratio (R)	*Stage Required (N)*
0.91	21
1.05	18
2.00	17

For a saturated vapour feed (q=0), the vapour flow rate reached a threshold value of 103.231 mol/hr from and above, which the rigorous method fails. This was as a result of entrainment of the reflux over flow due to high vapour flow rate (103.231 mol/hr) in the rectification section. This problem could be overcome by using a reflux factor of 1.3 (to achieve a reflux ratio greater than 2) or above for a water condenser as the heat sink.

q – factor does not give much effect on stage requirement, but as expected, it does have appreciable effect on the reflux overflow and vapour flow rates within the column as shown below in Table 4.11

Table 4.11 : Effects of q-factor on vapour and reflux overflow within column.

q-factor	*Rectification section (mol/hr)*		*Stripping section (mol/hr)*	
	Vapour	*Overflow*	*vapour*	*overflow*
0	103.231	68.785	37.514	68.785
0.5	83.893	49.447	51.035	82.305
1.00	70.633	36.188	70.633	101.904

The advantage of using results from the shortcut preliminary estimation method (FUG) as input data to the rigorous method (TDM) can be seen on figure 4.2. This figure shows the closeness between the initial temperature map estimate and the final converged temperature map from the computer. This greatly enhanced the speed of convergence. As convergence was achieved in four to five iterations, this reduces computer time and cost.

Correlation analysis of shortcut results obtained in this thesis with those presented by Onifade (2000) in his publication on CAD module for multi-component distillation column using Winn-Underwood-Gilliland shortcut and Thiele-Geddes rigorous methods compared very well as can be seen from the correlation coefficient of 0.999932.

All charts were drawn using Microsoft Excel 2000.

Figure 4.1 **Component Composition Profile**

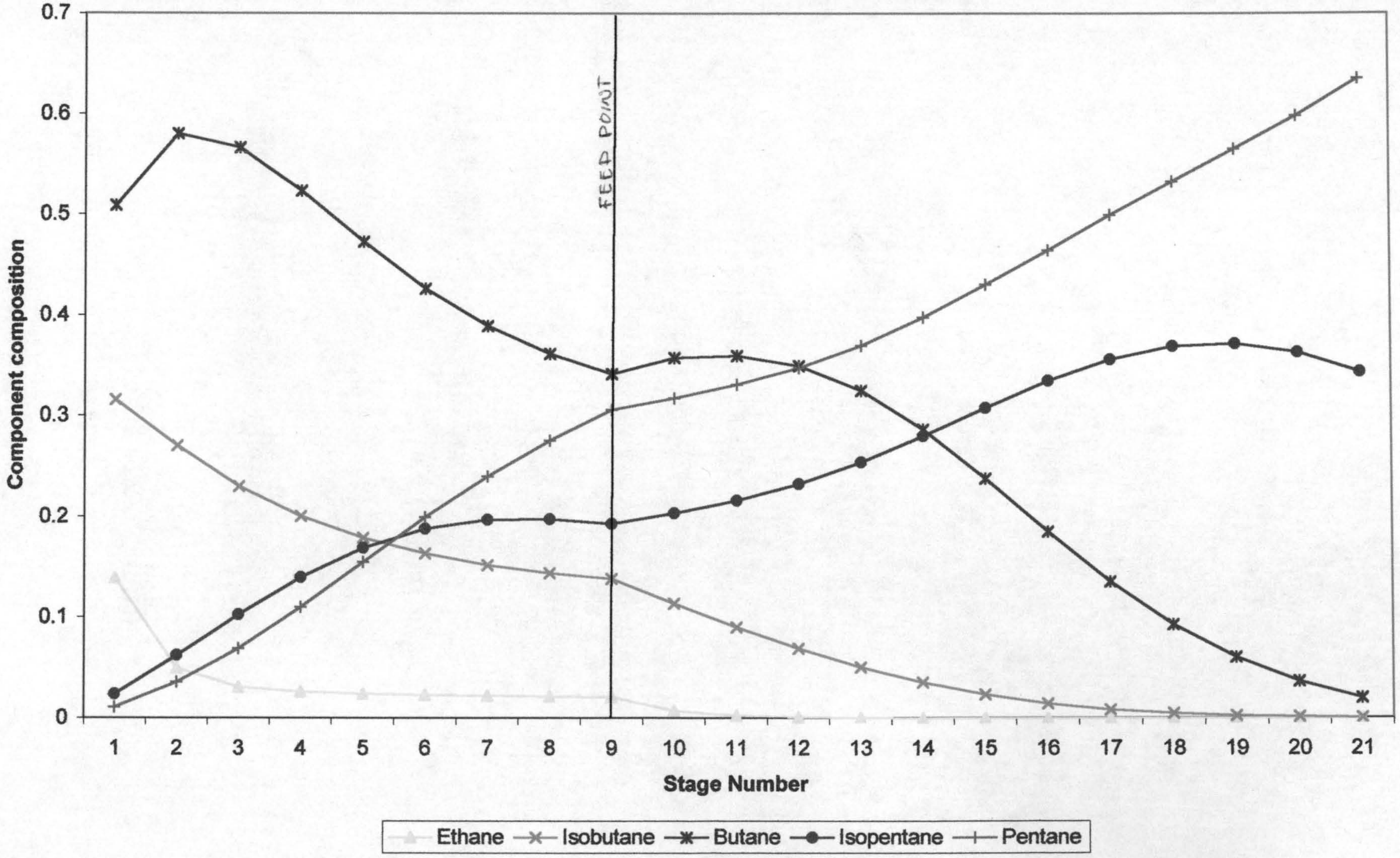
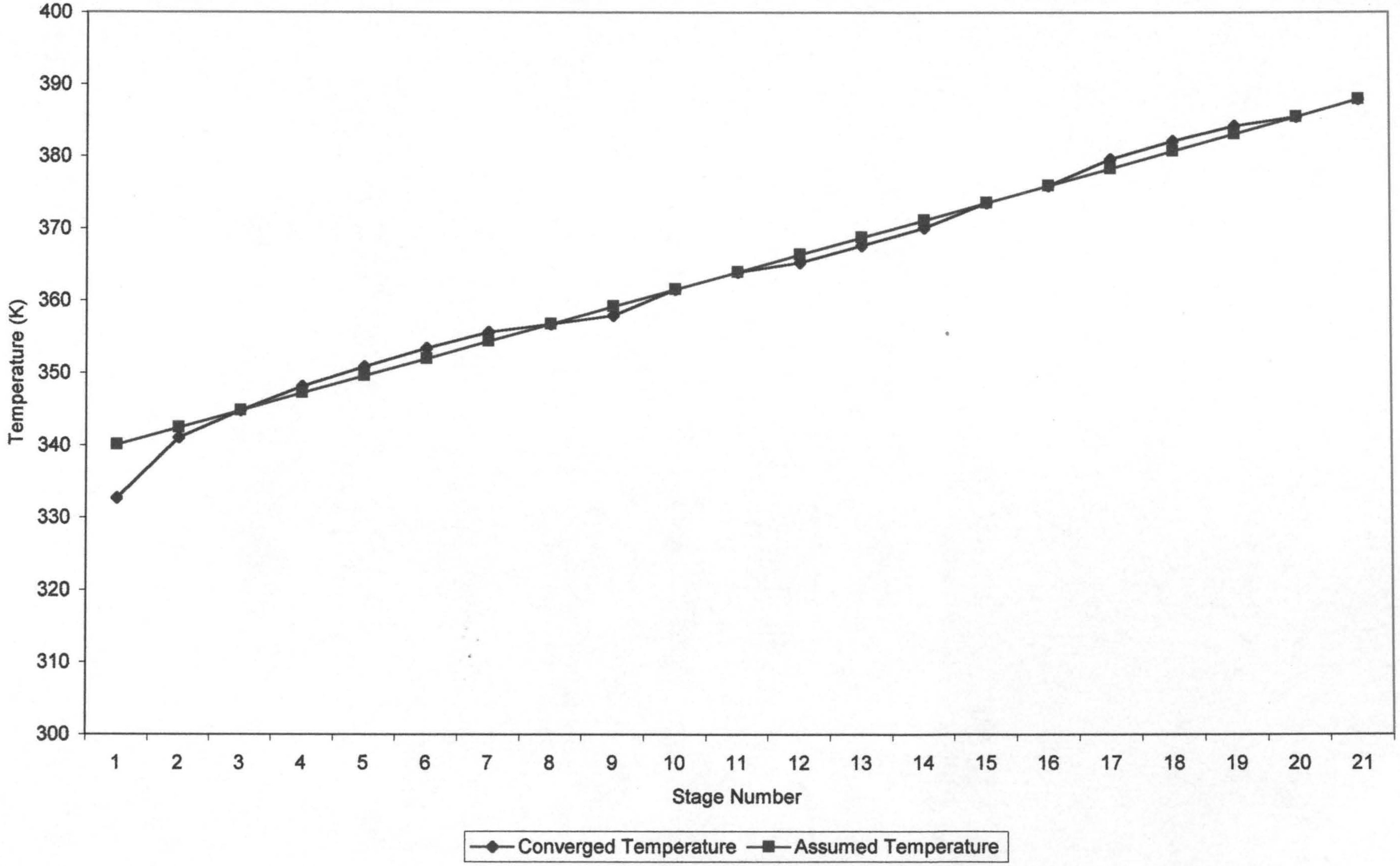


Figure 4.2 Assumed and Converged Temperature Profile



CHAPTER FIVE

5.1.0 CONCLUSION

A CAD module was developed for implementing the design of a multi-component distillation column. It employed Fenske, Underwood-Gilliland shortcut methods and Linear-Algebra rigorous solution. The module can be run either through a databank which contains mostly saturated straight chain hydrocarbons (C_1 to C_{20}) or through a provision within the module which the User can take to bypass the databank .By taking this path the User can supply all relevant data required for the design.

The module allows easy variation of the feed and product specifications, and design parameters of the shortcut method to obtain an optimal design.

Product purity of 3 wt% maximum iC_5 and 1wt% maximum C_4 in distillate and bottoms respectively was achieved in the shortcut method but not in the rigorous method. This is due to existence of components (especially the key components) having k-values < 1 in one section and k-values > 1 in another section of the cascade and also on the assumption of constant overall column pressure of 6112.98 mmHg.

The feed stage composition differs considerably from the feed stream composition as expected of most rigorous solution methods.

5.1.1 RECOMMENDATION

This CAD module could be further improved to handle wide range boiling mixtures by including enthalpy balance (i.e for non-constant molar overflow).

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APPENDIX A

SHORT CUT PROCEDURE

The problem statement gives the following:

1. Column total flow rate = 4200 kg/hr.
2. A maximum of 3 wt% Isopentane in the distillate product.
3. A maximum of 1 wt% Butane in the bottoms product.
4. Heat sink is air (design temperature 130°F)
5. Steam (5174 mmHg) to the reboiler.
6. Composition of various components are shown in Table A.1

Table A.1

Components	*Formula*	*wt%*
Propane	C_3	5
Isobutane	iC_4	15
Butane	C_4	25
Isopentane	iC_5	20
Pentane	C_5	35

DISTILLATE AND BOTTOMS COMPOSITION

Using the appropriate physical properties, the column feed is converted into molar and liquid volume units as shown on Table A.2.

Table A.2

Component	*WT%*	*kg/hr*	*Mol/WT.*	*Mol/hr*	*Mol%*
C_3	5	210.0	44.1	4.762	7.25
iC_4	15	630.0	58.1	10.843	16.50
C_4	25	1050.0	58.1	18.073	27.50
iC_5	20	840.0	72.1	11.651	17.73
C_5	35	1470.0	72.1	20.388	31.02
Total	100	4200.0	-	65.716	100.0

Reference liquid density is 60°F

Average molecular weight is 4200/65.716 = 63.91

Based on the given specifications the variables are assigned

X = mass, kg/hr C_4 in the bottoms products (1 wt%)

Y = mass, kg/hr iC_5 in the distillate products (3 wt%)

Assuming, (subject to later verification) that the C_3 and the iC_4 have negligible concentration in the bottoms, and that C_5 has negligible concentration in the distillate, the flow material balance can be prepared yielding the overall separation as shown in Table A.3.

Table A.3

Components	*Feed*	*Distillate*	*Bottoms*
C_3	210.0	210.0	0
iC_4	630.0	630.0	0
C_4	1050.0	1050 - X	X
iC_5	840.0	Y	840-Y
C_5	1470.0	0	1470
Total	4200.0	1890-X-Y	2310+X-Y

Distillate specification : 3 wt% iC_5 in distillate

$$3/100 = Y/(1890 - X + Y)$$

Bottoms specification : 1 wt% C_4 in bottoms

$$1/100 = X(2310 + X - Y)$$

solving these simultaneous linear equations yields

$$X = 22.75$$

$$Y = 57.75$$

Substituting the above values for X and Y in Table A.1 to obtain Table A.4

Table A.4

Components	*Feed*	*Distillate(kg/hr)*	*Bottoms(kg/hr)*
C_3	210.0	210.0	0
iC_4	630.0	630.0	0
C_4	1050.0	1027.25	22.75
iC_5	840.0	57.75	782.25
C_5	1470.0	0.00	1470
Total	4200.0	1925.00	2310.00

The result obtained above in terms of molar composition is shown on Table A.5 below.

Table 4.5

Components	*Feed*	*Distillate(Mol/hr)*	*Bottoms(Mol/hr)*
C_3	4.762	4.762	0.000
iC_4	10.843	10.843	0.000
C_4	18.072	17.680	0.392
iC_5	11.651	0.791	10.850
C_5	20.388	0.000	20.388
Total	65.716	34.067	31.630

4.[illegible].3 TEMPERATURE – PRESSURE OF TOP AND BOTTOM

For the fixed temperature 327.6K for air, the bubble point calculation requires pressure be determined. Design equation for bubble point calculation is :

$\Sigma K_i X_i = 1.0$

The characteristic component is iC_4 and

$P_{estimated} = P_{iC4}(327.6K) = 5622.198$ mmHg.

Components	*D.mol*	X_d	*K(5852.2 mmHg)*	*K(5852.2 mmHg)*
C_3	4.762	0.1398	2.46	2.36
iC_4	10.843	0.3180	1.00	0.96
C_4	17.680	0.5190	0.74	0.71
iC_5	0.791	0.0232	0.31	0.30
C_5	0.000	0.0000	0.24	0.23
Total	34.067	1.0000	-	-

For P = 5622.198 mmHg

$\Sigma K_i X_i = 1.0511$

For $P = 5852.198$ mmHg

$\Sigma K_i X_i = 1.0099$

The result of the distillate bubble point calculation for condenser are

$T = 327.6$ K and $P = 5852.198$ mmHg

The conditions at the top of the column must be evaluated, since the fractionator has a total condenser and not an equilibrium stage. The criteria for evaluation of the dew point conditions are:

Assumption of a pressure drop through the total condenser of 129.287 mmHg. Thus, the pressure at the top of the column is established as $P = 129.287 + 5852.199 = 5981.486$ mmHg.

The dew point design equation with the pressure specified is

$\Sigma [Y_i / K_i] = 1.0$

Since the fractionator has a total condenser, the column top vapour composition is identical to the distillate composition. Again using iC_4 as the characteristic component, vapour-pressure data can be used to estimate the column top temperature.

$P_{iC4}(T) = 5981.486$ mmHg

$T = 330.26$ K

Components	*Y_i*	*K(330.26 K)*	*K(334.26 K)*
C_3	0.1398	2.44	2.75
iC_4	0.3180	1.00	1.15
C_4	0.5190	0.74	0.85
iC_5	0.0232	0.31	0.37
C_5	0.0000	0.25	0.29
Total	1.0000	-	-

For T = 330.3 K; $\Sigma [Y_i / X_i] = 1.151$

For T = 334.3 K; $\Sigma [Y_i / X_i] = 1.046$

The result of the column top dew point calculation is

T = 334.3 K and P = 5981.48 mmHg

The column bottom conditions are evaluated at the reboiler, which is assumed to be an equilibrium stage. The criteria for establishing the condition at the bottoms of the column are: Assume a a column pressure drop of 258.574 mmHg. Thus, the column pressure is:

P = 258.374 + 5981.486 = 6240.06 mmHg

The bubble point design equation with temperature specified is

$\Sigma [K_i / X_i] = 1.0$

The bubble point calculation for a fixed pressure of 6240.06 mmHg requires that the temperature be determined. The average molecular weight can be determined from the product summary.

Average molecular weight = 2275.0/3163 = 71.93

The characteristic component is iC_5. Using vapour pressure data, an estimated bottoms temperature is obtained.

$P_{iC5}(T) = 6240.06$ mmHg; T = 380.68 K

Components	*B.mol*	X_d	*K(380.68 K)*	*K(383.68 K)*
C_3	0.000	0.0000	5.59	5.84
iC_4	0.000	0.0000	2.59	2.72
C_4	0.392	0.0124	2.06	2.16
iC_5	10.850	0.3430	1.00	1.06
C_5	20.388	0.6446	0.84	0.89
Total	31.630	1.0000	-	-

For T = 380.68 K; $\Sigma K_i X_i = 0.9094$

For T = 383.68 K; $\Sigma K_i X_i = 0.9676$

The result of the column bubble point calculation is

T = 383.68 K and P = 6240.06 mmHg.

From above and problem statement,

Reference component: Isopentane

Light key (LK) : Butane

Heavy key (HK) : Isopentane

a) The minimum number o stages is obtained using the Fenske equation.

$$N_{min} = \frac{\ln [(17.680/0.801) \times (10.850/0.392)]}{\text{Ln}\ (1.97/1.00)} = 9.461$$

b) The degree of separation for the nonkey components is estimated using the Fenske equation coupled with the overall material balance. To aid in the computational effort, the mean relative volatility is calculated.

$$\alpha_{mean} = \frac{\alpha_{LK} + \alpha_{HK}}{2} = \frac{1.97 + 1.00}{2} = 1.485$$

The separation of the nonkey components uses the data :

Propane (C_3) : $\alpha_{C_3} > \alpha_{mean}$

$\alpha_{C_3} = 4.90$

$f_{C_3} = 4.762$ mol/h

$$b_{C_3} = \frac{4.762}{1 + (0.801/10.850)\,(2.56/100)^{9.461}}$$

$= 0.020$ mol/h

$dc_3 = fc_3 - bc_3 = 4.762$ mol/h

The assumed and calculated separations of propane agree.

Isobutane (iC_4) : $\alpha_{iC_4} > \alpha_{mean}$

$A_{iC_3} = 2.56$

$F_{iC_4} = 10.843$

$$B_{iC_4} = \frac{10.843}{1 + (0.801/10.850)\,(2.56/100)^{9.461}}$$

$= 0.020$ mol/h

$d_{iC_4} = f_{ic_4} - b_{ic_4} = 10.823$ mol/h

The assumed separation had all of the iC_4 in the distillate. Since there is some iC_4 in the bottoms product, the column operating conditions and fractionation at infinite reflux must be recalculated.

Pentane (C_5) : $\alpha_{C_5} > \alpha_{mean}$

$$\alpha_{C_5} = 0.84$$

$$f_{C_5} = 20.388 \text{ mol/h}$$

$$d_{C_5} = \frac{20.388}{1 + (0.392/17.680)\,(1.97/0.84)^{9.461}}$$

$$= 0.285 \text{ mol/h}$$

$$b_{C_5} = f_{C_5} - d_{C_5} = 20.103 \text{ mol/h}$$

As with the iC_4 separation, the C_5 assumed and calculated separations do not agree.

c) The calculated separation is summarized below in both molar and mass units. Molar units, lb mol/h:

Component	*Feed*	*Distillate*	*Bottoms*
C_3	4.762	4.762	0.000
iC_4	10.843	10.843	0.020
C_4	18.072	17.680	0.392
iC_5	11.651	0.801	10.850
C_5	20.388	0.285	20.103
Total	65.716	34.351	31.365

Mass unit, lb/h:

Component	*Feed*	*Distillate*	*Bottoms*
C_3	210.0	210.0	0
iC_4	630.0	628.84	1.16
C_4	1050.0	1027.25	22.75
iC_5	840.0	57.75	782.25
C_5	1470.0	20.55	1449.45
Total	4200.0	1944.39	2255.61

d) For the calculated separation the specifications are compared and evaluated.

- Maximum of 3 wt% iC_5 in distillate

$$\text{Calculated value} = \frac{57.75}{1944.39} \times 100$$

$$= 2.97 \text{ wt\%}$$

since 2.97 < 3.00%, the specification is satisfied.

- Maximum of 1 wt% C_4 in the bottoms

$$\text{Calculated value} = \frac{22.75}{2255.61} \times 100$$

$$= 1.01 \text{ wt\%}$$

since 1.01 > 1.00%, the specification is not satisfied.

When the specifications are not satisfied, the separation assume is incorrect. A new separation must be assumed and the calculations must be repeated until the specifications are satisfied.

The revised separation is summarized below in molar units:

Table A11:

Component	*Feed*	*Distillate*	*Bottoms*
C_3	4.762	4.762	0.000
iC_4	10.843	10.822	0.021
C_4	18.072	17.684	0.388
iC_5	11.651	0.809	10.842
C_5	20.388	0.292	20.096
Total	65.716	34.369	31.347

Using equations 2.3.6 to 2.4.5 and the various empirical correlations the following parameters were determined:

Minimum number of stages = 9.00

Minimum reflux ratio = 0.91

Reflux ratio = 1.13

Feed point = 9 from the top

Number of stages = 21

APPENDIX B

RIGOROUS METHOD

Initial assumption

A temperature profile must first be assumed to start the rigorous method. This variable is referred to as tear variable and must be iterated until convergence is achieved.

Initial temperature profile for column assuming a linear increase from top to bottom.

Table B1:Initial temperature profile

Stage #	Temp(K)
1	340.09
2	342.49
3	344.88
4	347.27
5	349.66
6	352.05
7	354.44
8	356.84
9	359.23
10	361.62
11	364.01
12	366.40
13	368.79
14	371.19
15	373.58
16	375.97
17	378.36
18	380.75
19	383.14
20	385.54
21	387.93

Employing the stage temperature and equation 2.1 together with the overall column pressure (6239.00mmHg), K-values were computed for each of the components on each of the stages.

The following calculations were done for propane only.

Equations 2.74 to 2.76 were used to calculate Thomas parameters shown in the table below.

Table B2: Thomas parameters

An	Bn	Cn
0	-70.31722	199.1412
36.08079	-235.222	208.1281
36.08079	-244.2089	217.3782
36.08079	-253.4589	226.8937
36.08079	-262.9745	236.6774
36.08079	-272.7582	246.7317
36.08079	-282.8125	257.0587
36.08079	-293.1395	267.6609
101.7972	-369.4581	278.5401
101.7972	-380.3373	289.6987
101.7972	-391.4959	301.1385
101.7972	-402.9357	312.8611
101.7972	-414.6583	324.8687
101.7972	-426.666	337.1626
101.7972	-438.9598	349.7448
101.7972	-451.542	362.6165
101.7972	-464.4137	375.779
101.7972	-477.5762	389.234
101.7972	-491.0312	402.9823
101.7972	-504.7795	417.0256
101.7972	-448.5056	0

Equations 2.113 to 2.116 were used to calculate Jn and En shown in table B3

Table B3:

Jn	En
-2.832041	0
-1.564405	0
-1.15772	0
-1.071833	0
-1.055174	0
-1.051324	0
-1.049734	0
-1.048564	0
-1.060228	1.812559E-02
-1.063469	6.773395E-03
-1.0632	2.434395E-03
-1.061608	8.408908E-04
-1.059621	2.792017E-04
-1.057601	8.915305E-05
-1.055677	2.739377E-05
-1.053882	8.104607E-06
-1.052215	2.310147E-06
-1.050667	6.347897E-07
-1.049225	1.682474E-07
-1.047878	4.303603E-08
0	1.281599E-08

The mole fractions were computed using equations 2.117 and 2.118. Starting from the re-boiler stage.
At the re-boiler x_n = 1.281599E-08 which is approximately equals to zero

Table B4: mole fraction of propane

Stage#	x_n
21	0.0000
20	0.0000
19	0.0000
18	0.0000
17	0.0000
16	0.0000
15	0.0000
14	0.0001
13	0.0004

12	0.0013
11	0.0038
10	0.0108
9	0.0296
8	0.0310
7	0.0326
6	0.0342
5	0.0361
4	0.0387
3	0.0448
2	0.0701
1	0.1986

In the same way the mole fractions of the rest of the components were calculated, these mole fractions were adjusted using the theta convergence method, normalized and bubble point calculation done to determine the various stage temperatures. This is repeated until the mole fractions and temperature converged.

Table B5 below shows the converged mole fractions and temperatures for the entire components and stages.

Table B5: final converged mole fractions and temperature.

Stage	temp(K)	C_3	iC_4	C_4	iC_5	C_5
1	332.74	0.1391	0.3162	0.5093	0.0243	0.0111
2	341.12	0.0503	0.2707	0.5802	0.0627	0.0360
3	344.88	0.0313	0.2299	0.5669	0.1026	0.0693
4	348.22	0.0265	0.2004	0.5235	0.1396	0.1100
5	350.89	0.0245	0.1790	0.4729	0.1689	0.1547
6	353.51	0.0232	0.1632	0.4264	0.1880	0.1992
7	355.70	0.0223	0.1519	0.3891	0.1967	0.2400
8	356.84	0.0216	0.1440	0.3616	0.1973	0.2755
9	358.03	0.0210	0.1381	0.3416	0.1929	0.3064
10	361.62	0.0077	0.1137	0.3577	0.2032	0.3177
11	364.02	0.0027	0.0902	0.3600	0.2159	0.3312
12	365.31	0.0009	0.0691	0.3498	0.2324	0.3478
13	367.72	0.0003	0.0508	0.3250	0.2539	0.3700
14	370.16	0.0001	0.0355	0.2866	0.2800	0.3978
15	373.58	0.0000	0.0235	0.2379	0.3082	0.4302
16	375.97	0.0000	0.0147	0.1855	0.3350	0.4647
17	379.67	0.0000	0.0087	0.1356	0.3563	0.4994
18	382.19	0.0000	0.0049	0.0934	0.3691	0.5327
19	384.24	0.0000	0.0026	0.0606	0.3718	0.5651
20	385.54	0.0000	0.0013	0.0367	0.3635	0.5985
21	387.93	0.0000	0.0006	0.0202	0.3437	0.6356

APPENDIX C

```
FEED SPECIFICATION
Degree of vapourization (q): 1
Feed Temperature (K) : 351.76
  Component   Weight %
 1 Propane      5
 2 Iso-butane  15
 3 Butane      25
 4 Iso-pentane 20
 5 Pentane     35

 SHORT-CUT RESULT

Minimum number of stages :  9
Minimum reflux ratio : 0.85
Reflux factor :  1.24
Reflux ratio : 1.05
Feed point :  9
Total number of stages :  21

         Pressure (mmHg)   Temperature (K)
Condenser  :   6271.94          330.37
Column Top :   6401.94          340.10
Column Bottom :6660.44          387.93

Overall column Pressure (mmHg) :6531.19

  Component   X-distillate  X-bottom
 1 Propane    0.1391          0.0000
 2 Iso-butane 0.3162          0.0005
 3 Butane     0.5164          0.0124
 4 Iso-pentane0.0235          0.3446
 5 Pentane    0.0048          0.6426

Distillate product molar flowrate (mols/hr) :
34.236

Bottom product molar flowrate (mols/hr) : 31.480
```

```
Rectification Vapour flowrate (mols/hr) : 70.317

Stripping Vapour flowrate (mols/hr) : 70.317

Rectification Overflow (mols/hr) : 36.081

Stripping Overflow (mols/hr) :101.797
```

RIGOROUS METHOD RESULT

```
Stage Number :  1
Stage Temperature : 332.74

  Component      composition
 1 Propane         0.1391
 2 Iso-butane      0.3162
 3 Butane          0.5093
 4 Iso-pentane     0.0243
 5 Pentane         0.0111

Stage Number :  2
Stage Temperature : 341.12

  Component      composition
 1 Propane         0.0503
 2 Iso-butane      0.2707
 3 Butane          0.5802
 4 Iso-pentane     0.0627
 5 Pentane         0.0360

Stage Number :  3
Stage Temperature : 344.88

  Component      composition
 1 Propane         0.0313
 2 Iso-butane      0.2299
 3 Butane          0.5669
 4 Iso-pentane     0.1026
 5 Pentane         0.0693
```

```
Stage Number :  4
Stage Temperature : 348.22

  Component     composition
 1 Propane       0.0265
 2 Iso-butane    0.2004
 3 Butane        0.5235
 4 Iso-pentane   0.1396
 5 Pentane       0.1100

Stage Number :  5
Stage Temperature : 350.89

  Component     composition
 1 Propane       0.0245
 2 Iso-butane    0.1790
 3 Butane        0.4729
 4 Iso-pentane   0.1689
 5 Pentane       0.1547

Stage Number :  6
Stage Temperature : 353.51

  Component     composition
 1 Propane       0.0232
 2 Iso-butane    0.1632
 3 Butane        0.4264
 4 Iso-pentane   0.1880
 5 Pentane       0.1992

Stage Number :  7
Stage Temperature : 355.76

  Component     composition
 1 Propane       0.0223
 2 Iso-butane    0.1519
 3 Butane        0.3891
 4 Iso-pentane   0.1967
 5 Pentane       0.2400
```

```
Stage Number :  8
Stage Temperature : 356.84

Component     composition
 1 Propane        0.0216
 2 Iso-butane     0.1440
 3 Butane         0.3616
 4 Iso-pentane    0.1973
 5 Pentane        0.2755

Stage Number :  9
Stage Temperature : 358.03

  Component     composition
 1 Propane        0.0210
 2 Iso-butane     0.1381
 3 Butane         0.3416
 4 Iso-pentane    0.1929
 5 Pentane        0.3064

Stage Number :  10
Stage Temperature : 361.62

  Component     composition
 1 Propane        0.0077
 2 Iso-butane     0.1137
 3 Butane         0.3577
 4 Iso-pentane    0.2032
 5 Pentane        0.3177

Stage Number :  11
Stage Temperature : 364.02

  Component     composition
 1 Propane        0.0027
 2 Iso-butane     0.0902
 3 Butane         0.3600
 4 Iso-pentane    0.2159
 5 Pentane        0.3312
```

```
Stage Number :  12
Stage Temperature : 365.31

  Component    composition
 1 Propane       0.0009
 2 Iso-butane    0.0691
 3 Butane        0.3498
 4 Iso-pentane   0.2324
 5 Pentane       0.3478

Stage Number :  13
Stage Temperature : 367.72

  Component    composition
 1 Propane       0.0003
 2 Iso-butane    0.0508
 3 Butane        0.3250
 4 Iso-pentane   0.2539
 5 Pentane       0.3700

Stage Number :  14
Stage Temperature : 370.16

  Component    composition
 1 Propane       0.0001
 2 Iso-butane    0.0355
 3 Butane        0.2866
 4 Iso-pentane   0.2800
 5 Pentane       0.3978

Stage Number :  15
Stage Temperature : 373.58

  Component    composition
 1 Propane       0.0000
 2 Iso-butane    0.0235
 3 Butane        0.2379
 4 Iso-pentane   0.3082
 5 Pentane       0.4302
```

```
Stage Number :  16
Stage Temperature : 375.97

  Component    composition
 1 Propane       0.0000
 2 Iso-butane    0.0147
 3 Butane        0.1855
 4 Iso-pentane   0.3350
 5 Pentane       0.4647
Stage Number :  17
Stage Temperature : 379.69

  Component    composition
 1 Propane       0.0000
 2 Iso-butane    0.0087
 3 Butane        0.1356
 4 Iso-pentane   0.3563
 5 Pentane       0.4994

Stage Number :  18
Stage Temperature : 382.19

  Component    composition
 1 Propane       0.0000
 2 Iso-butane    0.0049
 3 Butane        0.0934
 4 Iso-pentane   0.3691
 5 Pentane       0.5327

Stage Number :  19
Stage Temperature : 384.24

  Component    composition
 1 Propane       0.0000
 2 Iso-butane    0.0026
 3 Butane        0.0606
 4 Iso-pentane   0.3718
 5 Pentane       0.5651
```

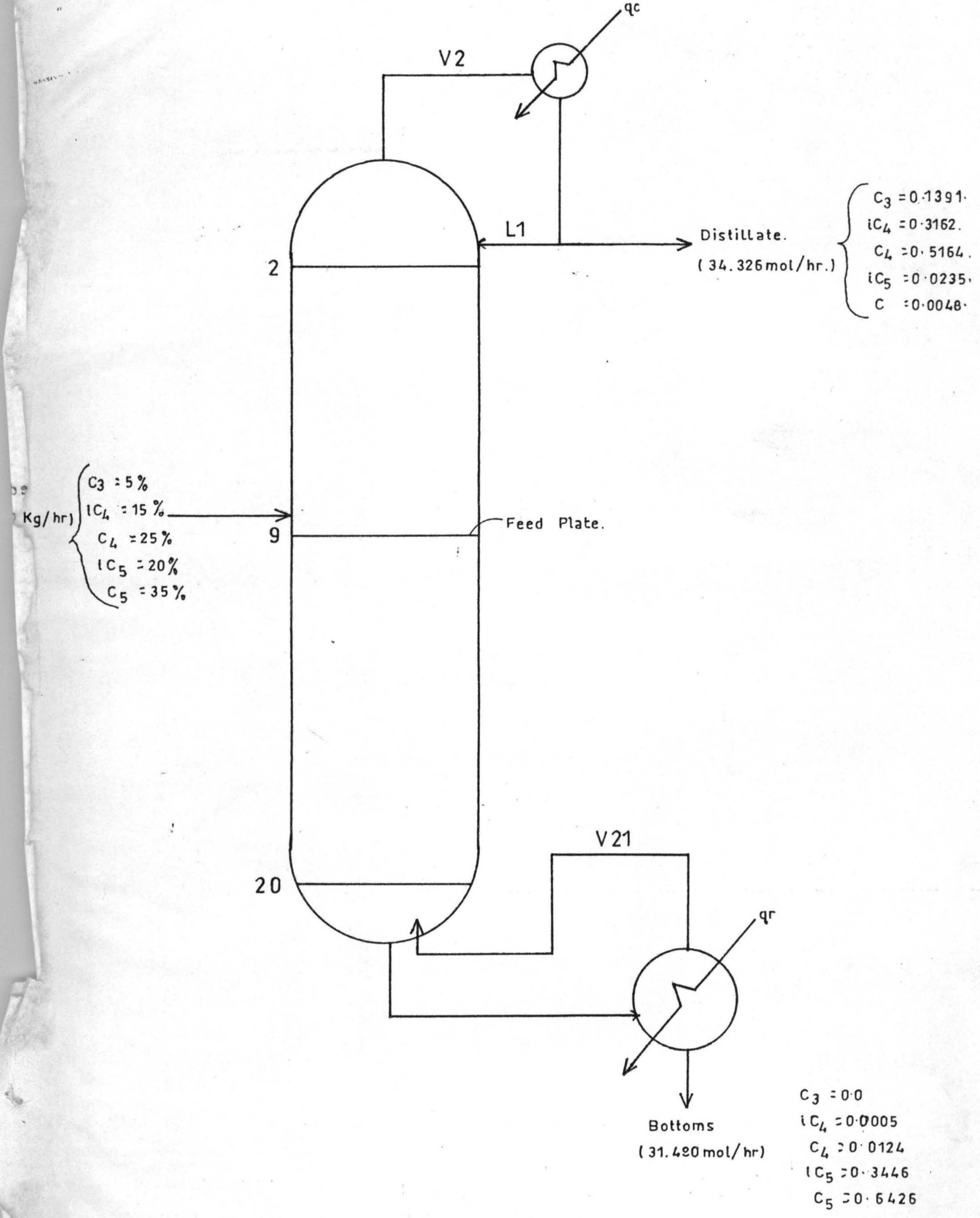
```
Stage Number :  20
Stage Temperature : 385.54

  Component      composition
 1 Propane          0.0000
 2 Iso-butane       0.0013
 3 Butane           0.0367
 4 Iso-pentane      0.3635
 5 Pentane          0.5985

Stage Number :  21
Stage Temperature : 387.93

  Component      composition
 1 Propane          0.0000
 2 Iso-butane       0.0006
 3 Butane           0.0202
 4 Iso-pentane      0.3437
 5 Pentane          0.6356
```

APPENDIX D·



e D- Schematic Diagram for Multi-component Distillation Column·