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DESIGN AND OPTIMIZATION OF DISTILLATION
SYSTEMS VIA. COMPUTER

A Thesis
Presented for the
Master of Science
Degree
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Shabbir K. Hussain

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ABSTRACT

A computer program has been written for the design of a binary distillation column. The program calculates the total annual operating cost at a specified reflux ratio. Other variables calculated include: number of trays, installed cost, energy usage, and optimum feed point.

The program can solve ideal as well as non-ideal systems. Well established UNIQUAQ correlations were used to get the vapor-liquid equilibria. The Yen-Alexander correlations were used to predict enthalpies. For the calculation of distillation column variables, the code used the method of Ponchon-Savarit. This is a more rigorous method than that of McCabe-Thiele.

The code was checked with Benzene-Toulene as an example of an ideal system and with Ethanol-Water as a non-ideal system. For the ideal system, the code gave 1.15579 as a minimum reflux, and 1.248 for the optimum reflux. This compared favorably to Peter's graphical solution (McCabe-Thiele) of 1.14 and 1.25 respectively. The code predicted a total annual operating cost at optimum reflux of \$103,580 compared to Peter's graphical result of \$99,000. For the non-ideal case, the code was checked with the problem solved by Manzoor. The results for feed plate position and total number of plates were in complete agreement with the Manzoor's results. The feed plate was predicted to be the fifth plate and the total number of plates was seven. The only difference was the minimum reflux ratio. The code gave this ratio as 0.454, compared to Manzoor's value of 0.434.

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NOMENCLATURE

B	Bottom Stream rate, Kmole/sec
b	Exponent in Equations (2.1.10, 11, and 12)
C_F	Flooding constant in Equation (2.3.4), empirical
C_p	Heat capacity, KJ/Kmole
D	Distillate rate, Kmole/sec
F	Feed rate, Kmole/sec
G	Vapor rate, enriching section, G' , stripping section, Kmole/sec
H	Enthalpy, H_M , heat of mixing, $H-H^\circ$, enthalpy departure function, H_V , Enthalpy of vaporization, KJ/Kmole
L	Liquid rate, enriching section, L' , stripping section, L_O , external reflux ratio, Kmole/sec
m	Slope of tie line
N	Number of trays
p	Vapor pressure, atm
P	Total pressure, atm
q	Uniquac surface parameter
Q_c	Heat removed at condenser, Q_B , heat added at reboiler KJ/hr, Q , Q' , quantities defined by Equations (2.2.8 and 9)
Q_T	Volumetric flow rate of gas, m^3 /sec
r	Uniquac volume parameter
R	Reflux ratio, gas constant
t	Tray spacing, meter
T_D	Tower diameter, meter
T	Temp, °K

NOMENCLATURE (continued)

u	Uniquac energy interaction parameter
V_{IL}	Liquid molal volume, cm^3/gmole
V_F	Flooding velocity, m/sec
W	Constant in Equations (2.1.11 and 12)
X	Mole fraction of more volatile component in liquid phase
Y	Mole fraction of more volatile component in vapor phase

Greek

β	Quantity defined by Equations (2.1.11, 12 and 2.3.3)
ρ	Density, Kg/m^2
α	Relative volatility, (non-dimensional), quantity defined by Equation (2.3.2)
λ	Latent heat of vaporization, KJ/Kmole
σ	Surface tension, N/m
γ	Activity coefficient

Subscripts

av	Average
b	Normal boiling point
B	Bottoms, component B
c	critical, number of components
D	Distillate
F	Feed
G	Vapor
i	Any component

NOMENCLATURE (continued)

L	Liquid
m	Plate in stripping section, minimum
n	Plate in enriching section
r	Reduced

Superscripts

°	Ideal
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CHAPTER 1

INTRODUCTION

1.1 Problems

A substantial number of the unit operations of chemical engineering are concerned with the problem of changing the composition of solutions through methods not necessarily involving chemical reactions. The purpose of such operations is directed towards separating a substance into its component parts. The separation or purification costs depends directly upon the ratio of final to initial concentration of the separated substances. If this ratio is large, cost of their separation is large and hence the final cost of the product is large.

The purpose of distillation is either to separate liquid mixtures into their original components or to split them up into other mixtures having compositions other than that of the original mixture. Here the new phase created differs from the original one by its heat content, which can be readily added or removed. Distillation is by far the most common separation technique used in the petroleum, natural gas and chemical industries. In an audit of distillation energy consumptions for the production of various large-volume chemicals, it was concluded that distillation consumes about 3% of the United States' energy (Mix, et al., 1978). According to statistics of the U.S. Department of Energy, 1980, total distillation energy consumption was 7965 BTU/lb. A 10% savings in distillation

energy would amount to a savings of about \$500 million in the national energy cost (King, 1980). There is a substantial incentive for developing and implementing ways of lessening the energy consumption of distillation.

Calculation methods, aimed principally at determining the number of plates and the operating conditions required for a specified separation, have well developed theoretical background (McCabe and Smith, 1976). As the reflux ratio is increased the number of theoretical stages required for the specified separation decreases (resulting in lower capital cost) but energy requirements increases (resulting in higher operating cost). Various combinations of stages and reflux ratios can be used to accomplish a desired separation. Today, energy costs are so high relative to fabricated materials cost that the economic optimum design reflux ratio falls less than 10% above the minimum allowable reflux. The best operating condition is therefore a compromise between the reflux ratio and the total number of plates.

1.2 Binary System

The principle object of distillation calculations is to determine the number of plates or height of column required in order to separate a mixture to a specified extent at an economic reflux ratio. This calculation can be carried out graphically when a binary mixture is distilled. When the boiling points of the pure components are close together, the latent and sensible heats of the mixtures vary only a little with composition and consequently it can be assumed

that the vapor and liquid molal flow rates do not change from plate-to-plate except at the feed point. This applies to the majority of distillations. It is then unnecessary to make heat balances, and the graphical application of material balances leads to the McCabe-Thiele method of calculation. For an ideal solution, the equilibrium partial pressure of a constituent at a fixed temperature equals the product of its vapor pressure, when pure at this temperature, and its mole fraction in the liquid phase. When a mixture is far from ideality the graphical method of Ponchon-Savarit should be used. This method accounts for the fact that vapor and liquid flow rates may change as they pass through the column. Like McCabe-Thiele, the Ponchon-Savarit graphical method for making stage-to-stage calculations is restricted to binary systems only. Hand calculation by these methods need quite an amount of time due to repetition of calculations and their complexity. To avoid this, the existing facility of different varieties of computers could be used to speed up accurate calculation by this complicated procedure.

1.3 Optimization

The design of a distillation unit is ordinarily based on specifications giving the degree of separation required for a feed supplied to the unit at a known composition, temperature and flow rate. The design engineer must determine the size of column and reflux ratio necessary to meet the specifications. At the minimum reflux ratio the column requires an infinite number of trays, and consequently the fixed cost is infinite. However, the operating costs (reboiler

heat supply, condenser coolant, etc.) are at the minimum. As the reflux ratio is increased, the number of theoretical stages required for the given separation decreases, but the column diameter increases owing to the larger quantities of recycled liquid and vapor. The fixed costs therefore fall through a minimum and rise to a maximum again at total reflux. The optimum reflux ratio occurs at the point where the sum of fixed charges and operating costs is a minimum (Figure 1).

1.4 Objectives, Methodology and Approach

The main aim of this work is to develop a computer program which can calculate operating variables of ideal and non-ideal binary distillation systems by the Ponchon-Savarit method. Once these variables are known, the code can go further and calculate tower diameter based on vapor velocity, and the annual cost of operating the tower. By varying different reflux ratios, a point is reached where total annual cost is minimized. The reflux ratio for minimum total cost is the main task of this work.

The successful application of distillation methods depends greatly upon the accuracy of vapor-liquid equilibria. The program has been developed in such a manner that it calculates saturation temperature and mole fraction of the more volatile component in vapor phase. For this type of calculation, the program is provided with the mole fraction of the component in the liquid phase and total pressure of the system. This program has been developed for the pressure of 1 atm only. The code uses the correlations of Antoine

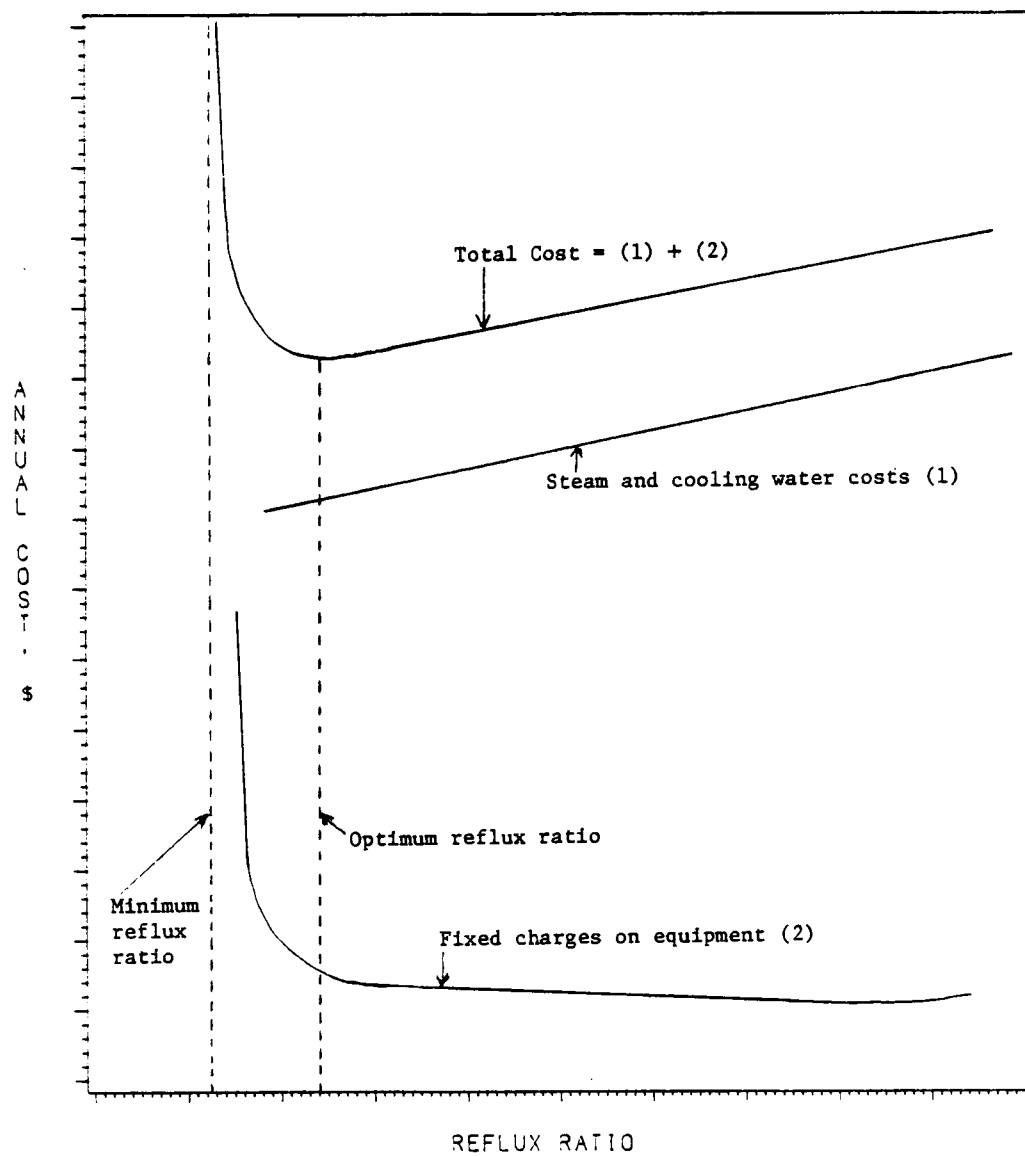


Figure 1. Optimum reflux ratio in distillation operation.

for the vapor pressure and UNIQUAC for the calculation of the vapor-liquid equilibria of both the systems.

The next step is the calculation of enthalpy-concentration data. Thermodynamic functions, being state functions, are independent of path. Thus, two different approaches have been taken to calculate the enthalpy at a specific concentration. For an ideal system, we have

$$H_L = \sum_{i=1}^c X_i C_{P_{iL}} \quad (1.4.1)$$

$$H_G = \sum_{i=1}^c Y_i C_{P_{iL}} + \sum_{i=1}^c Y_i \lambda_i \quad (1.4.2)$$

The enthalpy obtained by these correlations was checked with the Benzene-Toulene binary system.

For non-ideal system, the program has been developed to calculate those systems which show positive deviation from ideality, i.e., minimum-boiling mixtures/azeotropes. For such systems, the enthalpy departure function and heat of solution are also necessary.

Being acquainted with the above, the author decided to follow a different path for calculating the enthalpy of non-ideal systems. Basing enthalpy on ideal gas heat capacity, we have

$$H_G = \sum_{i=1}^c Y_i C_{P_{iG}}^\circ + (H_G - H_G^\circ) \quad (1.4.3)$$

In Equation 1.4.3, first term on the right represents ideal gas enthalpy at zero pressure. The second term is the pressure correction

for the vapor mixture enthalpy from zero pressure to saturation pressure. This term which is called enthalpy deviation from ideality is calculated by the Yen and Alexander correlations. For the liquid enthalpy, we have,

$$H_L = \sum_{i=1}^c X_i C_{P_{iG}}^{\circ} + (H_L - H_G^{\circ}) \quad (1.4.4)$$

where

$$H_L - H_G^{\circ} = (H_L - H_{SL}) - \sum_{i=1}^c X_i \lambda_i + (H_G - H_G^{\circ}) + H_M \quad (1.4.5)$$

In Equation 1.4.4, the second term is the function of vapor and liquid enthalpy deviation, latent heat of vaporization and the heat of mixing. In Equation 1.4.5, the first term on the right represents the correction to liquid enthalpy for pressure in excess of saturation pressure. For subcooled liquid, this term is the difference between the enthalpy deviation of saturated liquid at equilibrium pressure and the subcooled liquid enthalpy deviation at the pressure in excess of saturation/equilibrium pressure. The second, third and the fourth terms are the latent heat of vaporization, the gaseous mixture enthalpy deviation, and the heat of mixing respectively. For this system, the program was checked with Ethanol-Water as an example of a non-ideal system.

The next step was the calculation of the minimum reflux ratio, number of plates, heat taken out at the condenser, heat added at the reboiler and the feed plate location. The program also

calculates the tower diameter. The calculation is based on an initial estimation of tower diameter, based on maximum allowable vapor velocity. An already developed correlation for the cost of a plate versus diameter of the column curve (Manzoor, 1984) was tried. By doing regression analysis, two cubic polynomial equations were developed to predict cost of condenser and reboiler based on their heat transfer area. This development was carried out on the basis of cost versus heat transfer area data for condenser and reboiler provided by Peters and Timmerhaus.

Finally, the program calculates the cost of the tower based on actual number of total plates, cooling water cost, steam cost and the total annual cost of operating the tower for a given reflux ratio. The code is valid for the type of distillation systems where a total condenser is used.

CHAPTER 2

LITERATURE BACKGROUND

2.1 General Background

Important factors in the design and operation of plate column are the number of plates required to obtain the desired separation, the diameter of the column, the heat input to the reboiler, the heat output from the condenser, the tray spacing between the plates, the choice of type of plate and details of construction of the plates. In short, the performance of a plate column is generally based on material balance, energy balance, and phase equilibria.

Among the various calculational methods for the separation of binary mixtures by continuous distillation, McCabe-Thiele and Ponchon-Savarit are the most widely used. Before these, Lewis and Sorel proposed a method for the calculation of number of plates (Richardson, 1955). Expressing the material balance on the more volatile component, above the feed plate, they gave a relation between the composition of the vapor rising to a plate and the composition of the liquid on the plate above the feed plate. Mathematically,

$$Y_n = \frac{L_n X_{n+1}}{G_n} + \frac{DX_D}{G_n} \quad (2.1.1)$$

Similarly the corresponding relation between the compositions of the vapor rising to a plate and the liquid on the plate, for the

section below the feed plate, i.e., from the bottom to the above plate 'm' is

$$Y_m = \frac{L_m X_{m+1}}{G_m} - \frac{BX_B}{G_m} \quad (2.1.2)$$

Equation 2.1.1 and 2.1.2 are the operating line equations. In order to calculate the change in composition from one plate to the next, the equilibrium data is used to find the composition of the vapor above the liquid. The enrichment line is used to calculate the composition of the liquid on the next plate. The method can then be repeated up the column using Equations 2.1.1 and 2.1.2.

Assuming molal overflow and constant relative volatilities, an equation (Fenske, 1932) was developed for the calculation of minimum number of theoretical plates and minimum reflux ratio.

$$N_m + 1 = \frac{\log \frac{X_D}{1-X_D} \frac{1-X_B}{X_B}}{\log \alpha_{av}} \quad (2.1.3)$$

The equation shows that a plot of $\log(X_D/X_B)$ versus $\log \alpha_{av}$ will give a straight line having a slope numerically equal to the number of theoretical stages. The quantities and compositions of distillate and bottoms are determined by the overall balance equation

$$\frac{FX_F}{\left[\left(\frac{D}{B} \right) \left(\frac{X_D}{X_B} \right) + 1 \right]} = (BX_B)_i \quad (2.1.4)$$

where

$$\frac{D}{B}(\text{calculated}) = \frac{F - \sum (BX_B)_i}{\sum (BX_B)_i} \quad (2.1.5)$$

Equations 2.1.4 and 2.1.5 are solved by using various assumed values for D/B until a value of D/B is found which will give a consistent value for the calculated B.

One of the two basic equations proposed (Underwood, 1948) was

$$\frac{\sum (\alpha_i X_i)_F}{(\alpha_i - \Theta)} = 1 - q \quad (2.1.6)$$

Θ calculated from Equation 2.1.6 could be used in another equation to give a value of minimum reflux ratio

$$R_m + 1 = \sum \frac{(\alpha_i X_i)_D}{\alpha_i - \Theta} \quad (2.1.7)$$

The number for total reflux leads to the approximation of X_i in the distillate. Underwood's method assumes constant average α 's and constant liquid to vapor flow rate. The α 's are all computed at the average of the distillate dew point and the residue bubble point, which may require a few trial estimates. In case of hand calculation, values of Θ can be read directly from a graph (Van and Todd, 1971).

An empirical correlation (Gilliland, 1940) was presented for the number of theoretical stages N as a function of R , R_m and N_m . He plotted $R - R_m / R + 1$ as abscissa and $N - N_m / N + 1$ as ordinate. He suggested to calculate N_m by the Fenske equation.

An important development, to correlate R , R_m and N_m as a substitute for Gilliland's graphical correlation, was made in 1975 (Eduljee, 1975).

$$\frac{N-N_m}{N+1} = 0.75 - 0.75 \left(\frac{R-R_m}{R+1} \right)^{0.5668} \quad (2.1.8)$$

This correlation has facilitated the work of a computer programmer and one does not need to curve fit Gilliland's curve.

Using conventional calculations for minimum trays and minimum reflux as starting points, a method was devised (Erbar and Maddox, 1961) for reflux rate and number of plates. They plotted S_m/S as abscissa and L_o/G_1 as ordinate and the parameter was $(L_o/G_1)_m$. S_m being minimum number of stages and S being the number of stages in fractionator.

$$\frac{L_o}{G_1} = \frac{L_o}{L_o + D} = \frac{R}{R+1} \quad (2.1.9)$$

Knowing R and R_m (for parametric value) the minimum number of stages could be found.

A relation that relates the distribution coefficient K of one component to that of another is (Winn, 1958)

$$K = \beta(K')^b \quad (2.1.10)$$

The equation does not apply to mixtures forming azeotropes or at conditions near the critical. Winn also modified Fenske's equation

for the number of plates

$$\beta^{n+1} = \left(\frac{L_D}{B}\right) \left(\frac{B'}{L_D}\right)^b \left(\frac{W}{D}\right)^{1-b} \quad (2.1.11)$$

$$\beta^{n+2} = \left(\frac{G_D}{B}\right) \left(\frac{B'}{G_D}\right)^b \left(\frac{W}{D}\right)^{1-b} \quad (2.1.12)$$

Equation 2.1.11 is for liquid overhead product and 2.1.12 is for vapor overhead product. The number of plates by Winn's equation is less than the Fenske equation which assumes average values of α 's.

2.2 Ponchon-Savarit

The graphical calculation method of Ponchon-Savarit is based upon the calculation method of Sorel. The method is mainly used for binary mixtures with large heats of mixing. Here, since the total heat of the mixture varies with composition, it is necessary to make heat as well as material balances on the column. Compared to McCabe-Thiele method, this method is rigorous, accurate and can handle all situations, but requires detailed enthalpy data for its application. In this method no simplifying assumption of constant molar flow need to be made.

In the McCabe-Thiele construction, material balance equations are plotted on an x-y phase equilibrium diagram (Figure 2), the stages being calculated by alternate use of the material balance and equilibrium relationships. On the other hand, Ponchon-Savarit diagram has both enthalpy and material balance relationships as well as phase equilibrium conditions. Material balance for the enriching

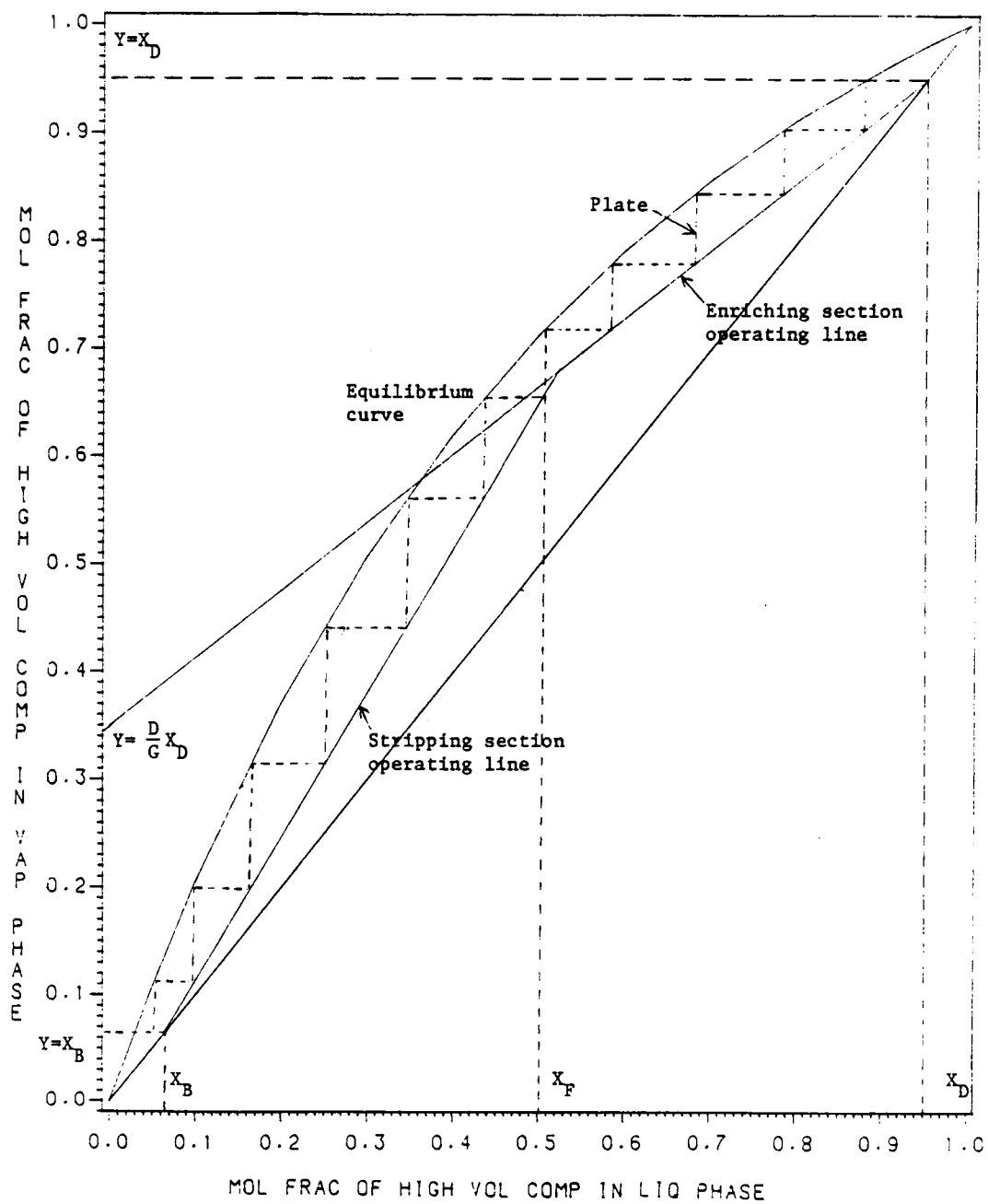


Figure 2. McCabe-Thiele construction.

section (Figure 3, Section A) based on more volatile component gives

$$G_{n+1} = L_n + D \quad . \quad (2.2.1)$$

An enthalpy balance in the enriching section gives

$$G_{n+1} H_{G_{n+1}} = L_n H_{L_n} + Q_c + D H_D \quad . \quad (2.2.2)$$

If Q' is the heat removed in the condenser and permanently removed distillate, per mole of distillate, then

$$G_{n+1} H_{G_{n+1}} - L_n H_{L_n} = D Q' \quad . \quad (2.2.3)$$

Eliminating D between Equations 2.2.1 and 2.2.2 and between 2.2.1 and 2.2.3, we get

$$\frac{L_n}{G_{n+1}} = \frac{X_D - Y_{n+1}}{X_D - X_n} = \frac{Q' - H_{G_{n+1}}}{Q' - H_{L_n}} \quad . \quad (2.2.4)$$

On the Hxy diagram, Equation 2.2.4 is the equation of a straight line through $(H_{G_{n+1}}, Y_{n+1})$ at G_{n+1} , (H_{L_n}, X_n) at L_n and (Q', X_D) at ΔD .

On the $x-y$ diagram, Equation 2.2.4 is the equation of a straight line of slope L_n/G_{n+1} , through (Y_{n+1}, X_n) and $Y=X=X_D$. This is the enriching section operating line.

Following the same procedure, for the stripping section (Figure 3, Section B), an equation similar to 2.2.4 is

$$\frac{L_m}{G_{m+1}} = \frac{Y_{m+1} - X_B}{X_m - X_B} = \frac{H_{G_{m+1}} - Q''}{H_{L_m} - Q''} \quad . \quad (2.2.5)$$

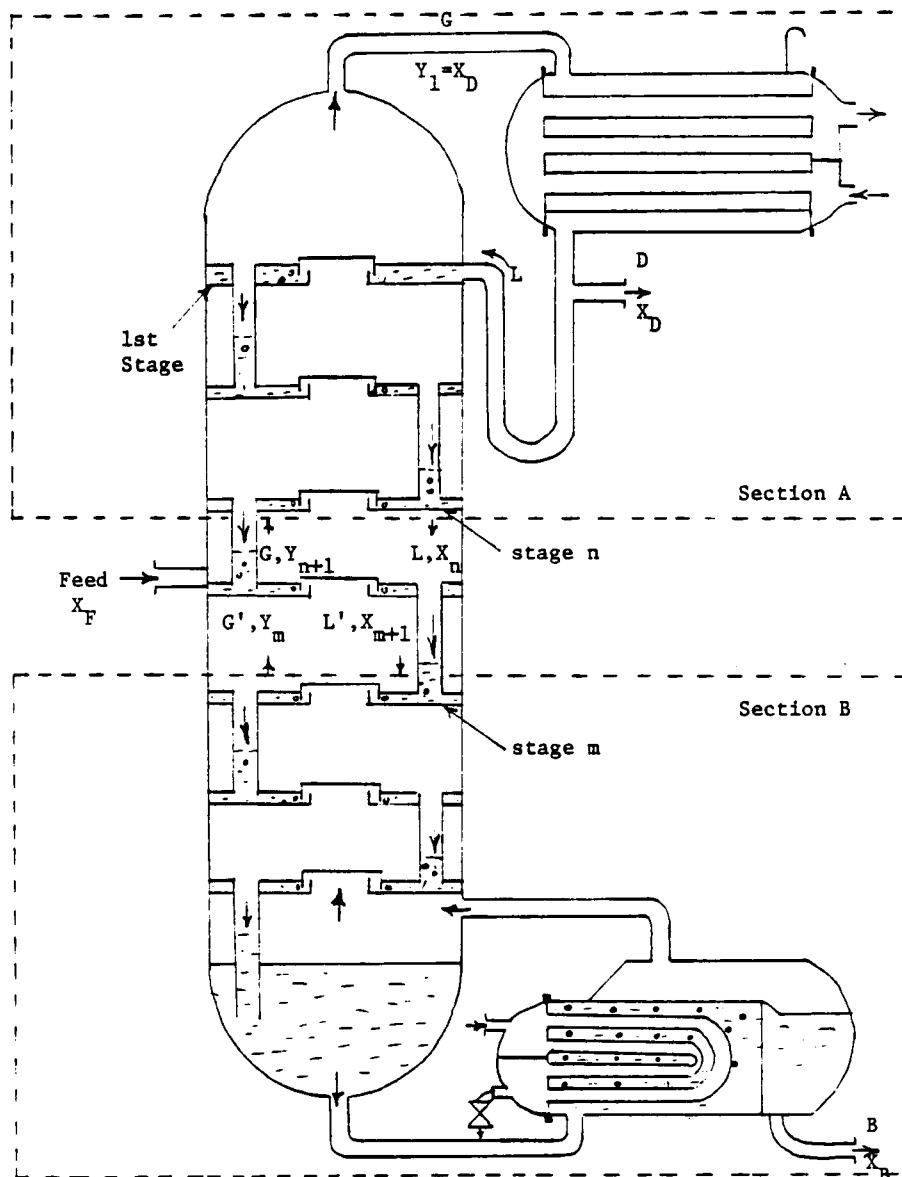


Figure 3. Distillation column.

On the Hxy diagram, Equation 2.2.5 is a straight line through $(H_{G_{m+1}}, Y_{m+1})$ at G_{m+1} , (H_{L_m}, X_m) at L_m and (Q'', X_B) at ΔB . On the x-y diagram 2.2.5 is a straight line of slope L_m/G_{m+1} , through (Y_{m+1}, X_m) and $Y=X=X_B$. The equation is the stripping section operating line.

In the absence of heat losses, following the same route of material and enthalpy balance, the equation is

$$\frac{D}{B} = \frac{X_F - X_B}{X_D - X_F} = \frac{H_F - Q''}{Q' - H_F} \quad (2.2.6)$$

This is the equation of a straight line on the Hxy diagram, through (Q', X_D) at D (H_F, X_F) at F, and (Q'', X_B) at ΔB . In other words

$$F = \Delta D + \Delta B \quad (2.2.7)$$

The location of F on the Hxy diagram represents the feed. After locating F, and the concentration abscissas X_D and X_B , corresponding to the products on the Hxy diagram, ΔD is located vertically on line $X=X_D$ by computation of Q' . From here one can calculate heat removed at the condenser Q_c by using the relation

$$Q' = H_D + \frac{Q_c}{D} \quad (2.2.8)$$

The line ΔDF extended to $X=X_B$ locates ΔB , the coordinates of which can be used to compute Q_B by using the relation

$$Q'' = H_B - \frac{Q_B}{B} \quad (2.2.9)$$

A straight operating line (Figure 4) from the known L_{n-1} to the fixed ΔD locates G_n on the saturated vapor curve. By definition, G_n is in equilibrium with L_n and L_n can be located by means of the equilibrium tie line which passes through G_n . If stage 'n' is assumed to be adiabatic, and no material is added or withdrawn through the column wall, no change in the difference point ΔD will occur across stage 'n'. Therefore, G_{n+1} can be located by means of a straight operating line from L_n to ΔD . While stepping down in the enriching section, the same difference point is used for each stage until the feed tray is reached. Enriching trays can thus be located on the Hxy diagram alone by alternating construction lines to ΔD and tie lines, each tie line representing an ideal tray. The same approach is used for the construction of operating line in the rectification section, the difference point now being ΔB (Figure 5). Switch from ΔD to ΔB is made after the tie line that crosses the overall enthalpy line given by Equation 2.2.7. This tie line also represents the tray where the feed is to be introduced.

For an ideal system, tie line passing through feed point and intersecting at $X=X_D$ give Q' and minimum reflux can thus be found out by the relation

$$R_m = \frac{Q' - H_{G_1}}{H_{G_1} - H_{L_o}} \quad . \quad (2.2.10)$$

For a non-ideal mixture, deviating positively from Raoult's law, an enriching section tie line which gives the highest

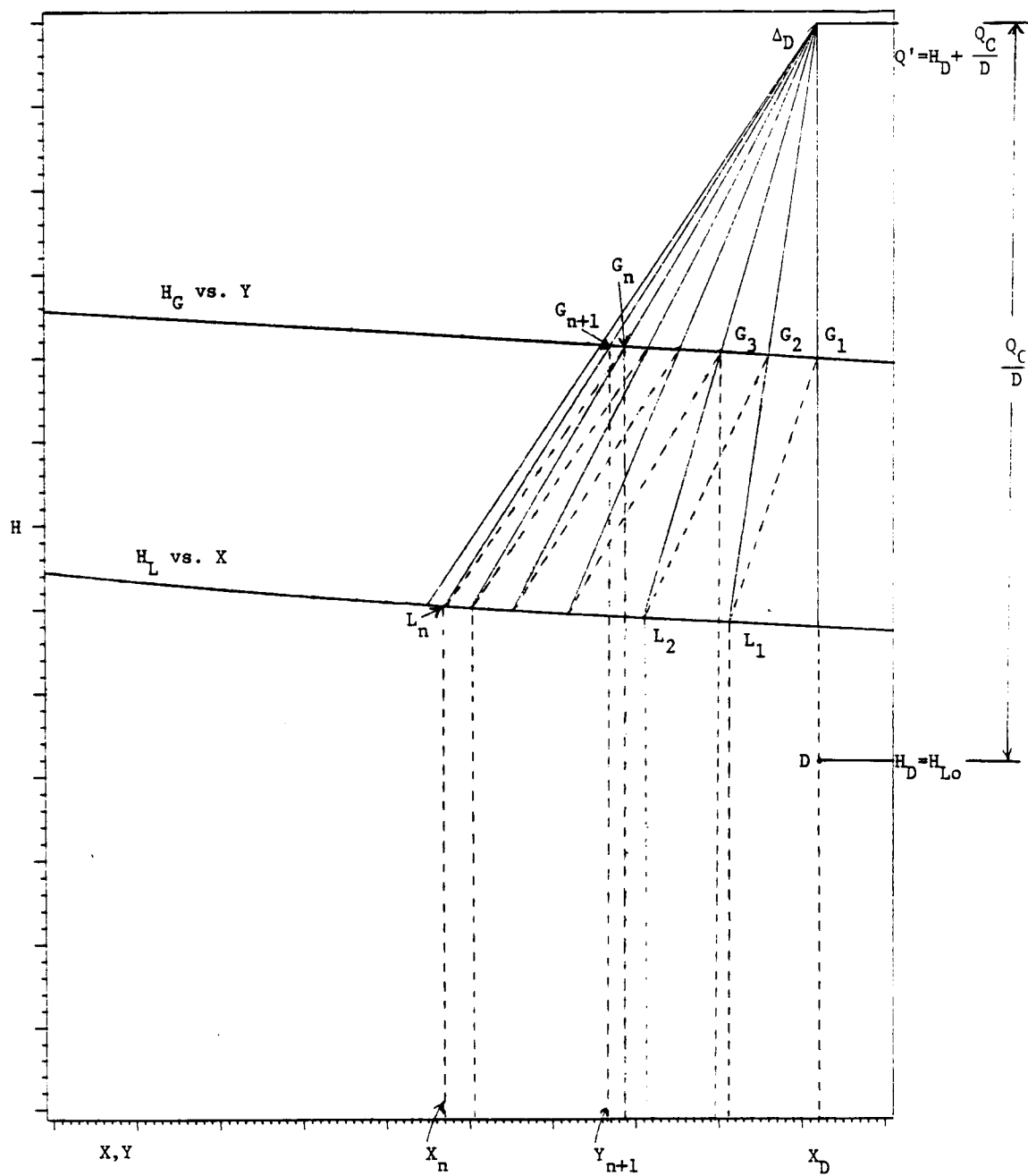


Figure 4. Ponchon-Savarit Hxy diagram (enriching section).

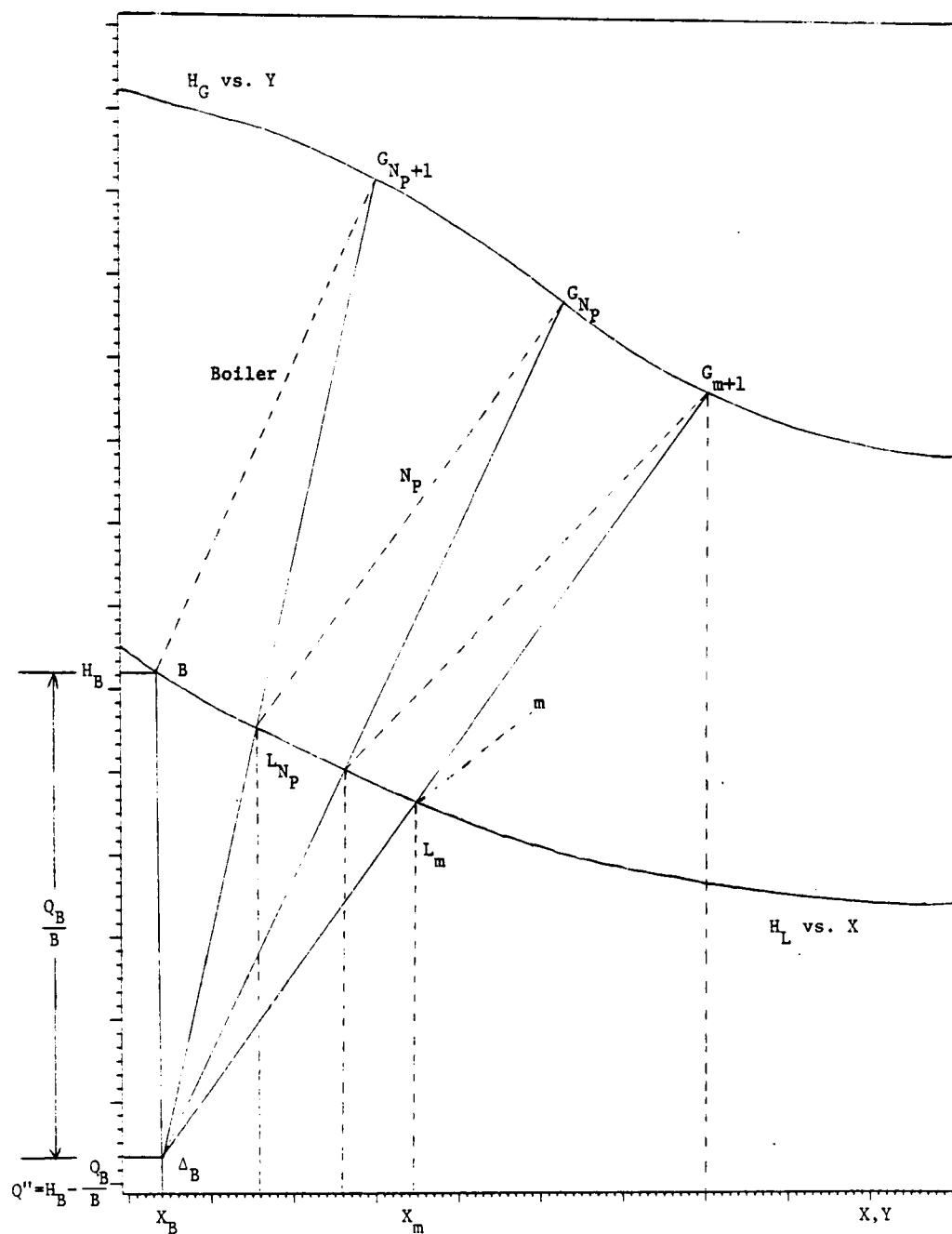


Figure 5. Ponchon-Savarit diagram (stripping section).

intersection with $X=X_D$ is the one which is used to locate Q' and thus the minimum reflux ratio.

A modified version of the Ponchon-Savarit and McCabe-Thiele (Ledanols and Fuentes, 1984) methods requires no extra effort and could be worked on the graphs obtained by the methods of Ponchon-Savarit and McCabe-Thiele. They have shown that for optimal effect, the liquid and vapor parts are introduced to separate but continuous stages. Numerical examples confirm that a small improvement in column performance is achieved but does not affect the number of stages or reflux ratio for a given separation.

2.3 Tower Diameter and Optimization

An initial estimate of the diameter of the column can be made on the basis of maximum allowable vapor velocity, V_{MAX} , and can be calculated by (Manzoor, 1984)

$$T_D = \sqrt{\frac{4QT}{\pi V_{MAX}}} \quad . \quad (2.3.1)$$

Treybal, 1980, recommended some correlations for sieve-tray towers. His correlations are meant for the calculation of empirical constants α and β which are involved in the calculation of the flooding constant. For plates having ratios of area of perforation to active area greater than 0.1, he suggested

$$\alpha = 0.0744t + 0.01173 \quad (2.3.2)$$

$$\beta = 0.0304t + 0.015 \quad . \quad (2.3.3)$$

For ratios less than 0.1, multiply Equations 2.3.2 and 2.3.3 by $5(\text{Ratio})+0.5$. The flooding constant can then be calculated by the empirical correlation

$$C_F = [\alpha \log \frac{1}{(\frac{L}{G}) (\frac{\rho_G}{\rho_L})^{0.5}} + \beta] [\frac{\sigma}{0.02}]^{0.2} \quad (2.3.4)$$

For a given type of tray at flooding, the superficial velocity of the gas is related to fluid densities by (Treybal, 1980)

$$V_F = C_F \left(\frac{\rho_L - \rho_G}{\rho_G} \right)^{\frac{1}{2}} \quad (2.3.5)$$

A smaller value of velocity is used in actual design practice. For nonfoaming liquids this is typically 80 to 85% of V_F . Volumetric flow rate when divided by this velocity leads to the cross-sectional area and hence diameter of the tower.

An optimum reflux ratio location technique in graphical form (Figure 1, page 5) has been very well explained by McCabe and Smith. This ratio is that point on the graph at which sum of fixed and operating cost is minimum. Fixed charges can be calculated graphically by calculating purchase cost of the material of construction in \$/plate for a known diameter of the column.

To implement these curves in a computer, there are two options. The program could be made interactive so that it could ask the user to provide the cost at a specific diameter. This value could be found by reading from the graph. In another option, regression

analysis could be done to do curve fitting. Manzoor did this regression analysis for the sieve tray tower (steel shell, stainless steel trays) curve and came up with the following cubic model equation.

$$\log(\text{COST}) = 5.165 - 0.0641\log(\text{DIA}) + 0.01761\log(\text{DIA})^2 - 0.0041\log(\text{DIA})^3 \quad (2.3.6)$$

where DIA is tower diameter in inches.

2.4 Physical Properties

Without physical properties, design problem of distillation cannot be solved. These properties along with the assumptions made in their calculations are discussed below.

Various methods are available for the calculation of ideal gas heat capacity. Some are the method of Thin, et al., 1971, method of Rihani and Doraiswamy, 1965, and Benson values, 1969, etc. Besides these methods, polynomial equations are widely used for heat capacity calculation.

$$C_p^\circ = A + BT + CT^2 + DT^3 \quad (2.4.1)$$

Constants used in the above equation can be very easily found in the literature.

For liquids at their boiling points, latent heat of vaporization is added to convert liquid to vapor. Similarly to convert gases to liquids, the same quantity is removed from gases. This heat

decreases with increase in temperature and is zero at the critical point. Fish and Lielmezs, 1975 suggested a way to correlate heat of vaporization with temperature. Their correlation is

$$\Delta H_V = \Delta H_{Vb} \frac{T_r}{T_{br}} \frac{X+X^q}{1+X} \quad (2.4.2)$$

where

$$X = \frac{T_{br}}{T_r} \frac{1-T_r}{1-T_{br}} \quad (2.4.3)$$

For organic and inorganic liquids $p=0.13856$ and $q=0.35298$.

For non-ideal systems, liquid enthalpy is given by Equation 1.4.4. The equation shows that it involves enthalpy departure and heat of mixing terms. Enthalpy departure terms checks for the deviation of gases and liquids from ideality. The departure functions could be calculated by analytical equations of state or Redlich-Kwong equations of state. Beside these, Yen and Alexander, 1965, also developed some equations for enthalpy departure. For saturated vapor, they gave

$$\frac{H-H^\circ}{T_c} = \frac{A P_r^B}{1+C(-\ln P_r)^D} \quad (2.4.4)$$

$H-H^\circ$ being enthalpy departure and A-D are constants which are different for different critical compressibility factors. Similarly for saturated liquids, they gave

$$\frac{H-H^\circ}{T_c} = \frac{U+V(-\ln P_r)^W}{1+X(\ln P_r)} \quad (2.4.5)$$

where constants U to X vary with compressibility factor. For sub-cooled liquid enthalpy departure, their relation is

$$\frac{H-H^0}{T_c} = A(P_r-B)+C(T_r-D)+E(T_r-F)^2-G(P_r-I)(T_r-J) \\ +K\ln P_r + L(\ln P_r)(\ln T_r) + M\ln(P_r)(\ln T_r)^2 + N \quad (2.4.6)$$

For superheated vapor

$$\frac{H-H^0}{T_c} = \frac{mP_r(1-\frac{P_r}{X_o})}{\exp(-C_1(P_r)^2)Q+C_4+C_5P_r+C_6P_r^2} \quad (2.4.7)$$

where

$$Q = 1-C_2-C_4-C_5P_r+C_2[\frac{1}{\pi} \arctan(C_3-C_3P_r)+0.5]^2 \quad (2.4.8)$$

Except $H-H^0$, T_r , T_c and P_r all alphabetical letters represent constants, which are different at different compressibility factors.

The above correlations are valid for compressibility factors of 0.23 to 0.29. Extrapolation to compressibility factors less than 0.23 or greater than 0.29 has not been recommended.

Another property of non-ideal systems is the heat of mixing. When two non-ideal substances are mixed, they either absorb or release heat. This property, which is function of temperature, can be calculated by

$$H_M = V_{iL}(\delta_i - \sum_{j=1}^c \phi_j \delta_j) \quad (2.4.9)$$

where

$$\delta_j = \left(\frac{\lambda_j}{V_{jL}} \right)^{-RT} \frac{1}{2} \quad (2.4.10)$$

and

$$\phi_j = \frac{X_j V_{jL}}{V_L} \quad (2.4.11)$$

The above equation for heat of solution assumes additive molal volumes in the calculation of volume fraction, and was proposed by Edmister, et al., (Henley and Seader, 1981).

The backbone of distillation problem solution is the vapor-liquid equilibria, i.e., moles of high volatile component in vapor phase in equilibrium with the same component in liquid phase. On the enthalpy concentration diagram of Ponchon-Savarit, this equilibria gives tie lines between the saturated liquid and vapor enthalpy curves. Many methods are available for their calculation but the one which is well established and uses activity coefficient is the UNIQUAC equation (Abrams and Prausnitz, 1975). This method uses the local area fraction as the primary concentration variable. The correlation consists of two parts, combinatorial and residual.

$$\ln \gamma_i = \ln \gamma_{ic} + \ln \gamma_{iR} \quad (2.4.12)$$

$$\ln \gamma_{ic} = \ln \frac{\phi_i}{X_i} + \frac{Z}{2} q_i \ln \frac{\theta_i}{\phi_i} + \phi_i \left(\ell_i - \frac{r_i}{r_j} \ell_j \right) \quad (2.4.13)$$

$$\ln \gamma_{iR} = -q_i \ln(\theta_i + \theta_j \tau_{ji}) + \theta_j q_i \left(\frac{\tau_{ji}}{\theta_i + \theta_j \tau_{ji}} - \frac{\tau_{ij}}{\theta_j + \theta_i \tau_{ij}} \right) \quad (2.4.14)$$

ℓ_i , θ , ϕ and τ_{ji} are given as:

$$\ell_i = \frac{Z}{2}(r_i - q_i) - (r_i - 1) \quad (2.4.15)$$

$$\theta = \frac{X_i q_i}{X_i q_i + X_j q_j} \quad (2.4.16)$$

$$\phi = \frac{X_i r_i}{X_i r_i + X_j q_j} \quad (2.4.17)$$

$$\ln \tau_{ji} = -\left(\frac{U_{ji} - U_{ii}}{RT}\right) \quad (2.4.18)$$

Equilibrium pressure expressed as a function of the activity coefficient is given by

$$P y_i = \gamma_i X_i P_i^s \quad (2.4.19)$$

Given liquid mole fraction and saturation temperature, activity coefficient can be obtained from Equation 2.4.12. Vapor pressure from the Antoine correlation and at known equilibrium pressure, Equation 2.4.19 can be used to get equilibrium mole fraction in the vapor phase.

2.5 Computer in Distillation

With the advent of large-capacity, high speed digital computers and sophisticated calculation techniques, many attempts have been made to revise fractionation column design techniques to include McCabe-Thiele and Ponchon Savarit for binary systems.

Using the McCabe-Thiele technique, Benenati calculated the minimum number of trays required for a binary separation (Benenati, 1977). He used a programmable pocket calculator for developing a program. His program determines the minimum reflux ratio, actual reflux ratio and then proceeds to step off plates from top to bottom. When all the plates are calculated, the computer displays the actual reflux ratio, the overhead product rate and then stops with the total number of real plates in the display.

A method was suggested for transferring the McCabe-Thiele method into computer mode (Prahl, 1979). He suggested to calculate the number of plates by calculating concentration at each plate by stepping down from the equilibrium curve to the operating line. For the case of varying relative volatility (α), he suggested

$$\alpha = \frac{P_B}{P_T} \quad (2.5.1)$$

where vapor pressure may be obtained by the Antoine equation.

Chein Henry has developed a method for use on high speed computers for calculating minimum reflux by a rigorous method (Henry, 1978). The limitation of the method is that it cannot solve problems in which the minimum reflux rate is determined by a point of tangency between the operating line and the equilibrium line on a McCabe-Thiele diagram.

Calculation of vapor-liquid equilibria is necessary for designing of distillation column. Taking the same fact into consideration a TI-59 program has been developed to determine the equilibrium

composition of a binary solution (Hunting and Robinson, 1984). With this program, the trial and error determination of composition can be made rigorous for non-ideal mixtures by including liquid activity coefficients in the calculation. Since the convergence is from both the zero and one mole fraction ends, the program detects azeotropic systems. Curves of pressure, temperature or activity coefficient versus mole fraction, for a constant temperature or constant pressure system can also be generated by means of this program.

A computer code for the design of the distillation column has been developed at The University of Tennessee, Knoxville (Manzoor, 1984). This code uses the McCabe-Thiele graphical technique. The author also proposed some model equations for the calculation of vapor-liquid equilibria of certain non-ideal binary mixtures.

CHAPTER 3

COMPUTER PROGRAM

3.1 Introduction to Program

For a binary system, the design and optimization problems of a distillation column can be solved by this program if the user has the following basic information:

1. feed rate and its thermal condition;
2. percentage of high volatile component in feed, top, and bottom products;
3. inlet and outlet temperatures of condenser and reboiler;
4. cost of steam and cooling water.

Along with this information, various other parameters are also required (see input variables in Appendix B). These parameters can be found from the literature. When all this information is fed to the code, it gives the number of plates in the rectification section, number of plates in stripping section, total number of plates, feed plate location from top, minimum reflux ratio, and the heat added and removed at reboiler and condenser respectively. Tower diameter and various other costs beside total annual cost are also calculated by the program. The program takes into consideration ideal as well as non-ideal binary systems and uses the plate-to-plate calculation technique of Ponchon-Savarit. Initially, to detect an azeotrope, the program looks for the point where the liquid mole fraction is equal to the vapor mole fraction. If it finds the point, it sets

flag $S0=1$ and informs the user by displaying a message. In case of failure, it sets flag $S0=0$ and informs the user of the ideality of the system. In the non-ideal case, only those systems deviating positively from Raoult's law are taken into account by the program. Liquid and vapor enthalpy of the two systems are calculated by the program through two different routes. Since the program is interactive, at various stages of its execution, it asks the user questions. The user is required to select and type an integer, as prompted. If the feed is subcooled liquid or superheated vapor, the user is required to provide the program with the temperature in degrees kelvin. For optimum cost of the tower, the user is required to vary the ratio of operating reflux to minimum reflux. This ratio is usually between 1.1 to 1.5. When this ratio is changed on every execution of the program, a point is reached when total annual cost of operating the tower is minimized. The operating reflux ratio at this point is the optimum reflux ratio. The main program is supported by a large number of subroutines. Each of these subroutines have been assigned the job of providing the main program with certain physical properties at a given mole fraction and temperature. For the ideal system, the program calls a series of subroutines and then a different series for the non-ideal one. The main program does the design with the help of subroutines. This section of the code is shown in Figure 6 and listing is given in Appendix A, Section 1. The optimization is done by the main program alone. The subroutines and their working is discussed below in detail.

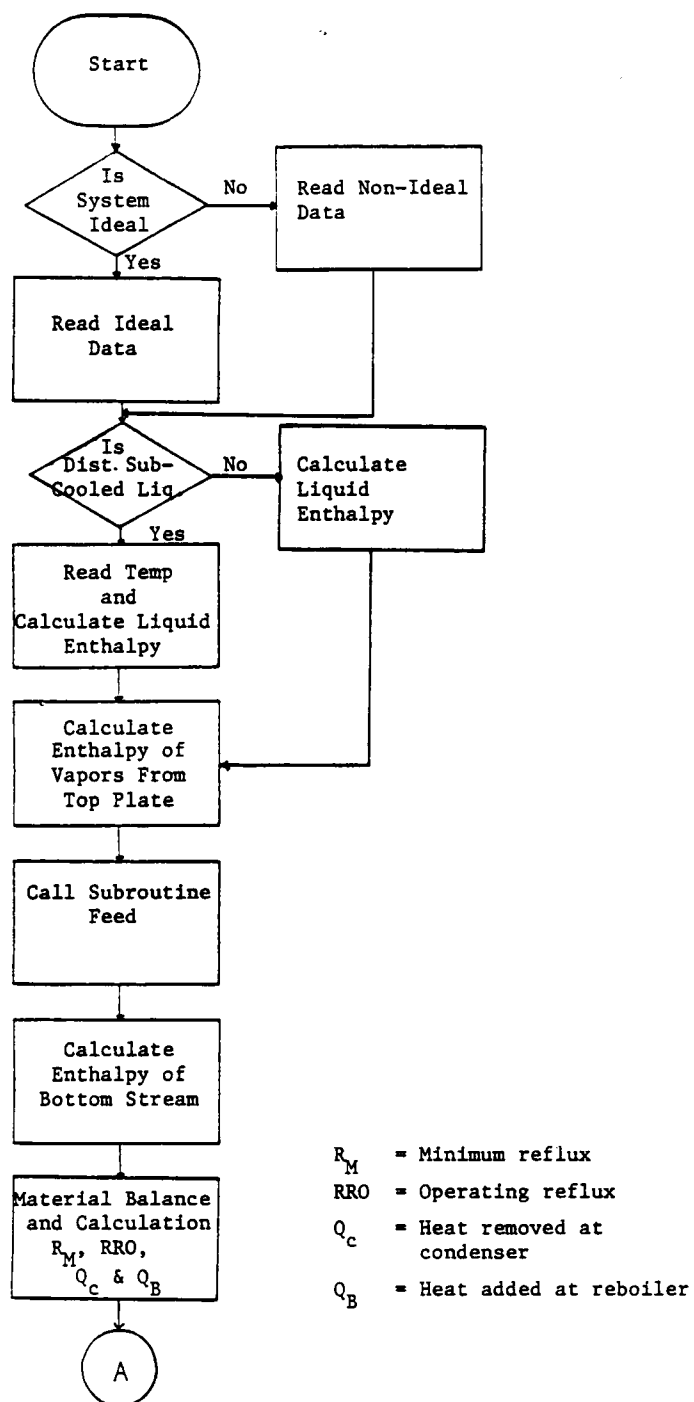


Figure 6. Flow chart of main program (design section).

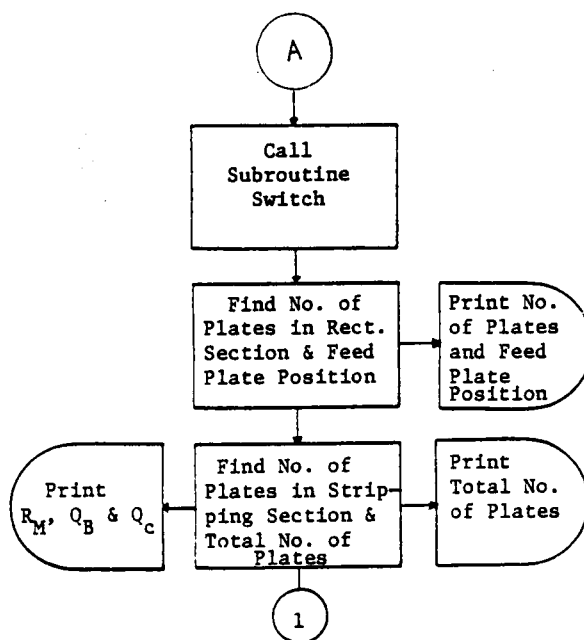


Figure 6. (Continued).

3.1.1 Subroutine UNIQAC. This routine has been developed to calculate vapor-liquid equilibria and saturation temperatures. The liquid mole fraction of more volatile component is supplied by the main program as an input argument. In response the routine supplies the main program the equilibrium mole fraction of the same component in the vapor phase and the saturation temperature at which this equilibrium exists. The UNIQAC volume, surface and energy interaction parameters, normal boiling points and the constants of the Antoine equation are passed to the subroutine through common statements. UNIQAC uses Equation 2.4.12, page 26, to calculate the activity coefficient of each component of an ideal as well as a non-ideal system. For a binary system, we know that

$$P = \gamma_A X_A P_A^S + \gamma_B X_B P_B^S \quad . \quad (3.1.1.1)$$

The subroutine calculates vapor pressure by using the Antoine vapor pressure equation

$$\ln p_{VP} = A - \frac{B}{T+C} \quad . \quad (3.1.1.2)$$

There exists one and only one saturation temperature at which activity coefficient of both the components satisfies the Equation 3.1.1.1. The subroutine looks for such a temperature by the bisection method. For this method to work, it is necessary that Equation 3.1.1.1 should change sign at two extreme limits, i.e., boiling points of the two components. If there is no sign change,

the routine exits by displaying an error message. The routine was used to calculate the vapor liquid equilibria and saturation temperature of the ideal Benzene-Toulene and the non-ideal Ethanol-Water system. Experimental and computer results of both systems are shown in Figures 7, 8, 9, and 10. This calculation was done at one atmosphere pressure. A flow chart and listing of the routine is given in Figure 11 and Appendix A, Section 2 respectively.

3.1.2 Subroutine LIQEPY. This subroutine is valid for calculation of liquid enthalpy of ideal systems only. The subroutine is supplied with the liquid mole fraction of more volatile component and the saturation temperature. The output arguments of this routine are the enthalpies of both the components and the mixture enthalpy at the given mole fraction.

Given some reference temperature and the temperature at which heat capacity is desired, the subroutine uses polynomial Equation 2.4.1, page 23. Enthalpy calculation is done with Equation 1.4.1, page 6. Constants of the heat capacity equation are passed by the main program through a common statement. A listing of the subroutine is given in Appendix A, Section 3.

3.1.3 Subroutine IENTPY. For an ideal system, this routine takes the vapor mole fraction and saturation temperature as its input arguments and as its output arguments gives gas mixture enthalpy, heat of vaporization, and enthalpies of individual components. Critical temperature, normal boiling point, heat of vaporization at

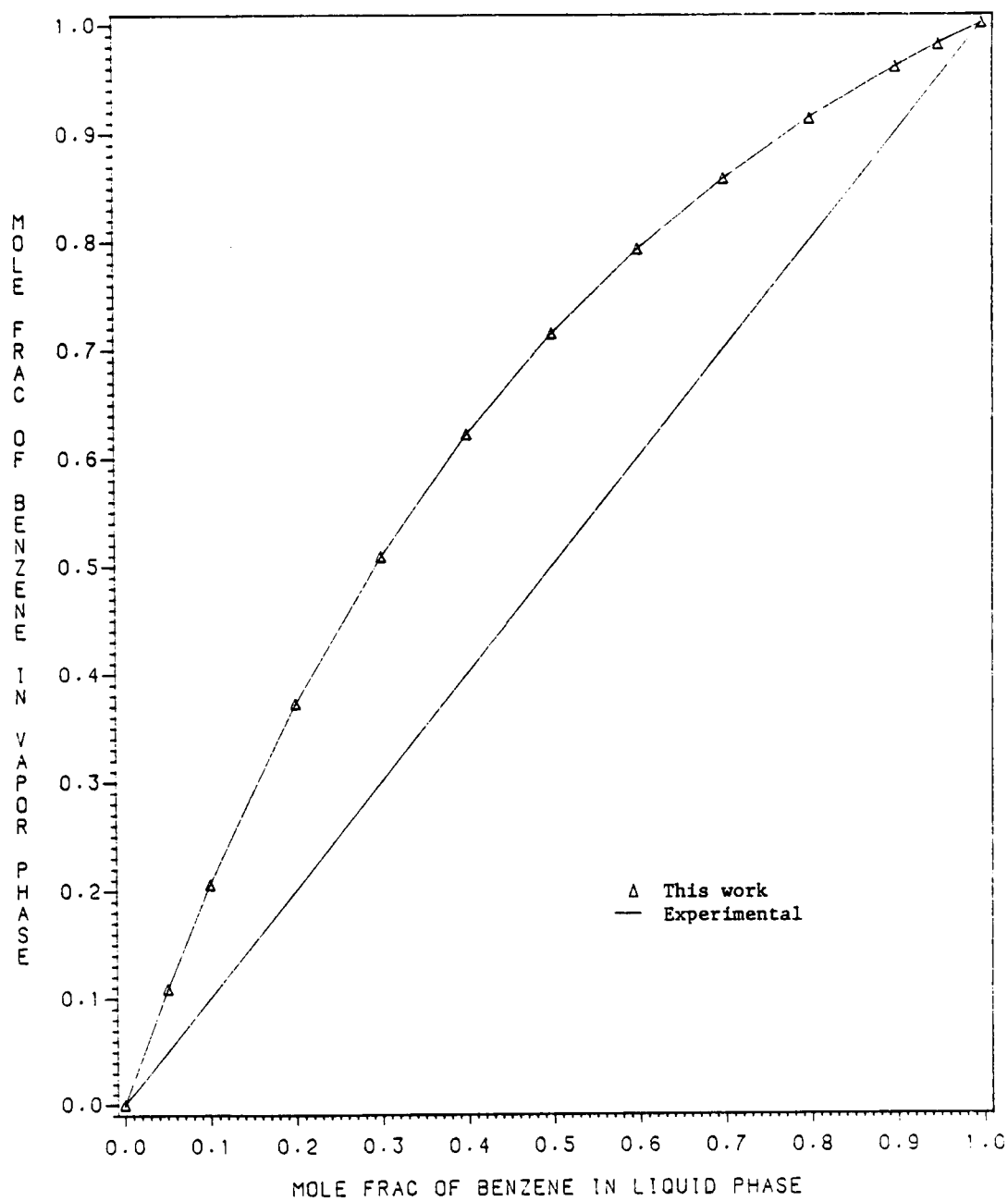


Figure 7. Vapor-liquid equilibria of Benzene-Toulene system.

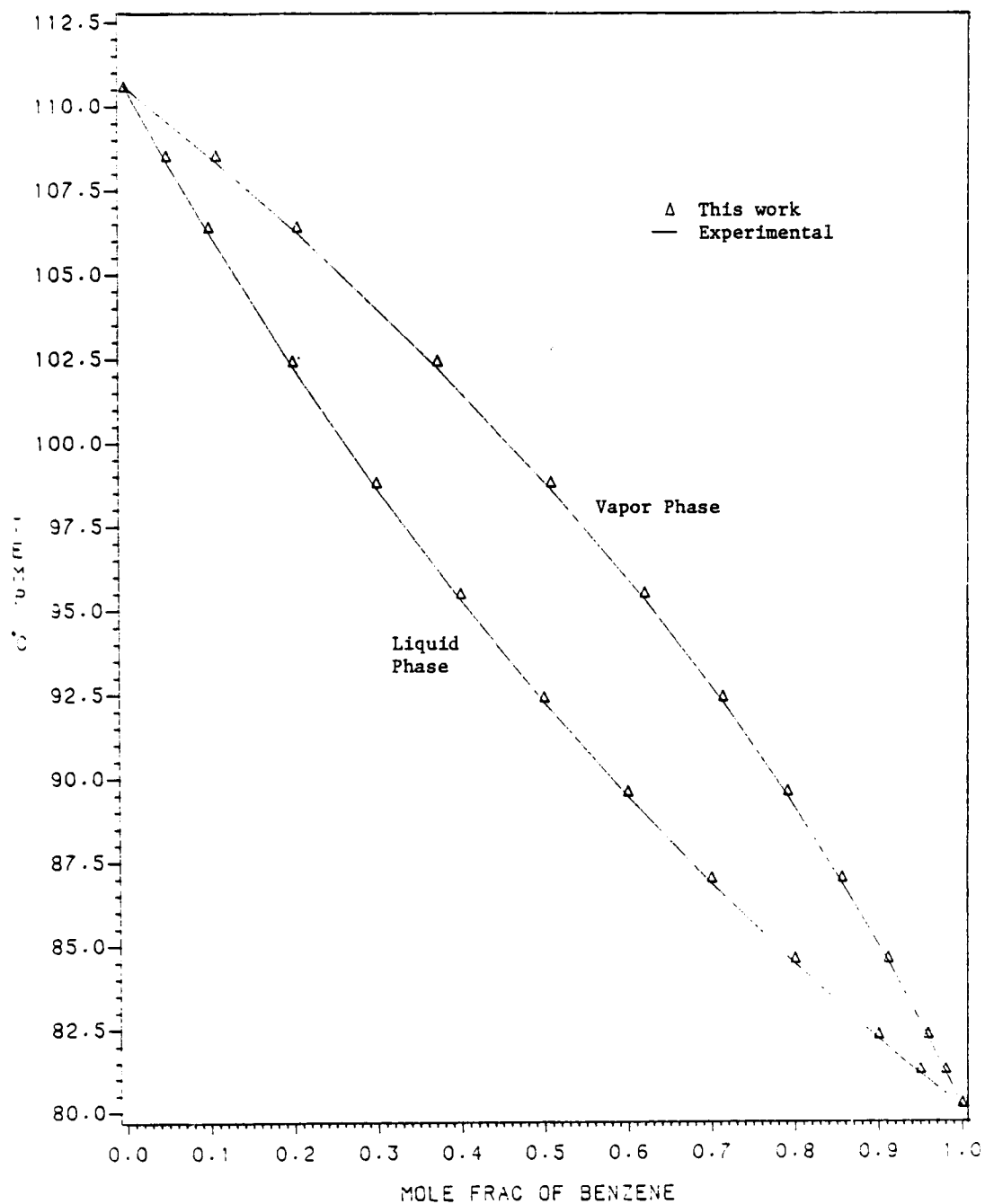


Figure 8. Boiling-point diagram for Benzene-Toulene system.

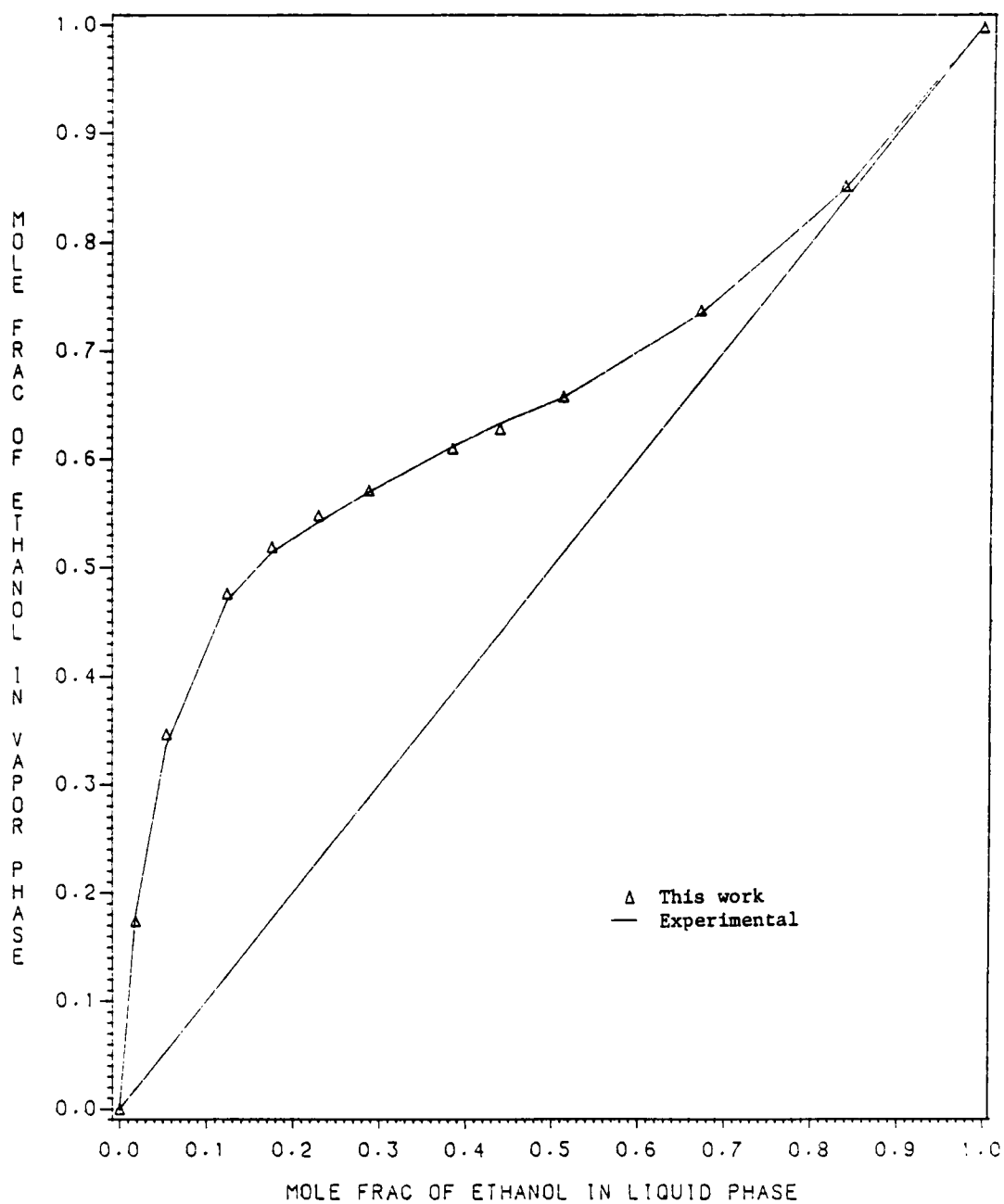


Figure 9. Vapor-liquid equilibria of Ethanol-Water system.

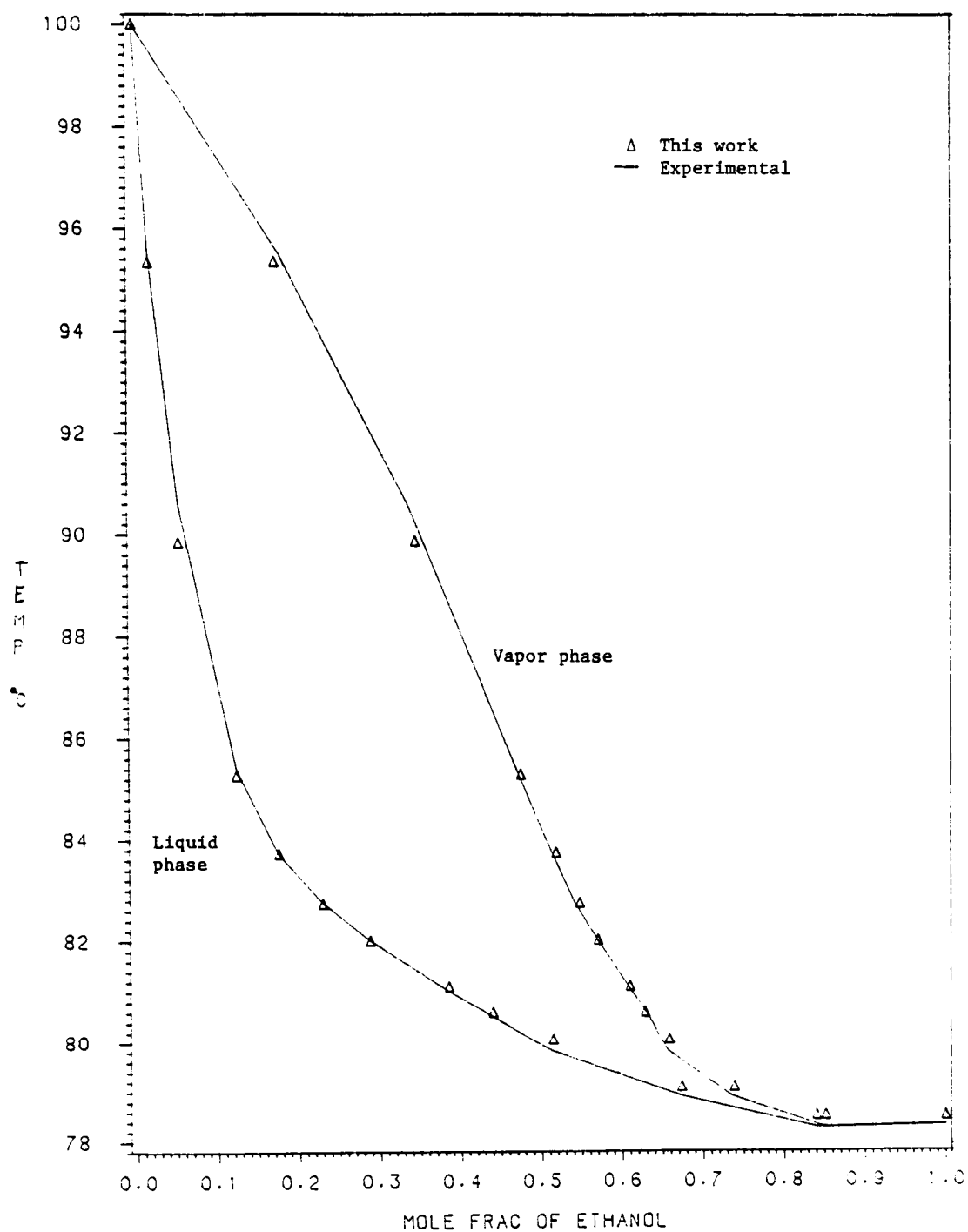


Figure 10. Boiling-point diagram for Ethanol-Water system.

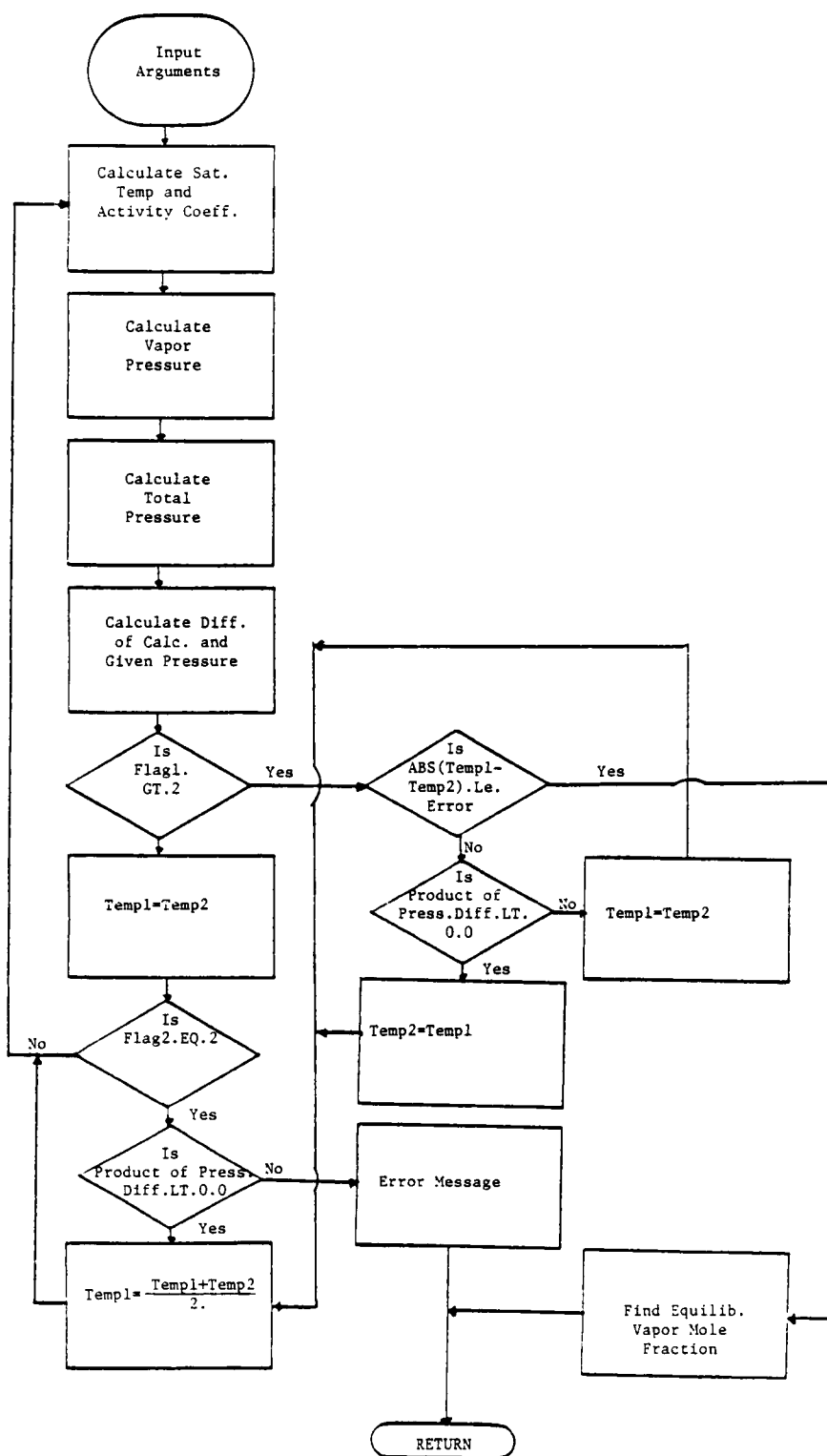


Figure 11. Flow chart of subroutine UNIQAC.

normal boiling point and constants W and Z are supplied through common statements.

Calculation of vapor enthalpy of an ideal system, as given by Equation 1.4.2, page 6, also requires liquid enthalpy at the same mole fraction. It calculates this by calling subroutine LIQEPY which provides it with the liquid phase enthalpy. The routine then calculates the latent heat of vaporization by Equation 2.4.2, page 24. On adding the latent heat to the liquid enthalpy, the routine returns with vapor phase enthalpy. A listing of the subroutine is given in Appendix A, Section 3.

3.1.4 Subroutine NONIDV. For a non-ideal system, a different approach to calculating liquid and vapor enthalpies has been taken. The input variables to this subroutine are vapor mole fraction, saturation temperature and an integer value of a flag by the name of TOPS. The output variables are the saturated gas mixture enthalpy and enthalpies of individual components.

The heat capacity of both the components is calculated with Equation 2.4.1, page 23. Multiplying by respective mole fractions and adding them together gives the enthalpy of an ideal gas mixture. To correct for departure from ideality, an enthalpy departure is required. The flag value taken by the subroutine as its input argument is passed to another subroutine QDVNV which provides the enthalpy departure value. When this departure is added to the ideal gas mixture enthalpy, the routine returns with the gas enthalpy of non-ideal system under consideration. The route taken for vapor enthalpy

calculation of non-ideal system is the one given by Equation 1.4.3, page 6. Appendix A, Section 4 shows the listing of the subroutine.

3.1.5 Subroutine NONIDL. There are three input and two output arguments in this subroutine. Liquid mole fraction, saturation temperature and one integrer, for flag, by the name of TOPS are the input and enthalpy of both the components and liquid mixture are the output variables.

The scheme shown by Equation 1.4.4, page 7, is used in this subroutine to calculate saturated liquid enthalpy. This routine calls subroutine NONIDV which provides the gas mixture enthalpy. The subroutine then calculates latent heat of vaporization as given by Equation 2.4.2, page 24. Since this subroutine is meant for non-ideal system, it also needs the heat of mixing. This is found by Equation 2.4.9, page 25. The routine exits by adding latent heat of vaporization, heat of mixing and non-ideal gaseous mixture enthalpy.

For listing of this subroutine, the reader is referred to Appendix A, Section 5.

3.1.6 Subroutine QDVNV. Given a vapor mole fraction, temperature, and a flag, this subroutine gives the enthalpy deviation of the vapor phase. The working range of the subroutine is 0.23 to 0.29 mixture compressibility factor. For value out of range, it gives an error message to the user. When the flag TOPS is set to

one, it calls another subroutine SUPVAP which calculates constants needed in the calculation of enthalpy deviation of superheated vapor mixture. TOPS value of zero is an indicator to the subroutine to calculate enthalpy departure of saturated vapor mixture. The deviation of enthalpy for both type of vapors is calculated by Yen and Alexander correlations. For saturated vapor, Equation 2.4.4, page 24, is used and for superheated vapors, the reader is referred to Equation 2.4.7, page 25. At a given temperature, the vapor pressure calculation is carried out by Equation 3.1.1.2, page 34. Figure 12 and Appendix A, Section 6 shows the flow chart and listing of the subroutine.

3.1.7 Subroutine QDVNL. This subroutine, in a similar fashion as subroutine QDVNV, takes liquid mole fraction, temperature and a flag value and provides enthalpy departure of the liquid phase. Depending on the flag value, it calculates the enthalpy departure of a saturated liquid mixture or subcooled liquid mixture, for non-ideal systems. The variable FLAGD has value of either zero or one. With the former value, it calculates the departure of saturated liquid. With the latter one it calculates subcooled liquid mixture departure.

Like QDVNV, its working range is also a 0.23 to 0.29 mixture compressibility factor. The Yen and Alexander correlation for saturated liquid departure is given by Equation 2.4.5, page 24. For subcooled liquid, the reader is referred to Equation 2.4.6, page 25. Working of this subroutine, which is similar to QDVNV,

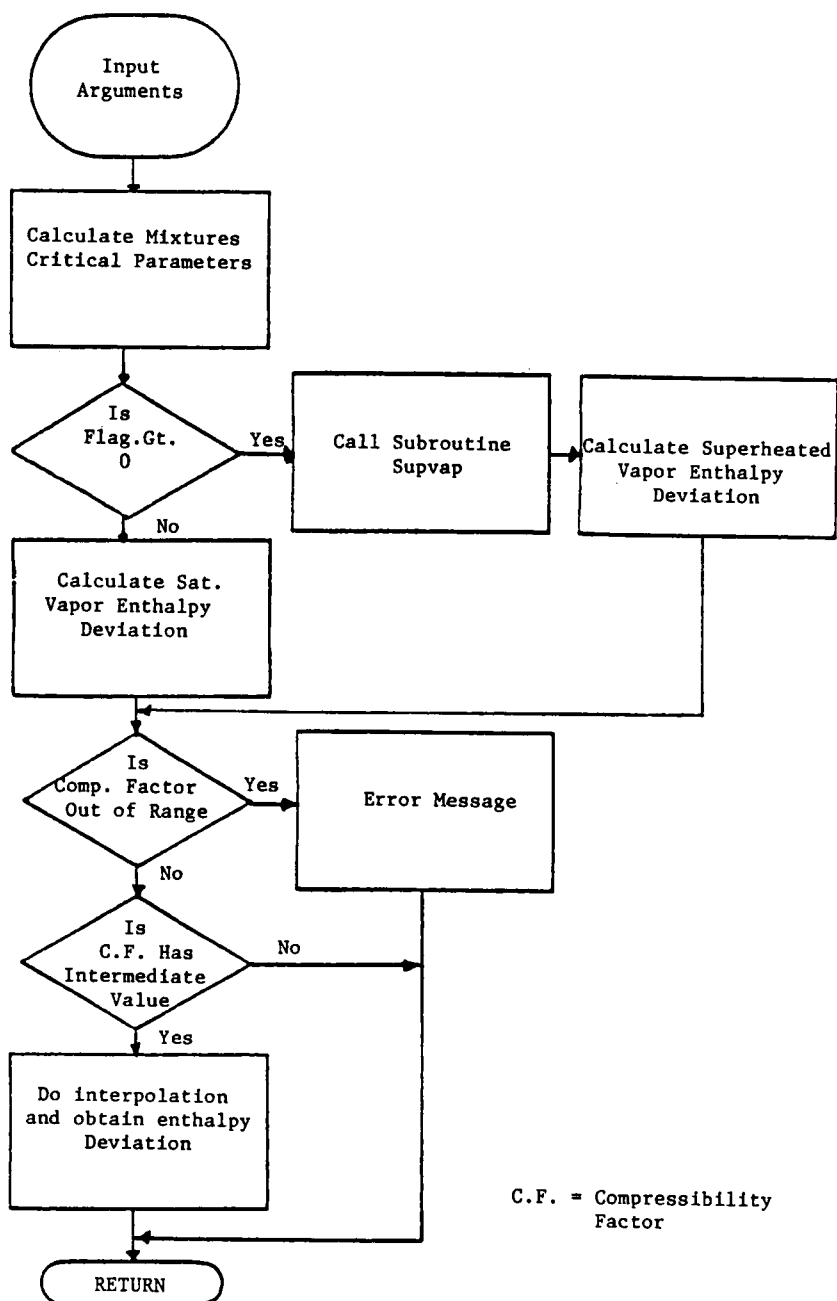


Figure 12. Flow chart of subroutine QDVNV.

could be very well understood if one refers to the flow chart of subroutine QDVNV in Figure 12. A listing is given in Appendix A, Section 7.

3.1.8 Subroutine SUPVAP. This subroutine contains a number of GO TO statements which enables it to calculate the constants needed in the enthalpy departure calculation of superheated vapor mixture. These GO TO statements work on the basis of an input argument 'N'. For N=1,2,3 and 4, the routine goes to the respective 0.23, 0.25, 0.27 and 0.29 compressibility factor and calculates constants. This routine is called by subroutine QDVNV, where enthalpy departure of superheated vapor mixture is calculated. A listing of the subroutine is given in Appendix A, Section 8.

3.1.9 Subroutine SWITCH. On the enthalpy concentration diagram, QBAR defines the quantity of heat removed in the condenser and the permanently removed distillate per unit weight of distillate. Similarly the quantity QDBAR defines the net flow of heat outward at the bottom, per mole of residue. An overall enthalpy line passing through these points intersect the saturated liquid curve at some point. The importance of this point comes from the fact that it determines the switching of operating lines from QBAR to QDBAR. Location of this point is done by this subroutine. In addition to QBAR and QDBAR, an input variable to this subroutine is SO which is a flag for either an ideal or a non-ideal system. The output from this subroutine is the intersection point discussed above.

At an assumed value of liquid mole fraction, it calls subroutine UNIQAC which provides saturation temperature. It then supplies this mole fraction and saturation temperature to LIQEPY or NONIDL as the case may be. The liquid enthalpy is compared with the liquid enthalpy obtained by Equation 2.2.6, page 17. The routine returns with the value of the liquid mole fraction, if the convergence criteria is met. This point is the one located at the intersection of the overall enthalpy line and saturated liquid enthalpy curve. The working of the subroutine can be seen in flow chart given in Figure 13. A listing of the routine is given in Appendix A, Section 9.

3.1.10 Subroutine YNRECT. Liquid mole fraction, saturation temperature, QBAR (heat removed in the condenser) and a flag for ideality or non-ideality are the input values to this subroutine. The routine uses the bisection method to find the point on the vapor enthalpy curve, which intersects the straight line given by Equation 2.2.4, page 15. This point is the output argument of the subroutine.

The subroutine first calculates liquid mixture enthalpy. It then assumes the vapor mole fraction equal to liquid mole fraction. By Equation 2.2.4, it calculates the vapor mixture enthalpy. This enthalpy is then used in Equations 1.4.2 or 1.4.3, page 6, as the case may be, and the mole fraction in vapor phase is calculated. If the assumed mole fraction and the calculated mole fraction are less than the convergence criteria, the routine returns with the value of mole fraction. In case of no convergence, the routine looks

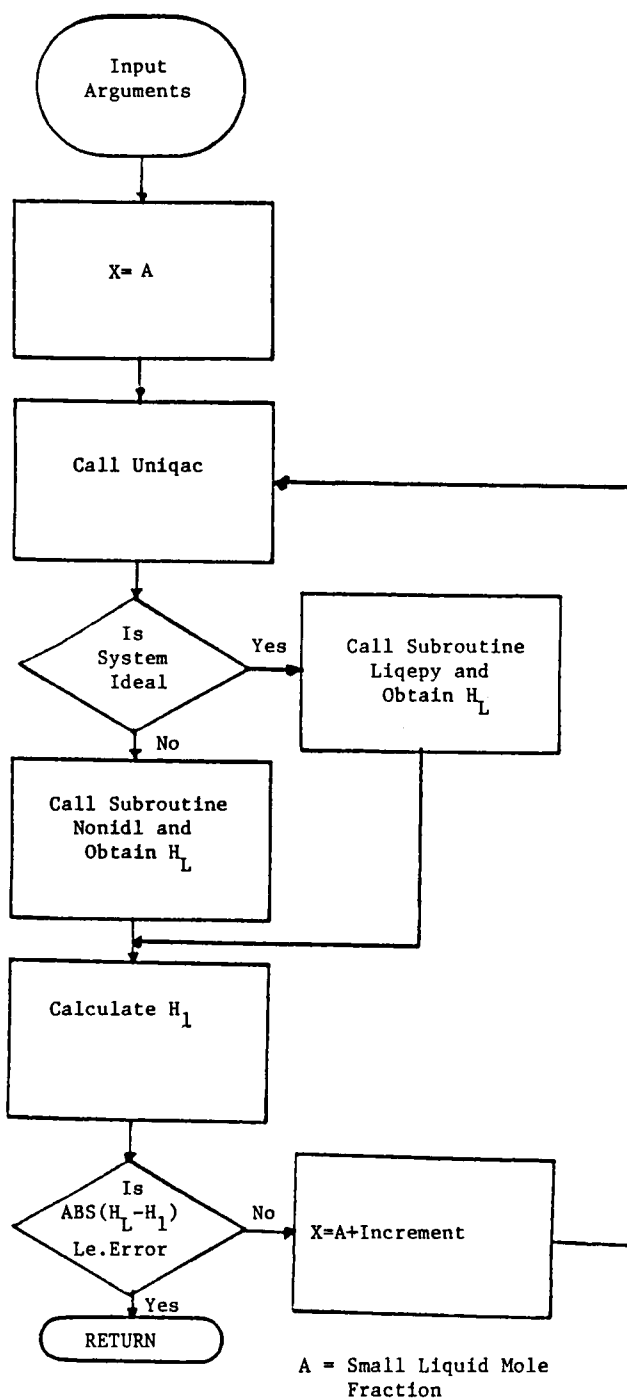


Figure 13. Flow chart of subroutine SWITCH.

for the mole fraction value by the bisection method. In case there is no sign change between two extreme limits of vapor mole fraction (assumed and vapor rising from top plate of the distillation column) then an error message is displayed on the screen. This subroutine finds the operating line only for the rectification section. Every time this subroutine returns, there is an addition of an operating line on the enthalpy concentration diagram. A flow sheet and listing of the subroutine is given in Figure 14 and Appendix A, Section 10 respectively.

3.1.11 Subroutine IDLSTP. For operating lines in the stripping section, this subroutine works in the same fashion as subroutine YNRECT. The input arguments are similar. In place of QBAR in YNRECT, QDBAR, the net flow of heat outward at the bottom is the input argument. For calculating the vapor mixture enthalpy at an assumed mole fraction, it uses Equation 2.2.5, page 15. Appendix A, Section 11 shows the listing of the subroutine.

3.1.12 Subroutine FEED. This subroutine has been developed such that it only needs a flag for ideality or non-ideality. The output variables are enthalpy of feed, and QM (the net heat removed in the condenser at minimum reflux ratio).

The routine is capable of calculating feed enthalpy (HF) and QM for every thermal condition of feed. To determine the thermal condition, it asks a question to the user. The user is required to type an integer. For example, in the case of subcooled feed the integer is '0', for saturated liquid feed, it is '1', etc. For

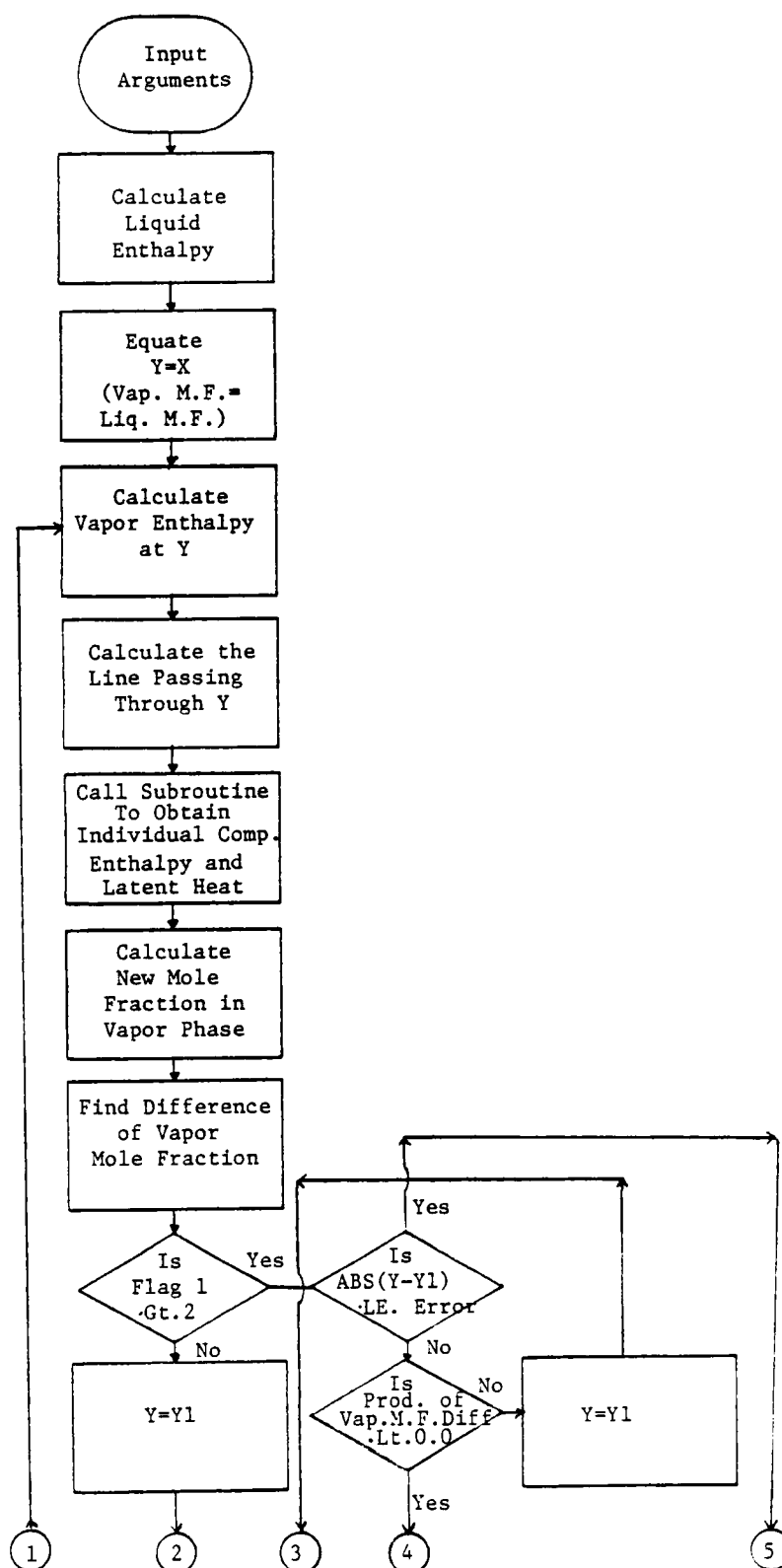


Figure 14. Flow chart of subroutine YNRECT.

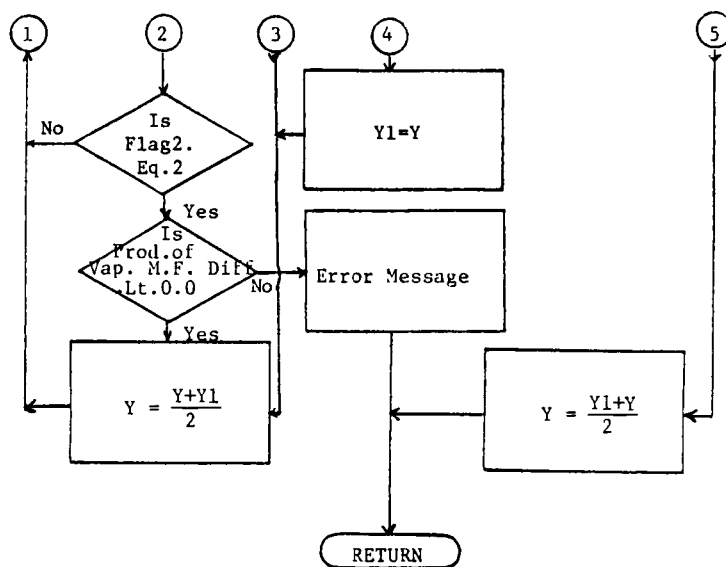


Figure 14. (Continued).

the case of subcooled and superheated feed, the temperature of the feed in degrees kelvin is provided by the user.

For subcooled feed, given mole fraction and temperature, it calculates feed enthalpy by calling subroutine LIQEPY for ideal, and NONIDL and QDVNL for non-ideal. It then calculates the slopes of the tie lines by

$$m = \frac{H_G - H_L}{Y - X} \quad (3.1.12.1)$$

Feed enthalpy and mole fraction values are then plugged in the above equation and a new slope calculated. If both slopes are very close, then the intercept of the tie line is found by the equation

$$H = mX + C \quad (3.1.12.2)$$

where H is enthalpy, and X is mole fraction.

A convergence criteria of 400.0 was found satisfactory for the example problems checked (see page 63). On evaluating the intercept, Q_M is found by

$$Q_M = X_D m + C \quad (3.1.12.3)$$

where X_D is the mole fraction in the distillate. For an ideal system, the intersection of this tie line with the line through X_D gives the highest location of Q_M . This may not be the case with a non-ideal system. For non-ideal case, the subroutine therefore goes into search of such a tie line. If it finds one, it calculates Q_M

and returns with the new value of Q_M . In case it fails, it returns with the QM value calculated initially.

For a saturated liquid feed, after calculating the feed enthalpy, it calculates the enthalpy of vapor which is in equilibrium with feed. It then calculates QM by using Equations 3.1.12.1, 3.1.12.2, and 3.1.12.3. For non-ideal, it then takes the same route as above.

For saturated vapor feed, it looks for that liquid mole fraction which is in equilibrium with feed. On location of that point, it follows the route of saturated liquid feed.

Partially vaporized feed contains a certain amount of liquid and a certain amount of vapor. For this feed, the subroutine looks for the tie line passing through the feed. On location of such tie line, pythagoruous theorem is used to find the length of the tie line.

$$\text{HYPTNS} = \sqrt{(H_G - H_L)^2 + (Y - X)^2} \quad (3.1.12.4)$$

On multiplying the percentage of vapors in the feed with HYPTNS and adding to liquid enthalpy leads to feed enthalpy. QM is then calculated in the same way as discussed above.

For superheated vapor feed, after calculating the vapor enthalpy at the given temperature, it follows the same procedure as subcooled liquid feed. Figure 15 and Appendix A, Section 12 shows the flow chart and listing of the subroutine respectively.

3.1.13 Diameter and cost estimation section. When the main program finishes the number of plates calculation in the stripping

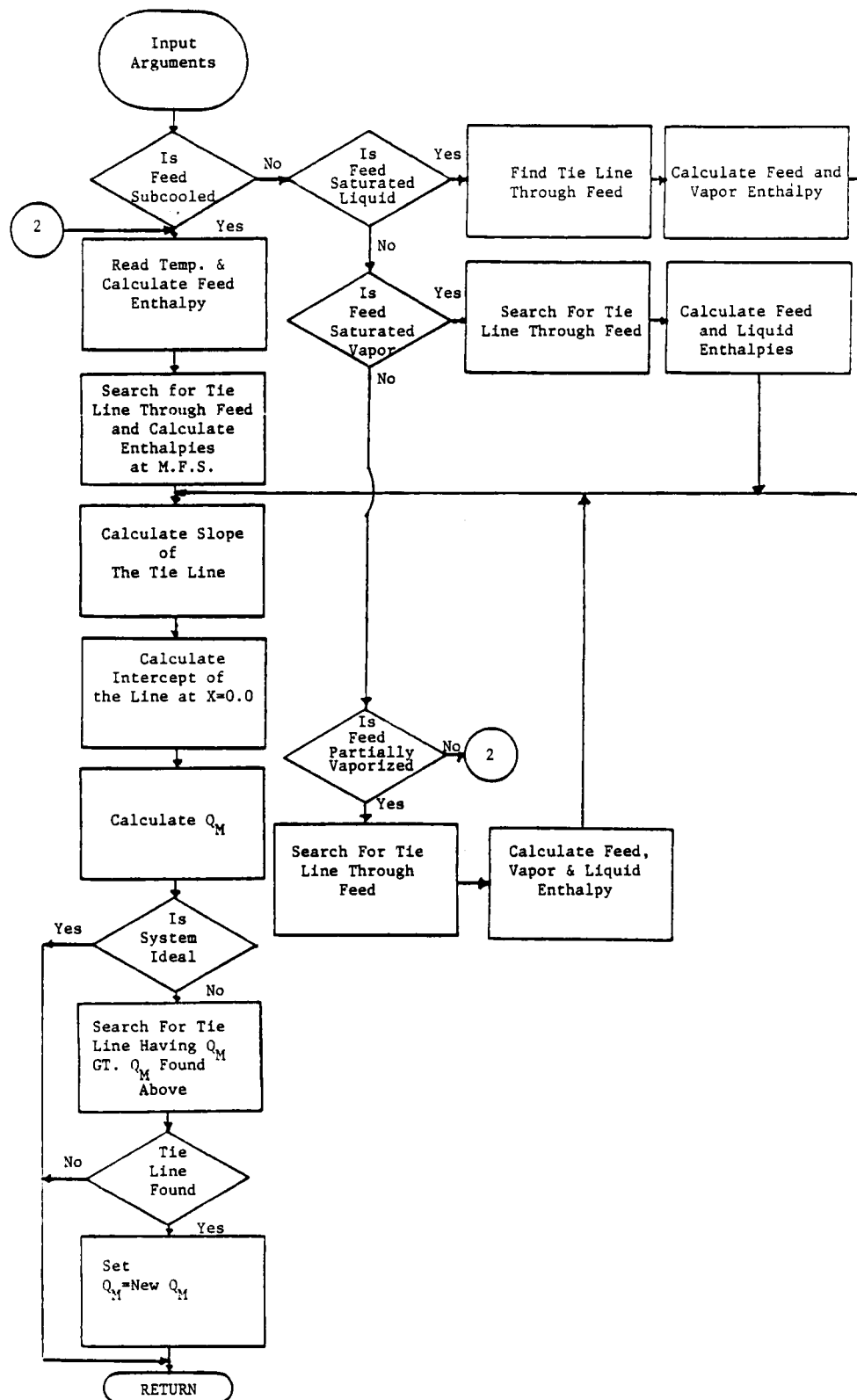


Figure 15. Flow chart of subroutine FEED.

section, it goes to the next stage of diameter and cost calculation. Here it first calculates the diameter of the tower based on maximum allowable vapor velocity. The tower diameter is used to find the tray spacing which in turn is used to calculate the constants α and β used in the empirical constant CF, Equation 2.3.4., page 22. At flooding the superficial velocity of the gas is given by the Equation 2.3.5., page 22. Eighty percent of this velocity is used to calculate new tower diameter. If both the diameters meet a convergence criteria the program goes to the next step of cost calculation. On performing 1000 iterations, if both the diameters do not converge, an error message is displayed.

In the next phase of calculation, it uses Equation 2.3.6, page 23, to predict the cost of a plate based on diameter. From this cost, annual cost of the column can be calculated by the relation

$$\text{Ann. Cost} = \left(\frac{\text{cost}}{\text{plate}} \right) (\text{Actual no. of plates}) \left(1 + \frac{\text{Ref. ratio}}{1 + \text{Ref. ratio}} \right) \\ (\% \text{ Fixed charges}) \quad . \quad (3.1.13.1)$$

The annual cost of the condenser was found by calculating the heat transfer area by

$$q = UA\Delta T \quad . \quad (3.1.13.2)$$

Cost versus heat transfer area data of condenser given by Peters were used to do regression analysis. For this purpose, SAS, a package program at the UTCC was used. A cubic polynomial equation

was tried and the correlation coefficient of 0.997 indicated it to be a good representation of the data. Cost of the condenser at the calculated area is then found by the following model equation.

$$\text{Cost} = 4741.43 + 59.94(\text{Area}) + 0.1873(\text{Area})^2 - 8.824 \times 10^{-4}(\text{Area})^3 \quad (3.1.13.3)$$

Replacing the cost/plate term in the Equation 3.1.13.1 by cost/area and the actual number of plates by area of the condenser, annual cost of condenser is found.

Regression analysis was also done to find a model equation to best represent the heat transfer area of reboiler versus cost data of Peters. Like condenser, in this case also a cubic polynomial equation was found as a good model equation.

$$\text{Cost} = 6792.09 + 115.29(\text{Area}) - 3.083 \times 10^{-4}(\text{Area})^3 \quad (3.1.13.4)$$

Equation 3.1.13.1 with the modification done for condenser is then used by the code to predict annual cost of reboiler. The annual cost of steam and cooling water are then added to these costs to get annual cost of operating the tower. Working of this section of the code is explained in a flow chart given in Figure 16. A listing is given in Appendix A, Section 13.

All these costs are directly or indirectly functions of reflux ratio. To find a reflux ratio at which minimum operating cost occurs,

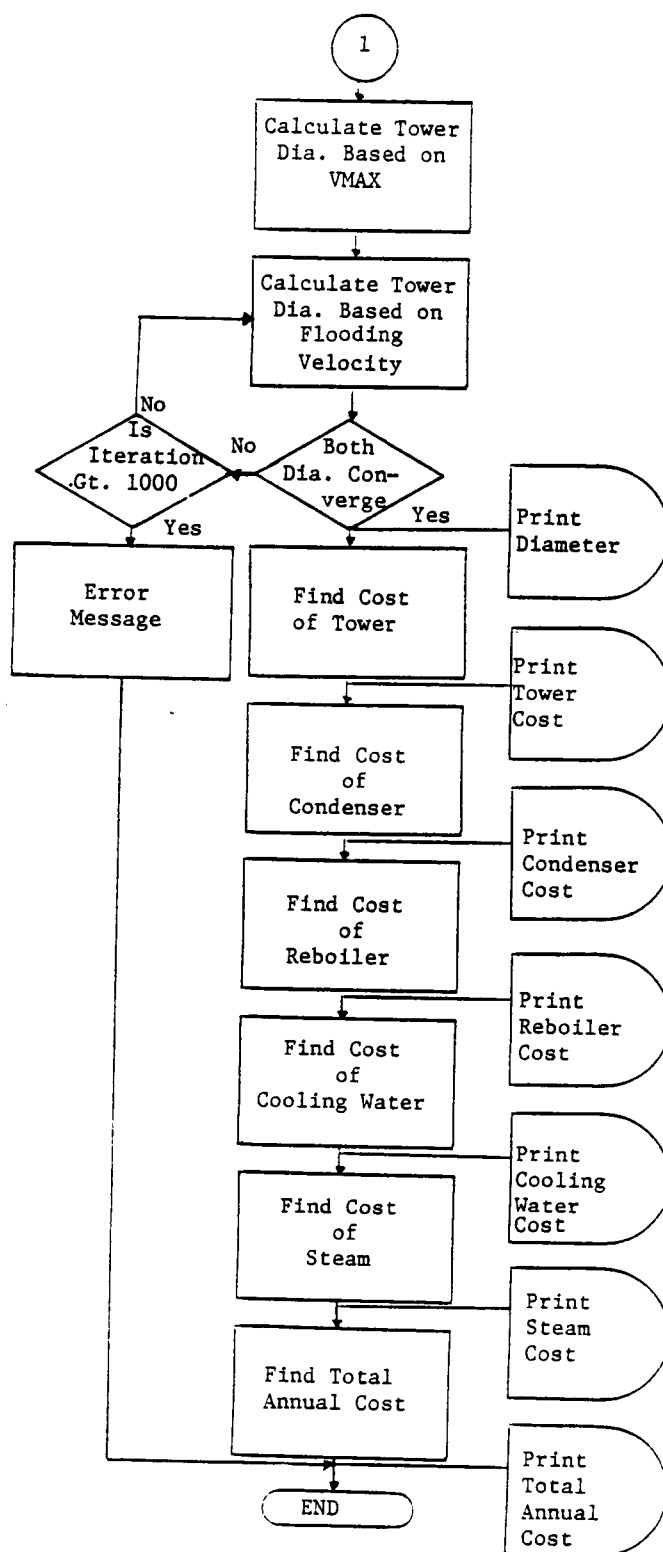


Figure 16. Flow chart of main program (diameter and cost estimation).

the user is required to vary in every run, the ratio of operating reflux and minimum reflux.

A complete listing of the main program with major variables is given in Appendix B.

CHAPTER 4

RESULTS

At atmospheric pressure and given liquid mole fractions of component 'x', saturation temperatures and equilibrium vapor mole fractions of the component were calculated by the use of the subroutine UNIQUAC. When a Benzene-Toulene system was used, the results were in agreement with the experimental results. For an Ethanol-Water system, equilibria deviation was found to be 2.79% in the low molefraction range. For high mole fractions, the result was the same as the experimental result. Tables 1 and 2 give a comparison of the experimental and the computer results for both the systems. Graphical representation of the results are given in Figures 7 and 9 (pages 36 and 38).

The cost versus heat transfer area data provided by Peters and Timmerhaus were used to do regression analysis. For predicting cost of the reboiler, a cubic polynomial equation was found to give quite close results to the actual data. This was further confirmed by the correlation coefficient of this regression which is 0.999.

From another model equation, developed for the condenser, the cost for 74.3 meter square area deviated by 1.23%. The correlation coefficient for the model equation was found to be 0.997, suggesting good fit of equation to the data. Costs predicted by both the model equations are compared with the data in Figures 17 and 18. An example problem described below was solved by the code.

TABLE 1
COMPARISON OF VAPOR-LIQUID EQUILIBRIA
OF BENZENE-TOULENE

Mol. Fraction of Benzene in Liquid Phase 'X'	Mol. Fraction of Benzene in Vapor Phase 'Y'	
	Experimental ^a	Computer
0.050	0.108	0.109
0.100	0.206	0.206
0.200	0.372	0.373
0.300	0.508	0.509
0.400	0.621	0.621
0.500	0.714	0.714
0.600	0.792	0.792
0.700	0.857	0.857
0.800	0.913	0.912
0.900	0.960	0.959
0.950	0.981	0.980
1.000	1.000	1.000

^aSource: Kojima, K., and K. Tochigi, Prediction of Vapor-Liquid Equilibria by the Asog Method, 3, 107 (1979).

TABLE 2
COMPARISON OF VAPOR-LIQUID EQUILIBRIA
OF ETHANOL-WATER

Mol. Fraction of Ethanol in Liquid Phase 'X'	Mol. Fraction of Ethanol in Vapor Phase 'Y'	
	Experimental ^a	Computer
0.018	0.179	0.174
0.054	0.337	0.347
0.124	0.470	0.476
0.176	0.514	0.519
0.230	0.542	0.548
0.288	0.570	0.571
0.385	0.612	0.610
0.440	0.633	0.628
0.514	0.657	0.658
0.637	0.735	0.738
0.840	0.850	0.852
1.000	1.000	0.999

^aSource: Kojima, K., and K. Tochigi, Prediction of Vapor-Liquid Equilibria by the Asog Method, 3, 170 (1979).

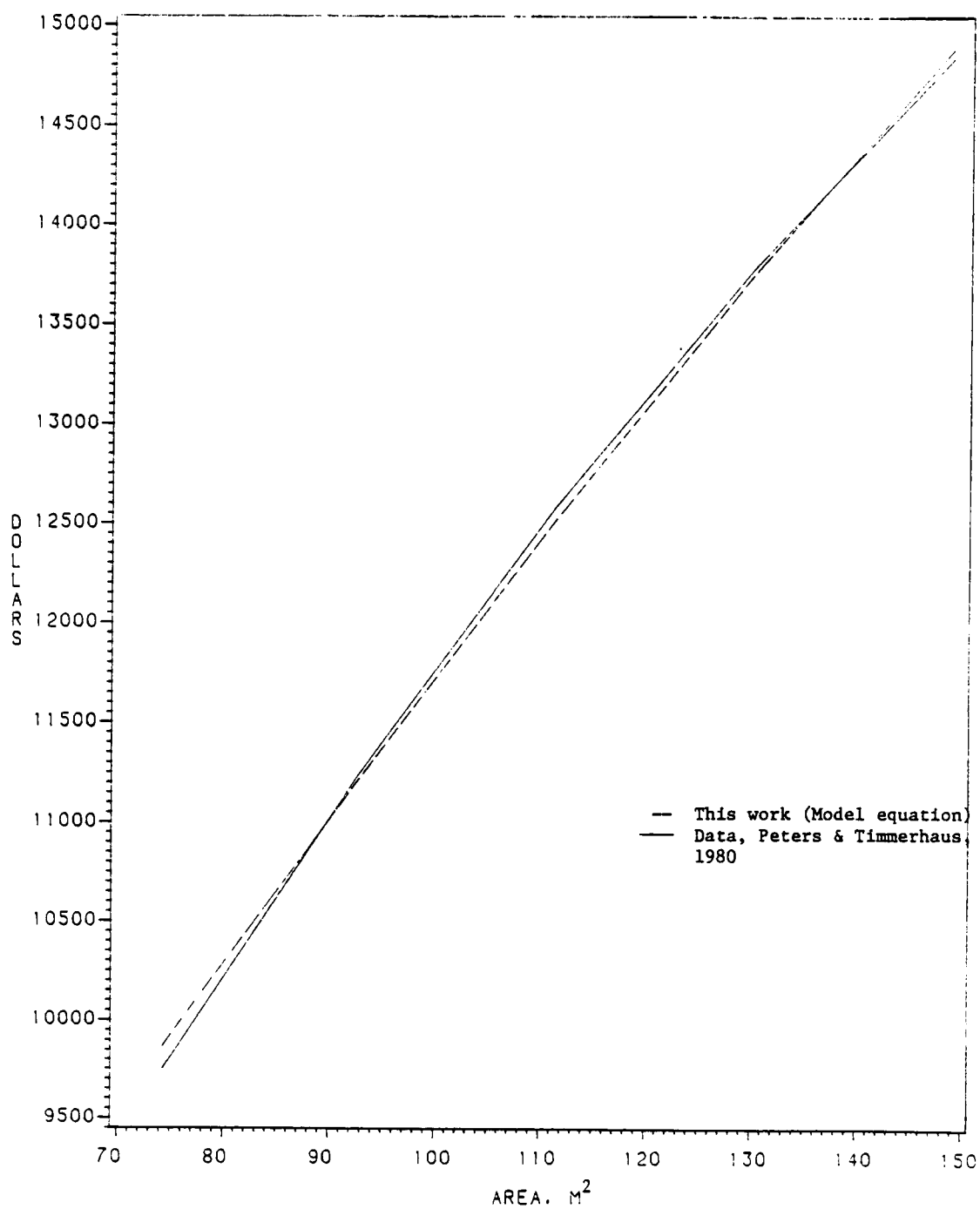


Figure 17. Condenser cost comparison.

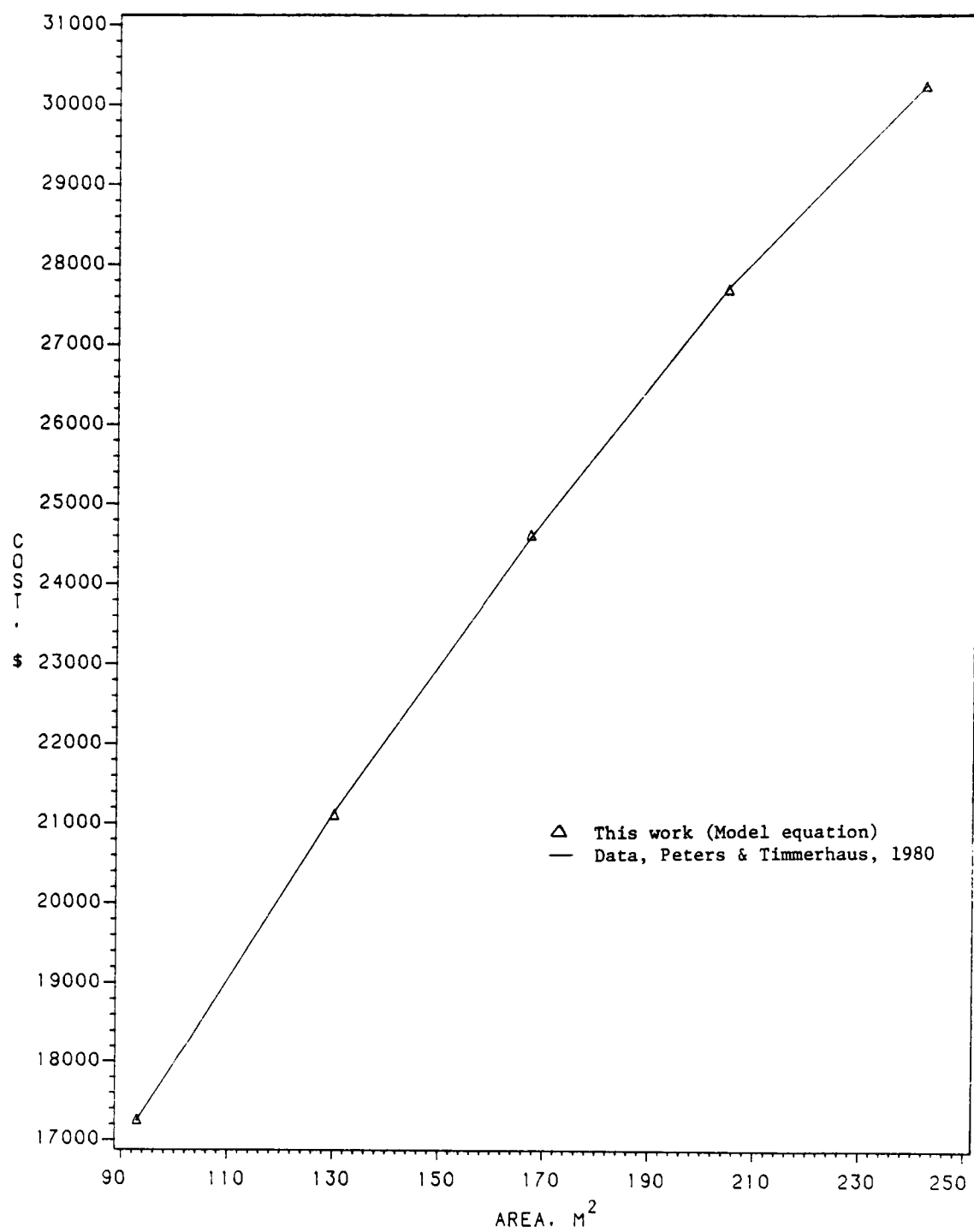


Figure 18. Reboiler cost comparison.

A sieve plate distillation column is to be designed to distill Benzene-Toulene using the following data:

Feed rate	= 318 K mole/hr
Benzene mole fraction in distillate	= 0.92
Benzene mole fraction in feed	= 0.45
Benzene mole fraction in bottoms	= 0.05
Thermal condition of feed	= saturated liquid
Total pressure	= 1 atm
Overall heat transfer coefficient in reboiler	= $454 \text{ J/m}^2\text{-s-}^\circ\text{K}$
Overall heat transfer coefficient in condenser	= $568 \text{ J/m}^2\text{-s-}^\circ\text{K}$

The same problem described above was solved by Peters and Timmerhaus, (Example 6, page 388). He used the McCabe-Thiele graphical technique to solve the problem. Using the same technique, Manzoor solved this problem with his computer code. The results of the problem, obtained by this work, is compared with the results of the above described works in Table 3. Graphical solution of this problem, using Ponchon-Savarut technique, is shown in Figure 19. Peter's solution is based on cost of plate where installation and auxiliaries costs are not considered. Due to this, total annual cost calculated by Peter is less than the computer results.

For optimum reflux, total annual cost at different reflux ratios was calculated and plotted in Figure 20. The curve shows that at all the reflux ratios, the code gives quite close agreement to the graphical result of Peters.

TABLE 3

COMPARISON OF RESULTS OF A BENZENE-TOULENE
SEPARATION FOR A SATURATED LIQUID FEED

Quantity	RESULTS		
	Manzoor ^a	Peters & Timmerhaus ^b	Computer
Minimum reflux	1.149	1.14	1.156
Optimum reflux	1.264	1.25	1.248
Diameter, meter	2.18	2.10	2.12
Number of theoretical plates	19	18	17
Total annual cost dollars	102,095	99,000	103,580

^aSource: Manzoor, Q. H., Computer Aided Distillation Design, Thesis, Univ. of Tenn., Knoxville, 79 (1984).

^bSource: Peters, M. S., and K. D. Timmerhaus, Plant Design and Economics for Chemical Engineers, III-Ed, 388 (1980).

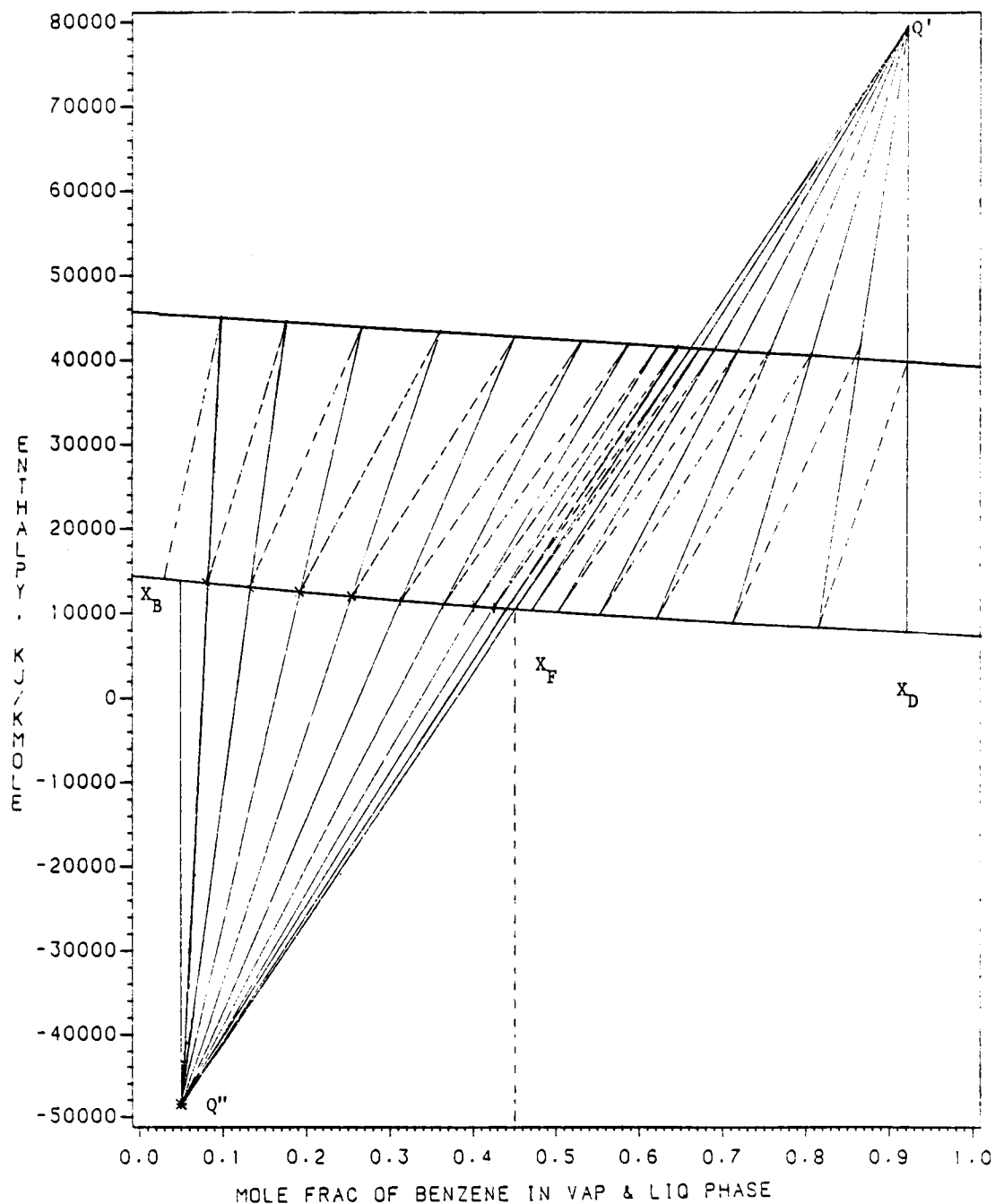


Figure 19. Graphical solution of Benzene-Toulene system (saturated liquid feed).

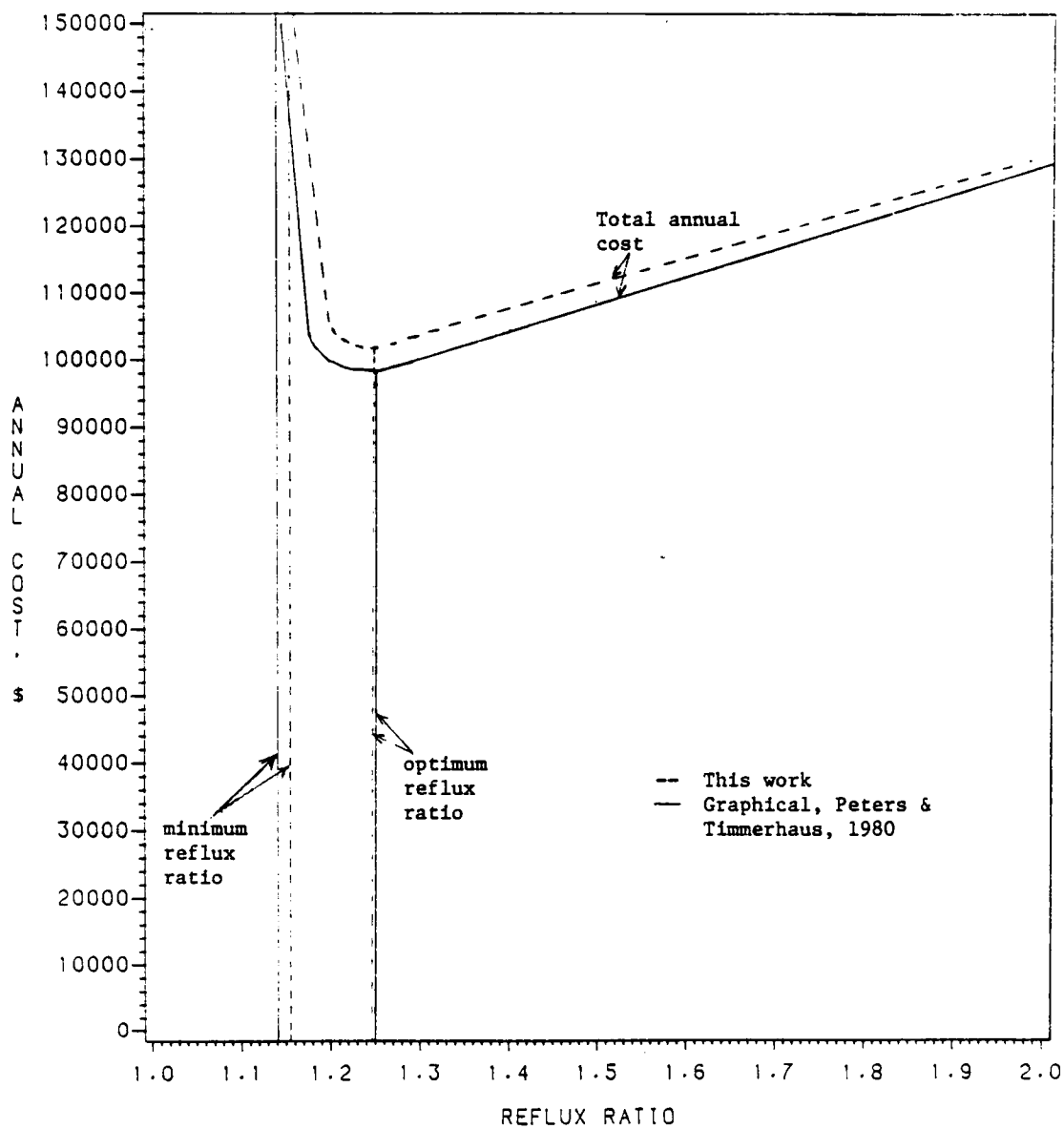


Figure 20. Annual cost comparison at optimum reflux ratios.

To check the working of the code at other thermal conditions of feed, another example problem from McCabe and Smith (Problem 19-4, page 560) was solved. By looking at the results in Tables 4 and 5, one can say that the code works quite well for other thermal conditions of feed too. The graphical solution of the problem for subcooled feed and partially vaporized feed is shown in Figures 21 and 22 respectively.

For the non-ideal case, a problem was solved with the following specified quantities.

Mole fraction of Ethanol in distillate	= 0.7
Mole fraction of Ethanol in feed	= 0.3
Mole fraction of Ethanol in bottoms	= 0.02
Ratio of operating to minimum reflux	= 1.5
Thermal condition of feed	= subcooled feed

The problem was solved graphically (Figure 23) as well as by the code. Manzoor also solved this problem with his code. Results of the two codes, with different approaches, are shown in Table 6. Total number of plates and the feed plate position being the same, the only difference was the minimum reflux ratio. For non-ideal case, the Ponchon-Savarit method is more accurate than the McCabe-Thiele as the former takes into consideration the heat effects. Therefore, it could be said that the code works quite well for non-ideal systems too.

TABLE 4
COMPARISON OF RESULTS OF A BENZENE-TOULENE
SEPARATION PROBLEM FOR A SUBCOOLED FEED

Quantity	RESULTS	
	Graphical Solution ^a	Computer Solution
Minimum reflux	1.17	1.19
<u>Number of theoretical plates</u>		
Enriching section	5	5
Stripping section	5	5
Feed tray location	5	5
Total number of plates including reboiler	11	11

^aSource: McCabe, W. L., and J. C. Smith, Unit Operations of Chemical Engineering, III-Ed, 560 (1976).

TABLE 5
COMPARISON OF RESULTS OF A BENZENE-TOULENE
SEPARATION PROBLEM FOR A PARTIALLY
VAPORIZED FEED

Quantity	RESULTS	
	Graphical Solution ^a	Computer Solution
Minimum reflux	2.16	2.23
<u>Number of theoretical plates</u>		
Enriching section	7	6
Stripping section	6	6
Feed plate location	7	6
Total number of plates including reboiler	13	12

^aSource: McCabe, W. L., and J. C. Smith, Unit Operations of Chemical Engineering, III-Ed, 560 (1976).

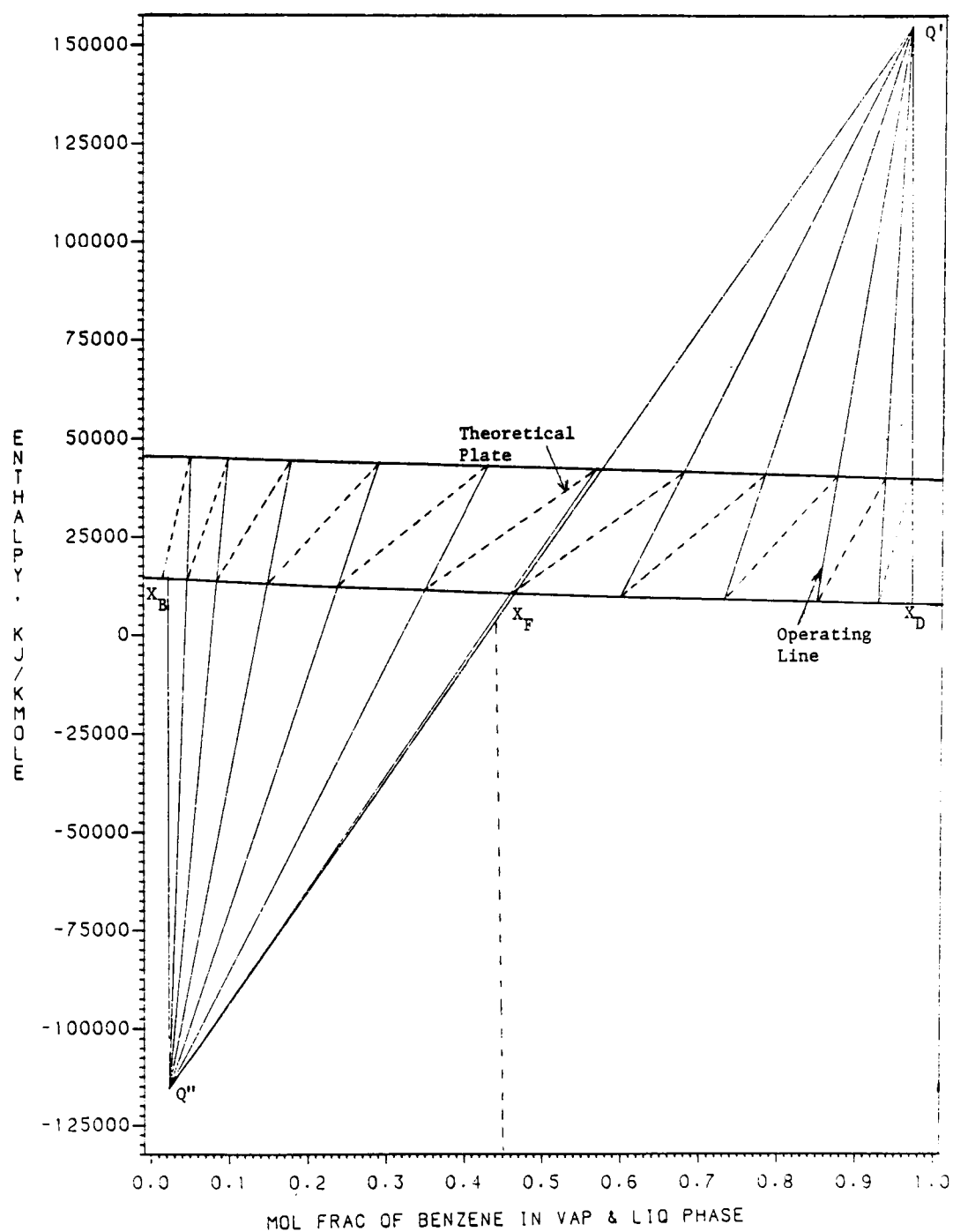


Figure 21. Graphical solution of Benzene-Toulene system (subcooled feed).

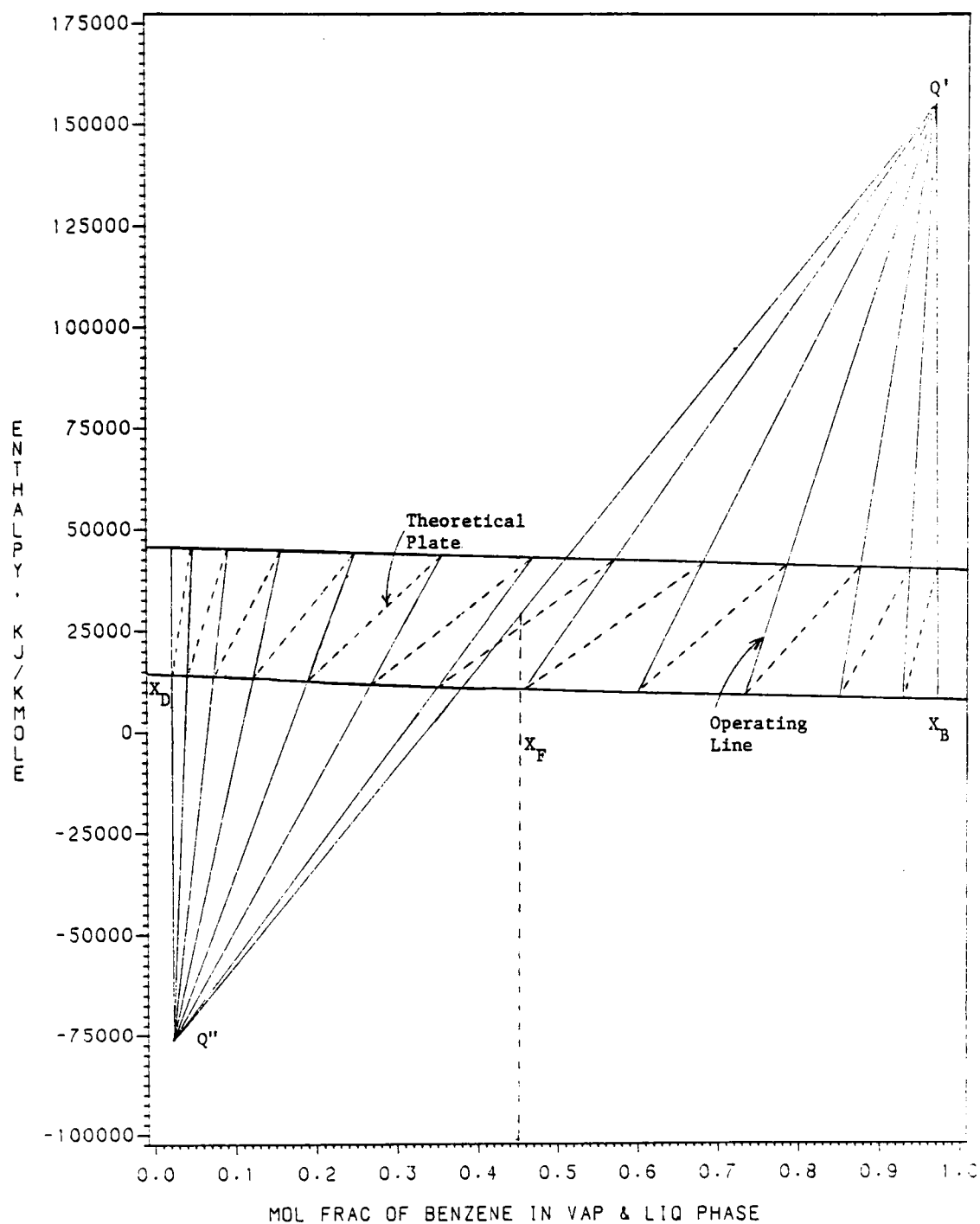


Figure 22. Graphical solution of Benzene-Toulene separation (partially vaporized feed).

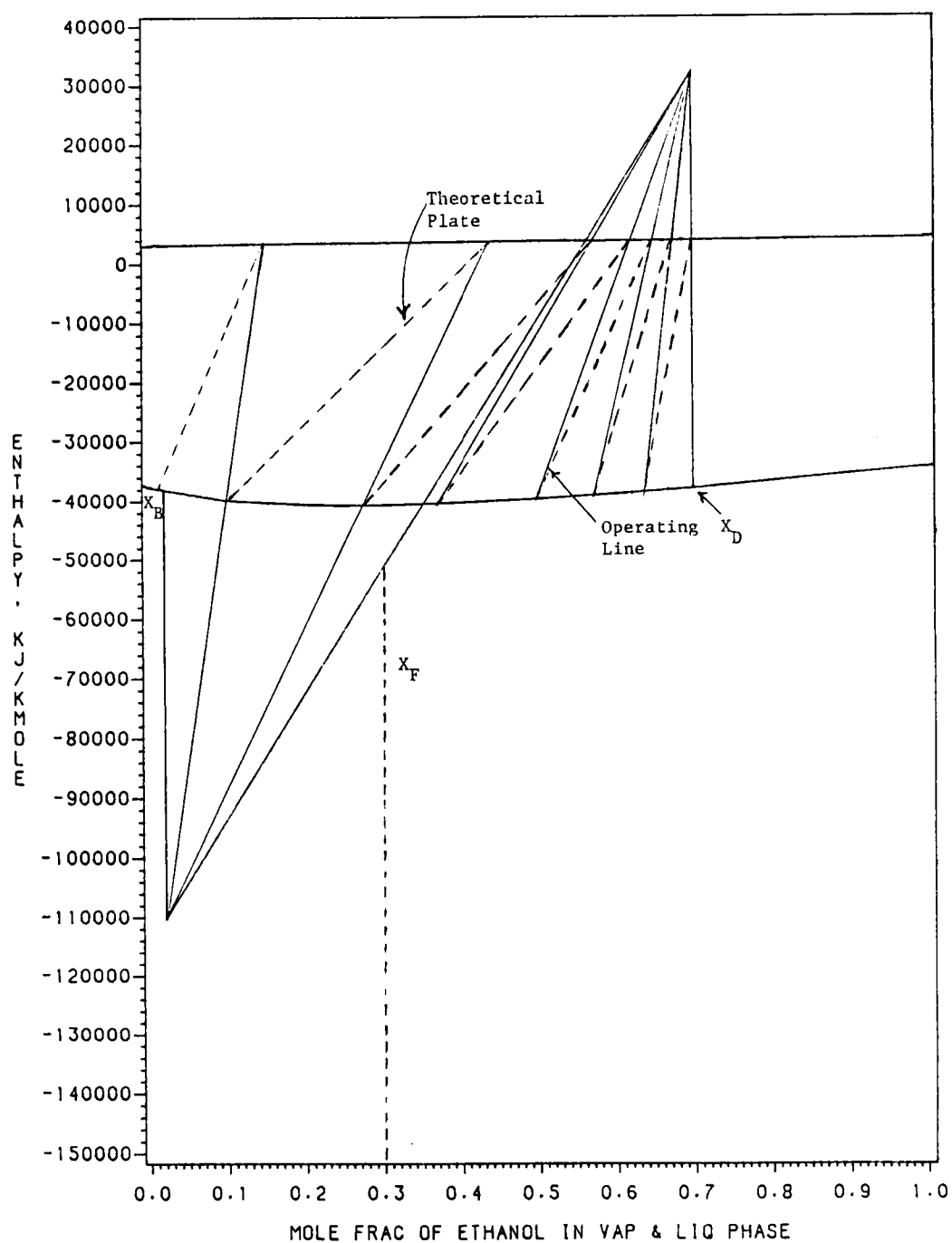


Figure 23. Graphical solution of Ethanol-Water separation (subcooled feed).

TABLE 6
COMPARISON OF RESULTS OF AN ETHANOL-WATER
SEPARATION PROBLEM FOR A SUBCOOLED FEED

Quantity	RESULTS	
	Manzoor solution ^a	Computer Solution
Minimum reflux	0.434	0.454
<u>Number of theoretical plates</u>		
Enriching section	5	5
Stripping section	1	1
Feed plate location	5	5
Total number of plates including reboiler	7	7

^aSource: Manzoor, Q. H., Computer Aided Distillation Design, Thesis, Univ. of Tenn., Knoxville, 63 (1984).

CHAPTER 5

SUMMARY AND CONCLUSIONS

A computer program has been written for the design and optimization of distillation systems. The program works at an atmospheric pressure for binary ideal and non-ideal systems. For design, the program used the plate-to-plate technique of Ponchon-Savarit.

For this technique, vapor-liquid equilibria and enthalpy at a given mole fraction was necessary. UNIQUAC correlations were used to calculate the equilibria. The enthalpy of non-ideal systems (Ethanol-Water) was obtained by the Yen-Alexander enthalpy departure correlations.

Plate characteristics, flooding constants, and superficial velocity were calculated by correlations given in Treybal. The tower diameter was based on maximum allowable vapor velocity. This diameter was used to calculate flooding velocity. A percentage of this velocity was used to calculate the actual diameter. The tower cost, based on number of plates and diameter, were calculated by Manzoor's cubic polynomial equation. By regression, two new correlations were developed from Peters and Timmerhaus cost data. These were used to predict the cost of reboiler and condenser for a given heat transfer area.

The code was checked for an ideal system with three different solutions of a Benzene-Toulene system. The results obtained were compared to a McCabe-Thiele graphical solution by Peters and

Timmerhaus, and McCabe and Smith. It was also checked with the computer solution of Manzoor.

For saturated feed, the code predicted 17 theoretical plates, 1.156 minimum reflux and 1.248 optimum reflux. Manzoor's work predicted 18 plates, 1.14 minimum and 1.25 optimum reflux while Peter's graphical solution predicted 19, 1.149 and 1.264 respectively. Total annual operating cost by these works was \$102,095, and \$99,000 respectively, while the code predicted \$103,580. Tower diameter by this code was 2.12 meter compared to Manzoor's and Peter's predicted diameter of 2.18 meter and 2.10 meter respectively.

For subcooled and partially vaporized feed, the code predicted fifth and sixth plate to be the feed points respectively, which is comparable to McCabe and Smith graphical solution of fifth and seventh respectively. Total number of plates was predicted to be 11 and 12, and minimum reflux ratio was 1.19 and 2.23 respectively. As compared to this, the graphical solution gave 11 and 13 to be the total number of plates and 1.17 and 2.16 respectively to be the reflux ratio.

For the non-ideal case, an example problem of Ethanol-Water separation was solved, and compared to the work of Manzoor. The code predicted fifth plate to be the feed plate, total number of plates was seven and the minimum reflux ratio was 0.454. This compares to Manzoor's results of fifth, seven and 0.434 respectively.

The Ponchon-Savarit technique for design is more difficult than the McCabe-Thiele technique. No assumption of constant molal overflow is an improvement, but good enthalpy-concentration data

is required. Since the results of this work are in good agreement with other works, it can be concluded that the code gives good results for both ideal and non-ideal systems.

CHAPTER 6

RECOMMENDATIONS FOR FUTURE WORK

This program can calculate the design variables of a distillation column only if the vapors from the top of the column are totally condensed. In the case of a partial condenser, this program cannot be used. This limitation could be removed with some minor modifications on this program.

The program only works for atmospheric pressure. Also, at a given liquid mole fraction, this program works quite well to calculate equilibrium vapor mole fraction. If the vapor mole fraction is provided, the program cannot calculate the equilibrium liquid mole fraction. A modification could be made to make it operate in both the directions for any given pressure.

Model equations for cost data do not represent current costs. It is recommended that the cost data be updated for inflation to correct cost of condenser, reboiler and tower to current dollars.

For determining the fixed annual cost of the tower, the method of Peters and Timmerhaus is not currently applicable. It is recommended that the 10% investment credit and ACRS (Annual Cash Return Scheme) depreciation method for a five year property be included.

All plate efficiencies were taken to be 70%. However, if plate characteristics are taken into consideration, modification can be made in the code to calculate plate efficiency.

The search for the minimum cost must be done manually. The ratio of operating reflux to minimum reflux must be changed every run. By adding an appropriate search technique, the program could automatically find the minimum cost.

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APPENDIX A

Section 1

```

REAL LAMDA(2),CP(2),MD,MB,LAMW,ML,MG,OPT,LR,HL
INTEGER SO,S1,TOPS,FLAGD
COMMON /WAAZ/W,Z
COMMON /NAYA/AC(2),AD(2),AE(2),AF(2),AG(2)
COMMON /ABC/A(2),B(2),C(2)
COMMON /VIL/VIL(2)
COMMON /PVC/PC(2),ZC(2)
COMMON /TLMT/ T(2)
COMMON /MOLFRN/ XT(3)
COMMON GC,PRESS,FR,TO
COMMON /RQU/R(2),Q(2),U(2,2)
COMMON /DEFG/D(2),E(2),F(2),G(2)
COMMON /TCT/TC(2),TBR(2),HOV(2)
COMMON /PUT/ PUT
DATA RR/1.5/
OPEN(UNIT=24,NAME='HUSS.DAT')
READ(24,*)GC,PRESS,FR,TO,T,A,B,C,R,Q,U
X=0.005
DO 1 I=1,990
  CALL UNIQAC(X,TEMP,Y)
  IF(ABS(X-Y).LE.0.0009)GO TO 2
  X=X+0.001
1  CONTINUE
  SO=0
  WRITE(5,*)' YOUR SYSTEM IS IDEAL'
  GO TO 3
2  SO=1
  WRITE(5,*)' YOUR SYSTEM IS AZEOTROPIC NON-IDEAL'
  GO TO 4
* Data reading
3  READ(24,*)XT,D,E,F,G,W,Z,HOV,TC,TBR,CS,CW,OPT,PFC,RA,SIGMA,
  1  TEMPB,TEMPS,TEMPT,DELTW,TEMPCW,UC,UR,VMAX,PE,HC,VFL,DL,LAMW,MG,
  2  ML,PUT,ZC
  GO TO 5
4  READ(24,*)XT,AC,AD,AE,AF,AG,W,Z,HOV,TC,TBR,VIL,PC,CS,CW,OPT,PFC,
  1  RA,SIGMA,TEMPB,TEMPS,TEMPT,DELTW,TEMPCW,UC,UR,VMAX,PE,HC,VFL,DL,
  2  LAMW,MG,ML,PUT,ZC
* Calculation starts with distillate
5  X=XT(1)
  XD=X
  YT=XD
  WRITE(5,6)
6  FORMAT(' TYPE 0 IF YOUR DISTILLATE IS SUBCOOLED LIQUID OR 1 IF
  1  IT IS SATURATED LIQUID')
  READ(5,*)S1
  IF(S1.EQ.1)GO TO 9
  WRITE(5,7)
7  FORMAT(' TYPE TEMPERATURE OF DISTILLATE IN DEGREES KELVIN')
  READ(5,*)TEMP
  IF(SO.EQ.1)GO TO 8
* Enthalpy calculation of subcooled distillate of ideal system
  CALL LIQEPY(X,TEMP,HL,CP)
  HLO=HL
  GO TO 14
* Enthalpy calculation of subcooled distillate of non-ideal system
8  TOPS=0
  CALL NONIDL (X,TEMP,TOPS,HL,CP)
  FLAGD=0
  CALL QDVNL(X,TEMP,FLAGD,DHL)
  HL=HL+DHL

```


Section 1 (continued)

```

        FLAGD=1
        CALL QDVNL (X,TEMP,FLAGD,DHL)
        HLO=HL-DHL
        GO TO 11
* Enthalpy calculation of saturated liquid distillate of ideal system
9      CALL UNIQAC (X,TEMP,Y)
        IF(SO.EQ.1)GO TO 10
        CALL LIQEPY(X,TEMP,HL,CP)
        HLO=HL
        GO TO 14
* Enthalpy calculation of saturated liquid distillate of non-ideal system
10     TOPS=0
        CALL NONIDL(X,TEMP,TOPS,HL,CP)
        HLO=HL
* Enthalpy calculation of ideal vapors from top of the column
11     X=0.005
        DO 12 I=1,1000
            CALL UNIQAC (X,TEMP,Y)
            IF(ABS(Y-XD).LE.0.001)GO TO 13
            X=X+0.001
12     CONTINUE
        WRITE(5,*)' CONVERGENCE CRITERIA IS NOT MET AT STMNT:11'
        GO TO 56
13     Y=XD
        CALL NONIDV(Y,TEMP,TOPS,HV,CP)
        HV1=HV
        GO TO 17
* Enthalpy calculation of non-ideal vapors from top of the column
14     X=0.005
        DO 15 I=1,1000
            CALL UNIQAC(X,TEMP,Y)
            IF(ABS(Y-XD).LE.0.001)GO TO 16
            X=X+0.001
15     CONTINUE
        WRITE(5,*)' CONVERGENCE CRITERIA IS NOT MET AT STMNT:14'
        GO TO 56
16     Y=XD
        CALL IENTPY(Y,TEMP,HV,LAMDA,CP)
        HV1=HV
* Feed enthalpy calculation starts
17     XF=XT(2)
        CALL FEED(SO,HF,QM)
* Enthalpy calculation of bottom stream starts
        X=XT(3)
        XB=X
        CALL UNIQAC(X,TEMP,Y)
        IF(SO.EQ.1)GO TO 18
        CALL LIQEPY(X,TEMP,HL,CP)
        CALL IENTPY(Y,TEMP,HV,LAMDA,CP)
        HLB=HL
        GO TO 19
18     TOPS=0
        CALL NONIDL(X,TEMP,TOPS,HL,CP)
        HLB=HL
* Material & Energy balance starts
19     DD=FR*(XT(2)-XT(3))/(XT(1)-XT(3))
        BB=FR-DD
        RM=(QM-HV1)/(HV1-HLO)
        RRO=RM*RR
        QBAR=(RRO*(HV1-HLO))+HV1
        QDBAR=(HF-(((XT(2)-XT(3))/(XT(1)-XT(2)))*(QBAR-HF)))

```

Section 1 (continued)

```

      QC=(QBAR-HLO)*DD
      QB=(HLB-QDBAR)*BB
      CALL SWITCH(SO,QBAR,QDBAR,XP)
* The program now starts stepping down in the rectification section from
* the top of the column
      KFLAG=1
20      X=0.005
      DO 21 I=1,1000
          CALL UNIQAC(X,TEMP,Y)
          IF(ABS(Y-YT).LE.0.001)GO TO 22
          X=X+0.001
21      CONTINUE
      WRITE(5,*)' CONVERGENCE CRITERIA FOR VAPOR MOLE FRACTION IN
1 RECTIFICATION SECTION IS NOT MET'
      GO TO 56
22      IF(X.LT.XP)GO TO 23
      CALL YNRECT(SO,X,TEMP,QBAR,YT)
      KFLAG=KFLAG+1
      GO TO 20
23      WRITE(5,24)KFLAG,KFLAG
      WRITE(23,24)KFLAG,KFLAG
24      FORMAT(' NUMBER OF PLATES IN RECTIFICATION SECTION IS',I5,' AND
1 FEED PLATE IS',I5)
* Stepping down in the stripping section starts
      IFLAG=1
      CALL IDLSTP(SO,X,TEMP,QDBAR,YT)
25      X=0.005
      DO 26 I=1,1000
          CALL UNIQAC(X,TEMP,Y)
          IF(ABS(Y-YT).LE.0.005)GO TO 27
          X=X+0.001
26      CONTINUE
      WRITE(5,*)' CONVERGENCE CRITERIA FOR VAPOR MOLE FRACTION IN
1 STRIPPING SECTION IS NOT MET'
      GO TO 56
27      IF(X.LT.XB)GO TO 29
      IF(X.EQ.XB)GO TO 28
      CALL IDLSTP(SO,X,TEMP,QDBAR,YT)
      IFLAG=IFLAG+1
      GO TO 25
28      JFLAG=KFLAG+IFLAG
      GO TO 30
29      JFLAG=KFLAG+IFLAG+1
30      WRITE(5,31)IFLAG,JFLAG
      WRITE(23,31)IFLAG,JFLAG
31      FORMAT(' NUMBER OF PLATES IN THE STRIPPING SECTION IS',I5
1 ' AND TOTAL NUMBER OF PLATES IS',I5)
      WRITE(23,32)QC,QB,RM
      WRITE(5,32)QC,QB,RM
32      FORMAT(' HEAT TAKEN OUT AT THE CONDENSER IS',F20.5/ ' HEAT
1 ADDED AT THEREBOILER IS',F20.5/ ' MINIMUM REFLUX RATIO IS'
2 ,F20.5)

```

Section 2

```

SUBROUTINE UNIQAC(X,TEMP,Y)
REAL BGT(2,2),PARL(2),THETA(2),PHI(2),AA(2),GAM(2),GAMT(2)
REAL PS(2),QSUM(2),RSUM(2),CAL(200)
INTEGER H
COMMON /RQU/R(2),Q(2),U(2,2)
COMMON GC,PRESS,FR,TO
COMMON /TLMT/T(2)
COMMON /ABC/ A(2),B(2),C(2)
H=1
FRAC=X
L=1
M=2
T1=T(L)
T2=T(M)
TA=T1
TB=T2
SUMQ=0.0
SUMR=0.0
DO 1 I=1,2
  PARL(I)=(5.*(R(I)-Q(I)))-(R(I)-1.0)! As defined by
*   ! eq 2.4.15
  QSUM(I)=X*Q(I)
  RSUM(I)=X*R(I)
  SUMQ=SUMQ+QSUM(I)
  SUMR=SUMR+RSUM(I)
  X=1.0-X
1 CONTINUE
K=1
2 DO 4 I=1,2
  THETA(I)=QSUM(I)/SUMQ! As defined by eq 2.4.16
  PHI(I)=RSUM(I)/SUMR! As defined by eq 2.4.17
  DO 3 J=1,2
    BGT(J,I)=EXP((-U(J,I)-U(I,I))/(GC*T1))! As defined
*   ! by eq 2.4.18
3 CONTINUE
4 CONTINUE
DO 5 I=1,2
  AA(I)=BGT(I,M)/(THETA(M)+(THETA(I)*BGT(I,M)))
  M=M-1
5 CONTINUE
X=FRAC
M=2
DO 6 I=1,2
  AC=THETA(M)*Q(I)
  P3=AC*(AA(M)-AA(I))
  AD=Q(I)*ALOG(THETA(I)+(THETA(M)*BGT(M,I)))
  AE=PHI(M)*(PARL(I)-((R(I)/R(M))*PARL(M)))
  P2=AE-AD
  AF=5.*Q(I)*ALOG(THETA(I)/PHI(I))
  AG=ALOG(PHI(I)/X)
  P1=AF+AG
  GAM(I)=P1+P2+P3
  GAMT(I)=EXP(GAM(I))! Activity coefficient
  X=1.0-X
  M=M-1
6 CONTINUE
DO 7 I=1,2
  PS(I)=EXP(A(I)-(B(I)/(T1+C(I))))! Vapor pressure
7 CONTINUE
X=FRAC
PT=0.0

```

Section 2 (continued)

```

      DO 8 I=1,2
        PT=PT+GAMT(I)*X*PS(I)! Total pressure
        X=1.0-X
8      CONTINUE
      CAL(H)=(PT/760.0)-PRESS! Difference of calculated and input
*      ! pressure
      X=FRAC
      M=2
      IF(H.GT.2)GO TO 12
      T1=T2
      H=H+1
      IF(K.EQ.2)GO TO 9
      K=K+1
      GO TO 2
9      H=2
      IF((CAL(L)*CAL(M)).LT.0.0) GO TO 11
      WRITE(5,10)FRAC
10     FORMAT(' FUNCTION DOES NOT CHANGE SIGN IN SUBROUTINE UNIQAC IN
1     THE BOILING POINTS RANGE FOR LIQUID MOLE FRACTION',F20.5)
      STOP
11     ERROR=0.001
      T1=(TA+TB)/2.0
      H=H+1
      GO TO 2
12     IF(ABS(TB-TA).LE.ERROR)GO TO 14
      IF((CAL(L)*CAL(H)).LE.0.0)GO TO 13
      CAL(L)=CAL(H)
      TA=T1
      GO TO 11
13     TB=T1
      GO TO 11
14     TEMP=T1! Saturation temperature at given liquid mole fraction
      Y=X*GAMT(L)*EXP(A(L)-(B(L)/(T1+C(L))))/(PRESS*760)! Equilibrium
*      !vapor mole fraction
      RETURN
      END

```

Section 3

```

SUBROUTINE LIQEPY(X,TEMP,HL,CP)
REAL CP(2),LAMDA(2)
COMMON /DEFG/D(2),E(2),F(2),G(2)
COMMON GC,PRESS,FR,TO
HL=0.0
DO 1 I=1,2
  CP(I)=(D(I)*(TEMP-TO))+(0.5*E(I)*((TEMP**2)-(TO**2)))+(0.333
1    *F(I)*((TEMP**3)-(TO**3)))+(0.25*G(I)*((TEMP**4)-(TO**4)))
  HL=HL+(X*CP(I))! Enthalpy of liquid mixture
  X=1.0-X
1 CONTINUE
RETURN
END

```

```

SUBROUTINE IENTPY(Y,TEMP,HV,LAMDA,CP)
REAL LAMDA(2),CP(2)
COMMON/WAAZ/W,Z
COMMON/TCT/TC(2),TBR(2),HOV(2)
COMMON/DEFG/D(2),E(2),F(2),G(2)
X=Y
CALL LIQEPY(X,TEMP,HL,CP)
SUM=0.0
DO 1 I=1,2
  TR=TEMP/TC(I)
  PARMTR=(TBR(I)/TR)*(1.0-TR)/(1.0-TBR(I))
  LAMDA(I)=((HOV(I)*TR)/TBR(I))*((PARMTR+(PARMTR**W))/(1.0+
1    (PARMTR**Z)))
  SUM=SUM+(Y*LAMDA(I))! Latent heat of vaporization of mixture
  Y=1.0-Y
1 CONTINUE
HV=SUM+HL! Enthalpy of vapor mixture
RETURN
END

```

Section 4

```

SUBROUTINE NONIDV(Y,TEMP,TOPS,HV,CP)
REAL CP(2)
COMMON /NAYA/ AC(2),AD(2),AE(2),AF(2),AG(2)
COMMON/TCT/ TC(2),TBR(2),HOV(2)
COMMON GC,PRESS,FR,TO
FRAC=Y
SUMHL=0.0
DO 1 I=1,2
    CP(I)=(AC(I)*(TEMP-TO))+(0.5*AD(I)*((TEMP**2.)-(TO**2.)))
1    +(0.333*AE(I)*((TEMP**3.)-(TO**3.)))+(0.25*AF(I)*((TEMP**4.)
2    -(TO**4.)))+(0.2*AG(I)*((TEMP**5.)-(TO**5.)))
    SUMHL=SUMHL+(Y*CP(I))! Ideal vapor enthalpy
    Y=1.-Y
1 CONTINUE
X=FRAC
CALL QDVNV(X,TEMP,TOPS,DHL)! Vapor enthalpy deviation
HV=SUMHL+DHL! Vapor enthalpy
RETURN
END

```

Section 5

```

SUBROUTINE NONIDL(X,TEMP,TOPS,HL,CP)
REAL CP(2),HL,SIG(2),PHISUM(2),LAMDA
INTEGER TOPS
COMMON /NAYA/ AC(2),AD(2),AE(2),AF(2),AG(2)
COMMON /WAAZ/W,Z
COMMON /TCT/TC(2),TBR(2),HOV(2)
COMMON GC,PRESS,FR,TO
COMMON /VIL/VIL(2)
FRAC=X
Y=X
CALL NONIDV(Y,TEMP,TOPS,HV,CP)! Vapor enthalpy
SUMLMD=0.0
SUMPFI=0.0
DO 1 I=1,2
    TR=TEMP/TC(I)
    PARMTR=(TBR(I)/TR)*(1.0-TR)/(1.0-TBR(I))
    LAMDA=((HOV(I)*TR)/TBR(I))*((PARMTR+(PARMTR**W))/(1.0+
1    (PARMTR**Z)))
    SIG(I)=(((LAMDA/4.187)-(GC*293.))/VIL(I))**0.5
    SUMLMD=SUMLMD+(X*LAMDA)! Latent heat of vaporization of mixture
    VIL(I)=(((LAMDA/4.187)-(GC*TEMP))/(SIG(I)**2.))
    PHISUM(I)=X*VIL(I)
    SUMPFI=SUMPFI+PHISUM(I)
    X=1.0-X
1    CONTINUE
    PHO=0.0
    DO 2 I=1,2
        PHEE=(PHISUM(I)/SUMPFI)*SIG(I)
        PHO=PHO+PHEE
2    CONTINUE
    X=FRAC
    HM=0.0
    DO 3 I=1,2
        HIE=X*(VIL(I)*((SIG(I)-PHO)**2.))*4.187
        HM=HM-HIE! Heat of mixing
        X=1.-X
3    CONTINUE
    HL=HV-SUMLMD+HM! Liquid enthalpy
    WRITE(20,*)HL,HM
    RETURN
END

```

Section 6

```

SUBROUTINE QDVNV(X,TEMP,TOPS,DHL)
REAL ENLIQ(4),A1(4),B1(4),C1(4),D1(4),RR1(4)
INTEGER TOPS
COMMON /TCT/ TC(2),TBR(2),HOV(2)
COMMON /PVC/ PC(2),ZC(2)
COMMON /ABC/A(2),B(2),C(2)
COMMON GC,PRESS,FR,TO
DATA A1/7.0,6.5,5.8,5.4/
DATA B1/0.65135,0.62252,0.63163,0.6747/
DATA C1/0.75727,0.76218,1.229,1.227/
DATA D1/0.46108,0.53042,0.55456,0.503/
DATA RR1/0.23,0.25,0.27,0.29/
TRM=0.0
PREST=0.0
SUMPRM=0.0
SUMTCM=0.0
SUMZCM=0.0
DO 1 I=1,2
  TRM=TRM+(X*(TEMP/TC(I)))! Reduced temperature of the mixture
  PREST=PREST+(X*(EXP(A(I)-(B(I)/(TEMP+C(I))))))! Vapor pressure
*   ! of the mixture
  SUMPRM=SUMPRM+(X*PC(I))! Critical pressure of the mixture
  SUMTCM=SUMTCM+(X*TC(I))! Critical temperature of the mixture
  SUMZCM=SUMZCM+(X*ZC(I))! Critical compressibility factor of
*   ! the mixture
  X=1.0-X
1  CONTINUE
  PRM=PREST/(SUMPRM*760.)! Reduced pressure of the mixture
  DO 4 J=1,4
    IF(TOPS.GT.0)GO TO 2
    ENLIQ(J)=- (A1(J)*(PRM**B1(J))*SUMTCM)/(1.+(C1(J)*((ALOG(1./
1    PRM))**D1(J))))! Saturated vapor enthalpy deviation
    GO TO 3
2    N=J
    CALL SUPVAP(N,TRM,PRM,CC1,CC4,CC5,CC6,XO,XM,BRKT)
    ENLIQ(J)=- ((XM*PRM*(1.-(PRM/XO)))/((EXP(-(CC1*(PRM**2.)))*
1    (BRKT))+CC4+CC5*PRM+(CC6*(PRM**2.)))*SUMTCM! Superheated
*    ! vapor enthalpy deviation
3    IF(SUMZCM.EQ.RR1(J)) GO TO 9
4  CONTINUE
  IF((0.23.LT.SUMZCM).AND.(SUMZCM.LT.0.25)) GO TO 5
  IF((0.25.LT.SUMZCM).AND.(SUMZCM.LT.0.27)) GO TO 7
  IF((0.27.LT.SUMZCM).AND.(SUMZCM.LT.0.29)) GO TO 8
  IF((SUMZCM.LT.0.23).OR.(SUMZCM.GT.0.29)) GO TO 10

```


Section 6 (continued)

```
5      K=1
      L=2
6      AA=RR1(L)-RR1(K)
      AB=ENLIQ(L)-ENLIQ(K)
      AC=AB/AA
      ZCMD=SUMZCM-RR1(K)
      AD=AC*ZCMD
      DHL=(AD+ENLIQ(K))*4.187! Interpolated enthalpy deviation
      GO TO 12
7      K=2
      L=3
      GO TO 6
8      K=3
      L=4
      GO TO 6
9      DHL=ENLIQ(J)*4.187
      GO TO 12
10     WRITE(5,11)
11     FORMAT(' YOUR SYSTEM CRITICAL COMPRESSIBILITY FACTOR IS OUT
1 OF RANGE IN SUBROUTINE QDVNV')
      STOP
12     RETURN
      END
```

Section 7

```

SUBROUTINE QDVNL(X, FLAGD, TEMP, DHL)
REAL ENLIQ(4), A1(4), B1(4), C1(4), D1(4), RR1(4), A2(4), B2(4), C2(4)
REAL D2(4), E2(4), F2(4), G2(4), H2(4), P2(4), Q2(4), R2(4), T2(4)
REAL U2(4)
INTEGER FLAGD
COMMON /ABC/A(2), B(2), C(2)
COMMON /TCT/TC(2), TBR(2), HOV(2)
COMMON /PVC/PC(2), ZC(2)
COMMON GC, PRESS, FR, TO
DATA A1/7.0, 6.5, 5.8, 5.4/
DATA B1/4.5688, 4.48, 5.19, 3.6485/
DATA C1/0.333, 0.3952, 0.4963, 0.33464/
DATA D1/0.004, -0.00185, -0.1, -0.0056942/
DATA RR1/0.23, 0.25, 0.27, 0.29/
DATA A2/0.08644293, 0.1074635, 0.1368774, 0.09572107/
DATA B2/4.2, 4.2, 4.664, 4.2/
DATA C2/12.93889, 15.80132, 14.56975, 9.501235/
DATA D2/0.77, 0.77, 0.79749, 0.77/
DATA E2/10.81311, 15.18611, 7.812724, 17.30389/
DATA F2/0.77, 0.77, 0.79749, 0.77/
DATA G2/0.1568094, 0.1476876, 0.1642482, 0.3195707/
DATA H2/4.2, 4.2, 4.664, 4.2/
DATA P2/0.77, 0.777, 0.79749, 0.77/
DATA Q2/0.7466842, 0.7800774, 1.036851, 1.368092/
DATA R2/3.17422, 3.154058, 4.463472, 4.227096/
DATA T2/2.930566, 2.988533, 4.525831, 3.181639/
DATA U2/12.72429, 12.28618, 10.86085, 9.707447/
TRM=0.0
PREST=0.0
SUMPRM=0.0
SUMTCM=0.0
SUMZCM=0.0
DO 1 I=1, 2
    TRM=TRM+(X*(TEMP/TC(I)))
    PREST=PREST+(X*(EXP(A(I))-(B(I)/(TEMP+C(I))))))
    SUMPRM=SUMPRM+(X*PC(I))
    SUMTCM=SUMTCM+(X*TC(I))
    SUMZCM=SUMZCM+(X*ZC(I))
    X=1.0-X
1 CONTINUE
IF(FLAGD.EQ.1)GO TO 2
PRM=PREST/(SUMPRM*760.)
GO TO 3
2 PRM=PRESS/SUMPRM
3 DO 6 J=1, 4
    IF(FLAGD.EQ.1)GO TO 4
    ENLIQ(J)=-((A1(J)+(B1(J)*((ALOG(1./PRM))**C1(J))))*SUMTCM)/
    (1.+D1(J)*ALOG(PRM))! Enthalpy deviation for saturated liquid
    GO TO 5
4 ENLIQ(J)=(A2(I)*(PRM-B2(I))+C2(I)*(TRM-D2(I))+E2(I)*((TRM-
1 F2(I))**2.))+G2(I)*(PRM-H2(I))*(TRM-P2(I))-Q2(I)*(ALOG(PRM))-
2 R2(I)*(ALOG(PRM))*(ALOG(TRM))-T2(I)*(ALOG(PRM))*((ALOG(TRM))
3 **2.))-U2(I))*SUMTCM! Enthalpy deviation for subcooled liquid
5 IF(SUMZCM.EQ.RR1(J))GO TO 11
6 CONTINUE
IF((0.23.LT.SUMZCM).AND.(SUMZCM.LT.0.25))GO TO 7
IF((0.25.LT.SUMZCM).AND.(SUMZCM.LT.0.27))GO TO 9
IF((0.27.LT.SUMZCM).AND.(SUMZCM.LT.0.29))GO TO 10
IF((SUMZCM.LT.0.23).OR.(SUMZCM.GT.0.29))GO TO 12

```

Section 7 (continued)

```
7      K=1
      L=2
8      AA=RR1(L)-RR1(K)
      AB=ENLIQ(L)-ENLIQ(K)
      AC=AB/AA
      ZCMD=SUMZCM-RR1(K)
      AD=AC*ZCMD
      DHL=(AD+ENLIQ(K))*4.187! Interpolated enthalpy deviation
      GO TO 14
9      K=2
      L=3
      GO TO 8
10     K=3
      L=4
      GO TO 8
11     DHL=ENLIQ(J)*4.187
      GO TO 14
12     WRITE(5,13)
13     FORMAT(' YOUR SYSTEM CRITICAL COMPRESSIBILITY FACTOR IS OUT
1      OF RANGE IN SUBROUTINE QDVNL')
      STOP
14     RETURN
      END
```

Section 8

```

SUBROUTINE SUPVAP(N,TRM,PRM,CC1,CC4,CC5,CC6,XO,XM,BRKT)
  IF(N.EQ.1)GO TO 5
  IF(N.EQ.2)GO TO 4
  IF(N.EQ.3)GO TO 1
  CC1=166.*EXP(-5.16*TRM)+0.017! For compressibility factor of 0.29
  CC2=0.62*EXP(-18.4*(TRM-1.0))+0.05
  CC3=EXP((38.8/TRM)-34.2)
  CC4=0.989*((TRM-0.75)**1.63)*EXP(-0.3175*(TRM-0.75))
  CC5=0.215*EXP(-0.1045*(TRM**4.935))
  CC6=0.0564*((TRM-0.5)**4.67)*EXP(-2.869*(TRM-0.5))
  XO=1.15-0.314*((TRM-8.0)**3.0)
  XM=(1.0-(0.0001499*(TRM**9.17)*EXP(-1.297*TRM)))/(0.1879+(
1  1.0826*((TRM-0.65)**1.1726)))
  GO TO 6
1  CC1=((40.*EXP(-5.7*TRM))/(TRM-0.81))+0.01! For compressibility
*  ! factor
*  ! of 0.27
  CC2=((0.35*EXP(-26.2*(TRM-1.0)))/TRM)+0.31
  CC3=(17.25*EXP(-16.7*(TRM-1.0)))+2.75
  CC4=0.444*(TRM-2.)-0.0215*((TRM-2.)**2.)+0.0610*((TRM-2.0)**3.)
1  -0.0404*((TRM-2.)**4.)+0.6564
  IF(TRM.LE.2.25)GO TO 2
  CC5=0.0
  GO TO 3
2  CC5=-0.0697*(TRM-2.)+0.0734*((TRM-2.)**2.)-0.0533*((TRM-2.)**5.)
1  +0.0125
3  CC6=0.00301*(TRM-0.8)*EXP(-0.87*((TRM-0.8)**2.0))
  XO=8.5+(10.5*((TRM-4.0)**2.0))
  SM=1./(0.1052+(1.2044*((TRM-0.4429)**2.135)))
  GO TO 6
4  CC1=0.89*EXP(9.845*(1.0-TRM))+0.023955*EXP(1.2405*TRM)! For
*  ! compressibility factor of 0.25
  CC2=0.47148*EXP(39.35*(1.0-TRM))+0.142
  CC3=3918.0*EXP(122*(1.0-TRM))+2.0
  CC4=1.1938*TRM-0.20726*(TRM**2.)-0.90649
  CC5=3.0*EXP(-2.52*TRM)
  CC6=0.004277*(TRM-0.895)*EXP(-0.946*((TRM-0.895)**2.0))
  XO=-60.0*TRM+(170.0)
  XM=1./(0.0853+(1.5078*((TRM-0.5952)**1.7336)))
  GO TO 6
5  CC1=TRM/(0.003147*EXP(6.0759*TRM)-61.12*(TRM-1.0)*EXP(-19.933*
1  (TRM-1.0))+1.9936*EXP(-0.911*(10.*((TRM-0.88)**10.))))! For
*  ! compressibility factor of 0.23
  CC2=EXP(17.671-(17.63*TRM))+0.17-1.1738*EXP(-17.193*(ABS(TRM-
1  1.05)))
  CC3=EXP(52.268-(49.188*TRM))+24.249*EXP(-920.5*((TRM-1.1)**2.))
  CC4=0.0032456*EXP(3.2917*TRM)-EXP((17.3*TRM)-30.6)
  CC5=1.9772*EXP(-2.1839*TRM)
  CC6=0.000336*EXP(1.61*TRM)-0.0000054*(TRM**11.5)
  XO=515.0-(250.0*TRM)
  XM=1./(-0.023+(1.0743*(TRM-0.4146)*1.8103))
6  BRKT=1.0-CC2-CC4-(CC5*PRM)+CC2*((1./3.1416)*(1./TAN(CC3-(
1  CC3*PRM)))+0.50)**2.0)
  RETURN
END

```

Section 9

```

SUBROUTINE SWITCH(SO,QBAR,QDBAR,XP)
REAL CP(2),LAMDA(2),HL
INTEGER TOPS,SO
COMMON/MOLFRN/XT(3)
X=0.005
DO 3 I=1,1000
  CALL UNIQAC(X,TEMP,Y)
  IF(SO.EQ.1)GO TO 1
  CALL LIQEPY(X,TEMP,HL,CP)! Enthalpy of ideal saturated
  ! liquid at given mole fraction
  GO TO 2
1  TOPS=0
  CALL NONIDL(X,TEMP,TOPS,HL,CP)! Enthalpy of non-ideal
  ! saturated liquid at given mole fraction
2  H1=(QBAR*(X-XT(3))+QDBAR*(XT(1)-X))/(XT(1)-XT(3))! Enthalpy by
  ! overall enthalpy line eq 2.2.7, at the same mole fraction
  IF(ABS(H1-HL).LE.200.)GO TO 4! Check for intersection of both
  ! the curves
  X=X+0.001
3  CONTINUE
  WRITE(5,*)' CONVERGENCE CRITERIA IS NOT MET IN SUBROUTINE
1 SWITCH'
  STOP
4  XP=X
  RETURN
END

```

Section 10

```

SUBROUTINE YNRECT(SO,X,TEMP,QBAR,YT)
REAL ARK(200),LAMDA(2),CP(2)
INTEGER H,TOPS,SO
COMMON /MOLFRN/XT(3)
H=1
L=1
M=2
T1=X
T2=XT(L)
IF(SO.EQ.1)GO TO 1
CALL LIQEPY(X,TEMP,HL,CP)
GO TO 2
1 TOPS=0
CALL NONIDL(X,TEMP,TOPS,HL,CP)
2 XK=X
HLP=HL! Saturated liquid enthalpy
YY=X! Assumption of vapor mole fraction equal to liquid
* ! mole fraction
K=1
3 HVV=QBAR-(((XT(L)-YY)/(XT(L)-XK))*(QBAR-HLP))! Eq 2.2.4
X=0.005
DO 4 J=1,1000
CALL UNIQAC(X,TEMP,Y)
IF(ABS(Y-YY).LE.0.005)GO TO 5
X=X+0.005
4 CONTINUE
WRITE(5,*)' CONVERGENCE CRITERIA FOR VAPOR MOLE FRACTION
1 IN SUBROUTINE YNRECT IS NOT MET'
GO TO 10
5 X=YY
IF(SO.EQ.1)GO TO 6
CALL IENTPY(Y,TEMP,HV,LAMDA,CP)
YI=(HVV-CP(2)-LAMDA(2))/(CP(1)-CP(2)+LAMDA(1)-LAMDA(2))! Eq
* ! 1.4.2
GO TO 7
6 CALL NONIDL(X,TEMP,TOPS,HL,CP)
CALL QDVNV(X,TEMP,TOPS,DHL)

```

Section 10 (continued)

```

      YI=(HVV-CP(2)-DHL)/(CP(1)-CP(2))! Eq 1.4.3
7     ARK(H)=YI-YY! Difference of assumed and calculated mole fractions
      IF(H.GT.2)GO TO 12
      YY=XT(L)
      H=H+1
      IF(K.EQ.2)GO TO 8
      K=K+1
      GO TO 3
8     H=2
      IF((ARK(L)*ARK(M)).LT.0.0)GO TO 11
      WRITE(5,9) XK
9     FORMAT(' NO SIGN CHANGE IN SUBROUTINE YNRECT AT LIQUID MOLE
1     FRACTION',F20.5)
10    STOP
11    ERROR=0.0095
      YY=(T1+T2)/2.
      H=H+1
      GO TO 3
12    IF(ABS(T1-T2).LE.ERROR)GO TO 14
      IF((ARK(L)*ARK(H)).LE.0.0)GO TO 13
      ARK(L)=ARK(H)
      T1=YY
      GO TO 11
13    T2=YY
      GO TO 11
14    YT=(T1+T2)/2.0! Vapor mole fraction at which operating line and
*    ! vapor enthalpy curve intersects
      RETURN
      END

```

Section 11

```

SUBROUTINE IDLSTP(SO,X,TEMP,QDBAR,YT)
REAL RAK(200),CP(2),LAMDA(2)
INTEGER H,SO,TOPS
COMMON /TCT/TC(2),TBR(2),HOV(2)
COMMON /WAAZ/W,Z
COMMON GC,PRESS,FR,TO
COMMON /VIL/VIL(2)
COMMON/MOLFRN/ XT(3)
H=1
N=1
M=2
L=3
T1=X
T2=XT(N)
IF(SO.EQ.1)GO TO 1
CALL LIQEPY(X,TEMP,HL,CP)
GO TO 2
1 TOPS=0
CALL NONIDL(X,TEMP,TOPS,HL,CP)
2 XK=X
HLP=HL! Saturated liquid enthalpy
YY=X! Assumption of vapor mole fraction equal to liquid
* ! mole fraction
K=1
3 HVV=((YY-XT(L))/(XK-XT(L))*(HLP-QDBAR))+QDBAR! Eq 2.2.5
X=0.005
DO 4 J=1,1000
CALL UNIQAC(X,TEMP,Y)
IF(ABS(YY-Y).LE.0.009)GO TO 5
X=X+0.001
4 CONTINUE
WRITE(5,*)' CONVERGENCE CRITERIA FOR VAPOR MOLE FRACTION IS NOT
1 MET IN SUBROUTINE IDLSTP'
GO TO 10
5 X=(YY+Y)/2.
IF(SO.EQ.1)GO TO 6
CALL IENTPY(Y,TEMP,HV,LAMDA,CP)
YI=(HVV-CP(2)-LAMDA(2))/(CP(1)-CP(2)+LAMDA(1)-LAMDA(2))! Eq
* ! 1.4.2
GO TO 7
6 CALL NONIDL(X,TEMP,TOPS,HL,CP)
CALL QDVNV(X,TEMP,TOPS,DHL)
YI=(HVV-CP(2)-DHL)/(CP(1)-CP(2))! Eq 1.4.3
7 RAK(H)=YI-YY! Difference of assumed vapor mole fraction
* ! and calculated
* !mole fraction

```


Section 11 (continued)

```

      IF(H.GT.2)GO TO 12
      YY=XT(N)
      H=H+1
      IF(K.EQ.2)GO TO 8
      K=K+1
      GO TO 3
8     H=2
      IF((RAK(N)*RAK(M)).LT.0.0)GO TO 11
      WRITE(5,9) XK
9     FORMAT(' NO SIGN CHANGE IN SUBROUTINE IDLSTP AT LIQUID MOLE
1    FRACTION',F20.5)
10    STOP
11    ERROR=0.0095
      YY=(T1+T2)/2.0
      H=H+1
      GO TO 3
12    IF(ABS(T1-T2).LE.ERROR)GO TO 14
      IF((RAK(N)*RAK(H)).LE.0.0)GO TO 13
      RAK(N)=RAK(H)
      T1=YY
      GO TO 11
13    T2=YY
      GO TO 11
14    YT=(T1+T2)/2.0! Vapor mole fraction at the intersection of
*    ! operating line and saturated vapor curve
      RETURN
      END

```

Section 12

```

SUBROUTINE FEED(SO,HF,QM)
REAL LAMDA(2),CP(2)
INTEGER SO,S2,FLAGD,TOPS
COMMON /MOLFRN/XT(3)
COMMON /PUT/ PUT
X=XT(2)
XF=X
XD=XT(1)
WRITE(5,1)
1  FORMAT(' PLEASE TYPE APPROPRIATE NUMBER AS MENTIONED BELOW'/
1  ' 0 = SUBCOOLED FEED'/' 1 = SATURATED LIQUID FEED'/
2  ' 2 = SATURATED VAPOR FEED'/' 3 = PARTIALLY VAPORIZED FEED'/
3  ' 4 = SUPERHEATED FEED')
READ(5,*)S2
IF(S2.EQ.1)GO TO 14
IF(S2.EQ.2)GO TO 19
IF(S2.EQ.3)GO TO 24
WRITE(5,2)
2  FORMAT(' TYPE TEMPERATURE OF THE FEED IN DEGREES KELVIN')
READ(5,*)TEMP
IF(S2.EQ.4)GO TO 29
IF(SO.EQ.1)GO TO 3
* Subcooled feed calculation
CALL LIQEPY(X,TEMP,HL,CP)
HF=HL! Subcooled feed enthalpy of ideal system
GO TO 4
3  TOPS=0
CALL NONIDL(X,TEMP,TOPS,HL,CP)
FLAGD=0
CALL QDVNL(X,FLAGD,TEMP,DHL)
HL=HL+DHL
FLAGD=1
CALL QDVNL(X,FLAGD,TEMP,DHL)
HF=HL-DHL! Subcooled feed enthalpy of non-ideal system
4  X=XF+0.001! Search for tie line passing through feed starts
*  ! from here
5  CALL UNIQAC(X,TEMP,Y)
IF(SO.EQ.1)GO TO 6
CALL LIQEPY(X,TEMP,HL,CP)
CALL IENTPY(Y,TEMP,HV,LAMDA,CP)
GO TO 7
6  TOPS=0
CALL NONIDL(X,TEMP,TOPS,HL,CP)
CALL NONIDV(Y,TEMP,TOPS,HV,CP)
7  USLOPE=(HV-HL)/(Y-X)
FSLOPE=(HV-HF)/(Y-XF)
IF(ABS(USLOPE-FSLOPE).LT.500.0)GO TO 8
IF(X.GT.XD)GO TO 37
X=X+0.001
GO TO 5
8  XFF=X! Tie line found
P=(USLOPE+FSLOPE)/2.0! Slope of the tie line
CINTCP=HV-(Y*P)! Intercept of the tie line
QM=(P*XD)+CINTCP! Heat removed at minimum reflux i.e., intersection
* !of the tie line with the line through distillate mole fraction
IF(SO.EQ.1)GO TO 9
GO TO 39! For ideal system

```

```

9      X=XFF+0.001! Search for any other tie line expected to give highest
*      ! intersection with the line through distillate
10     TOPS=0
      FLAG=QM
      DO 11 I=1,1000
          CALL UNIQAC(X,TEMP,Y)
          CALL NONIDL(X,TEMP,TOPS,HL,CP)
          CALL NONIDV(Y,TEMP,TOPS,HV,CP)
          P=(HV-HL)/(Y-X)
          CINTCP=HV-(Y*P)
          QM=(P*XD)+CINTCP
          IF(QM.GT.FLAG)GO TO 12
          IF(ABS(Y-XD).LT.0.001)GO TO 13
          X=X+0.001
11     CONTINUE
      GO TO 13
12     FLAG=QM! Such tie line found
      X=X+0.005
      GO TO 11
13     QM=FLAG! Such tie line not found
      GO TO 39
* Saturated liquid feed calculation
14     CALL UNIQAC(X,TEMP,Y)
      IF(SO.EQ.1)GO TO 15
      CALL LIQEPY(X,TEMP,HL,CP)
      CALL IENTPY(Y,TEMP,HV,LAMDA,CP)
      GO TO 16
15     TOPS=0
      CALL NONIDL(X,TEMP,TOPS,HL,CP)
      CALL NONIDV(Y,TEMP,TOPS,HV,CP)
16     HF=HL! Saturated liquid feed enthalpy
17     P=(HV-HL)/(Y-X)! Slope of the tie line through feed
      CINTCP=HV-(Y*P)! Intercept of the tie line through feed
      QM=(P*XD)+CINTCP! Intersection of the tie line with the line
*      ! through distillate
      IF(SO.EQ.1)GO TO 18
      GO TO 39! For ideal system
18     X=XF+0.001! For non-ideal system
      GO TO 10
* Saturated vapor feed calculation
19     X=0.005! Tie line search passing through feed
      DO 20 I=1,1000
          CALL UNIQAC(X,TEMP,Y)
          IF(ABS(Y-XF).LT.0.001)GO TO 21
          X=X+0.001
20     CONTINUE
      WRITE(5,*)' IN SUBROUTINE FEED, CONVERGENCE CRITERIA FOR
1 VAPOR MOLE FRACTION IS NOT MET AT STMT:19'
      GO TO 38
21     IF(SO.EQ.1)GO TO 22
      CALL LIQEPY(X,TEMP,Y,HL,CP)
      CALL IENTPY(Y,TEMP,HV,LAMDA,CP)
      GO TO 23
22     TOPS=0
      CALL NONIDL(X,TEMP,TOPS,HL,CP)
      CALL NONIDV(Y,TEMP,TOPS,HV,CP)
23     HF=HV! Saturated vapor feed enthalpy
      XF=X
      GO TO 17
* Partially vaporized feed calculation
24     X=0.005! Tie line search passing through feed

```

Section 12 (continued)

```

DO 27 I=1,10000
  CALL UNIQAC(X,TEMP,Y)
  IF(SO.EQ.1)GO TO 25
  CALL LIQEPY(X,TEMP,HL,CP)
  CALL IENTPY(Y,TEMP,HV,LAMDA,CP)
  GO TO 26
25  TOPS=0
  CALL NONIDL(X,TEMP,TOPS,HL,CP)
  CALL NONIDV(Y,TEMP,TOPS,HV,CP)
26  USLOPE=(HV-HL)/(Y-X) ! Slope of tie line
  HYPTNS=SQRT(((HV-HL)**2.)+(Y-X)**2.))! Magnitude of the
  *   ! tie line
  HF=HL+(((100.-PUT)/100.)*HYPTNS)! Feed enthalpy
  FSLOPE=(HV-HF)/(Y-XF)! Slope of line through feed and saturated
  *   ! vapor
  IF(ABS(USLOPE-FSLOPE).LE.50.0)GO TO 28! Check to see if both
  *   ! the lines are same or very near
  X=X+0.0001
27  CONTINUE
  GO TO 37
28  X=XF
  GO TO 8
* Superheated vapor feed calculation
29  Y=XF
  IF(SO.EQ.1)GO TO 30
  CALL IENTPY(Y,TEMP,HV,LAMDA,CP)
  HF=HV! Enthalpy of superheated ideal feed
  GO TO 32
30  TOPS=0
  CALL NONIDV(Y,TEMP,TOPS,HV,CP)
  X=Y
  HV=0.0
  DO 31 I=1,2
    HV=HV+(X*CP(I))
    X=1.0-X
31  CONTINUE
  X=Y
  TOPS=1
  CALL QDVNV(X,TEMP,TOPS,DHL)
  HF=HV-DHL! Enthalpy of superheated non-ideal feed
32  X=0.005! Search for tie line through feed starts
33  CALL UNIQAC(X,TEMP,Y)
  IF(SO.EQ.1)GO TO 34
  CALL LIQEPY(X,TEMP,HL,CP)
  CALL IENTPY(Y,TEMP,HV,LAMDA,CP)
  GO TO 35
34  TOPS=0
  CALL NONIDL(X,TEMP,TOPS,HL,CP)
  CALL NONIDV(Y,TEMP,TOPS,HV,CP)
35  USLOPE=(HV-HL)/(Y-X)! Tie line slope
  FSLOPE=(HF-HL)/(XF-X)! Slope of the line through feed and saturated
  *   ! liquid
  IF(ABS(USLOPE-FSLOPE).LE.400.)GO TO 36
  IF(X.GT.XD)GO TO 37
  X=X+0.001
  GO TO 33
36  GO TO 8! Tie line found
37  WRITE(5,*)' CONVERGENCE CRITERIA FOR DIFFERENCE OF USLOPE
1 AND FSLOPE IS TOO SMALL TO BE MET'
38  STOP
39  RETURN
  END

```

Section 13

```

* Tower diameter calculation starts
MD=(FR*(XT(2)-XT(3)))/(XT(1)-XT(3))
MB=FR-MD
VD=MD*(RRO+1.0)
QT=(VD*22.41*(TEMPT))/(273.0*3600.0)
TD=((4.0*QT)/(VMAX*3.1416))**0.5
DO 42 I=1,1000
    IF(TD.LE.1.0)GO TO 33
    IF(TD.LE.3.0)GO TO 34
    IF(TD.LE.4.0)GO TO 35
    IF(TD.LE.8.0)GO TO 36
    GO TO 54
33    SMT=0.5
    GO TO 37
34    SMT=0.6
    GO TO 37
35    SMT=0.75
    GO TO 37
36    SMT=0.9
37    IF(RA.GE.0.1)GO TO 38
    ALFA=(0.0744*SMT+0.01173)*((5.*RA)+0.5)
    BETA=(0.0304*SMT+0.015)*((5.*RA)+0.5)
    GO TO 39
38    ALFA=0.0744*SMT+0.01173
    BETA=0.0304*SMT+0.015
39    AMWG=(XD*MG)+((1.0-XD)*ML)
    AMWL=(XB*MG)+((1.-XB)*ML)
    DG=(AMWG*273.)/(22.41*(TEMPT))
    VR=(MD*22.41*(TEMPT))/(273.*3600.0)
    LR=(MB*AMWL)/(DL*3600.0)
    DEN=((LR*DL)/(VR*DG))*((DG/DL)**0.5)
    IF(DEN.GT.0.1)GO TO 40
    DEN=0.1
40    CF=(ALFA*(ALOG10(1./DEN))+BETA)*((SIGMA/0.02)**0.2)
    VF=CF*((DL-DG)/DG)**0.5
    V=VF*(VFL/100.)
    AREA=QT/V
    DIA=((4.*AREA)/3.1416)**0.5
    ERR=0.05
    WRITE(5,41)TD,DIA
    WRITE(23,41)TD,DIA
41    FORMAT(' TD AND DIA ARE',2F10.2)
    IF(ABS(TD-DIA).LE.ERR)GO TO 43
    DELTD=0.01
    TD=TD+DELTD
42    CONTINUE
43    IF(I.EQ.1000)GO TO 45
    WRITE(5,44)DIA
    WRITE(23,44)DIA
44    FORMAT(' THE DIAMETER OF TOWER IS',F10.2)
    GO TO 47
45    WRITE(5,46)
    WRITE(23,46)
46    FORMAT(' THE VALUES OF ASSUMED AND CALCULATED DIAMETER DO NOT
1    CONVERGE')
    GO TO 56

```

Section 13 (continued)

```

* Cost estimation starts
47  DIAIN=DIA*39.36
    COST=EXP(5.16474-0.06366*(ALOG(DIAIN))+0.1755*((ALOG(DIAIN))
      1  **2.)-0.004*((ALOG(DIAIN))**3.))
    SLOPE=RRO/(RRO+1.)
    TL=(JFLAG-1.)/(PE/100.)
    ACOST=COST*TL*(1.+SLOPE)*(PFC/100.)
    WRITE(5,48)ACOST
    WRITE(23,48)ACOST
48  FORMAT(' ANNUAL COST FOR DISTILLATION COLUMN IS',F10.2)
    HAC=QC/(UC*(TEMPT-TEMPCW))
    CC=4741.43+(59.94*HAC)+(0.1873*(HAC**2.))-(0.0008824*(HAC**3.))
    ACC=(CC/HAC)*HAC*(1.+SLOPE)*(PFC/100.)
    WRITE(5,49)ACC
    WRITE(23,49)ACC
49  FORMAT(' ANNUAL COST OF CONDENSER IS',F10.2)
    HAR=QB/(UR*(TEMPS-TEMPB))
    CR=9712.681+(79.99*HAR)+(0.118*(HAR**2.))-(0.0003663*(HAR**3.))
    AR=(CR/HAR)*HAR*(1.+SLOPE)*(PFC/100.)
    WRITE(5,50)AR
    WRITE(23,50)AR
50  FORMAT(' ANNUAL COST OF REBOILER IS',F10.2)
    AW=(QC*CW*OPT)/(LAMW*DELTW)
    WRITE(5,51)AW
    WRITE(23,51)AW
51  FORMAT(' ANNUAL COST OF COOLING WATER IS',F15.2)
    AS=(QB*CS*OPT)/HC
    WRITE(5,52)AS
    WRITE(23,52)AS
52  FORMAT(' ANNUAL COST OF STEAM IS',F10.2)
    TAC=ACOST+ACC+AR+AW+AS
    WRITE(5,53)TAC
    WRITE(23,53)TAC
53  FORMAT(' TOTAL ANNUAL COST IS',F15.2)
    GO TO 56
54  WRITE(5,55)
55  FORMAT(' ESTIMATED TOWER DIAMETER IS GREATER THAN 8 METERS
      1 THEREFORE TRAY SPACING ESTIMATION FOR CONSTANTS ALPHA AND BETA
      2 CANNOT BE MADE')
56  STOP
    END

```

APPENDIX B

```

* Program      : Design & Optimization of Binary distillation system
*
* Programmer: Shabbir K. Hussain
*
* For the separation of ideal or non-ideal binary mixture, this
* program designs tray type distillation column. For a specified
* separation, it calculates minimum reflux ratio, number of theoretical
* plates required for the separation, feed plate position from the top of
* the column, heat added and removed from the system, diameter of the
* tower based on superficial velocity and total annual cost of operating
* the tower.
*
* This program uses the plate-to-plate regression technique of Ponchon-
* Savarit. Vapor-liquid equilibria is calculated by the UNIQUAC
* correlations.
*
* The main program does the designing part with the help of subroutines
* which provides it physical properties at specified mole fraction.
* Followed by designing is tower diameter and cost estimation which is
* done by the main program itself. For physical properties of ideal
* system, the main program calls different set of subroutines than the
* the one which it calls for non-ideal case. Subroutines and their
* purpose are briefly discussed below:
*
* UNIQAC: Calculates vapor-liquid equilibria
* LIQEPY: Calculates liquid enthalpy of ideal system
* IENTPY: Calculates vapor enthalpy of ideal system
* SWITCH: Calculates intersection of overall enthalpy and liquid
*          enthalpy curve
* NONIDL: Calculates liquid enthalpy of non-ideal system
* QDVNV : Calculates enthalpy departure of non-ideal vapors
* NONIDV: Calculates vapor enthalpy of non-ideal system
* YNRECT: Calculates operating line in rectification section
* IDLSTP: Calculates operating line in stripping section
* QDVNL : Calculates enthalpy departure of non-ideal liquid
* FEED  : Calculates feed enthalpy and heat removed in the condenser at
*          minimum reflux
* SUPVAP: Calculates variables for superheated vapor enthalpy
*          deviation
*
* The data to be read are contained by free format in the file
* "HUSS.DAT". The input data for an ideal system are less than
* a non-ideal system.
*
*          *****
*          Input Variables
*          *****
*
* GC          = Gas Constant, Cal/g-mole-°K
* PRESS       = Pressure, atm
* FR          = Feed rate, Kmole/Hr
* TO          = Reference temperature in equation 2.4.1, °K
* T           = Boiling points, °K
* XT          = Mole fractions of high volatile component in
*              distillate feed and bottom streams
*
* A,B,C       = Antoine vapor pressure constants (In mmHg units)
* D,E,F,G     = Constants in equation 2.4.1, for ideal system
*              (In KJ/Kmole-°K units)
* AC,AD,AE,AF,AG = Heat capacity constants for non-ideal system
*              (In KJ/Kmole-°K units)
* R,Q,U       = UNIQUAC volume, surface and energy interaction

```



```

*           parameters respectively
*   W,Z      = Constants in equation 2.4.2
*   HOV      = Latent heat of vaporization at normal boiling point,
*             KJ/Kmole
*   TC       = Critical temperature, °K
*   TBR      = Reduced temperature at normal boiling point
*   VIL      = Liquid molal volume, cm**3/g-mole
*   PC       = Critical pressure, atm
*   CS       = Cost of steam, $/kg
*   CW       = Cost of cooling water, $/kg
*   OPT      = Operating time, Hr/year
*   PFC      = Percentage of fixed charges
*   RA       = Ratio of hole area to active area
*   SIGMA    = Surface tension, N/m
*   TEMPB    = Temperature at the bottom of the tower, °K
*   TEMPS    = Temperature of steam, °K
*   TEMPT    = Temperature at the top of the tower, °K
*   DELTW    = Change in cooling water temperature, °K
*   TEMPCW   = Cooling water temperature, °K
*   UC       = Condenser heat transfer coefficient, KJ/hr-°K-m**2
*   UR       = Reboiler heat transfer coefficient, KJ/hr-°K-m**2
*   VMAX     = Maximum allowable vapor velocity, m/sec
*   PE       = Plate efficiency
*   HC       = Heat of condensation of steam, KJ/kg
*   VFL      = Percentage of superficial velocity
*   DL       = Density of liquid, Kg/m**3
*   LAMW     = Molal heat capacity of water, KJ/kmole-°C
*   MG       = Molecular weight of gas, component 1
*   ML       = Molecular weight of liquid, component 2
*   PUT      = Percentage of vapors in feed
*   ZC       = Critical compressibility factor
*   RR       = Ratio of operating to minimum reflux
*
*           *****
*           MAJOR VARIABLES
*           *****
*
*   HLO      = Enthalpy of liquid distillate
*   HV1      = Enthalpy of vapors from the top of the column
*   HF       = Enthalpy of feed
*   QM       = Heat removed in condenser at minimum reflux
*   HLB      = Enthalpy of saturated liquid bottoms
*   RM       = Minimum reflux
*   RRO      = Operating reflux
*   QC       = Heat removed in condenser
*   QB       = Heat added at reboiler
*   XP       = Intersection point of overall enthalpy and saturated
*             liquid enthalpy curve
*   KFLAG    = Number of plates in rectification section of
*             the tower
*   IFLAG    = Number of plates in stripping section including
*             reboiler
*   JFLAG    = Total number of plates in the column
*   TD       = Tower diameter based on maximum allowable vapor
*             velocity
*   SMT      = Tray spacing
*   ALFA, BETA = Constants in equation 2.3.4
*   DG       = Density of gas
*   VR       = Vapor rate
*   LR       = Liquid rate
*   CF       = Flooding constant

```

```

*      VF                      = Superficial velocity
*      QT                      = Volumetric flow rate of gas
*      DIA                    = Tower diameter based on superficial velocity
*      ACOST                  = Annual cost of distillation column
*      ACC                    = Annual cost of condenser
*      AR                     = Annual cost of reboiler
*      AW                     = Annual cost of cooling water
*      AS                     = Annual cost of steam
*      TAC                    = Total annual operating cost of operating the tower
*
*      Component 1 = High volatile component
*      Component 2 = Low volatile component
*
      REAL LAMDA(2),CP(2),MD,MB,LAMW,ML,MG,OPT,LR,HL
      INTEGER SO,S1,TOPS,FLAGD
      COMMON /WAAZ/W,Z
      COMMON /NAYA/AC(2),AD(2),AE(2),AF(2),AG(2)
      COMMON /ABC/A(2),B(2),C(2)
      COMMON /VIL/VIL(2)
      COMMON /PVC/PC(2),ZC(2)
      COMMON /TLMT/ T(2)
      COMMON /MOLFRN/ XT(3)
      COMMON GC,PRESS,FR,TO
      COMMON /RQU/R(2),Q(2),U(2,2)
      COMMON /DEFG/D(2),E(2),F(2),G(2)
      COMMON /TCT/TC(2),TBR(2),HOV(2)
      COMMON /PUT/ PUT
      DATA RR/1.5/
      OPEN(UNIT=24,NAME='HUSS.DAT')
      READ (24,*)GC,PRESS,FR,TO,T,A,B,C,R,Q,U
      X=0.005
      DO 1 I=1,990
          CALL UNIQAC(X,TEMP,Y)
          IF (ABS(X-Y).LE.0.0009)GO TO 2
          X=X+0.001
1      CONTINUE
      SO=0
      WRITE(5,*)' YOUR SYSTEM IS IDEAL'
      GO TO 3
2      SO=1
      WRITE(5,*)' YOUR SYSTEM IS AZEOTROPIC NON-IDEAL'
      GO TO 4
* Data reading
3      READ(24,*)XT,D,E,F,G,W,Z,HOV,TC,TBR,CS,CW,OPT,PFC,RA,SIGMA,
1      TEMPB,TEMPS,TEMPT,DELTW,TEMPCW,UC,UR,VMAX,PE,HC,VFL,DL,LAMW,MG,
2      ML,PUT,ZC
      GO TO 5
4      READ(24,*)XT,AC,AD,AE,AF,AG,W,Z,HOV,TC,TBR,VIL,PC,CS,CW,OPT,PFC,
1      RA,SIGMA,TEMPB,TEMPS,TEMPT,DELTW,TEMPCW,UC,UR,VMAX,PE,HC,VFL,DL,
2      LAMW,MG,ML,PUT,ZC
* Calculation starts with distillate
5      X=XT(1)
      XD=X
      YT=XD
      WRITE(5,6)
6      FORMAT(' TYPE 0 IF YOUR DISTILLATE IS SUBCOOLED LIQUID OR 1 IF
1      IT IS SATURATED LIQUID')
      READ(5,*)S1
      IF(S1.EQ.1)GO TO 9
      WRITE(5,7)
7      FORMAT(' TYPE TEMPERATURE OF DISTILLATE IN DEGREES KELVIN')

```

```

      READ(5,*)TEMP
      IF(SO.EQ.1)GO TO 8
* Enthalpy calculation of subcooled distillate of ideal system
      CALL LIQEPY(X,TEMP,HL,CP)
      HLO=HL
      GO TO 14
* Enthalpy calculation of subcooled distillate of non-ideal system
8     TOPS=0
      CALL NONIDL (X,TEMP,TOPS,HL,CP)
      FLAGD=0
      CALL QDVNL(X,TEMP,FLAGD,DHL)
      HL=HL+DHL
      FLAGD=1
      CALL QDVNL (X,TEMP,FLAGD,DHL)
      HLO=HL-DHL
      GO TO 11
* Enthalpy calculation of saturated liquid distillate of ideal system
9     CALL UNIQAC (X,TEMP,Y)
      IF(SO.EQ.1)GO TO 10
      CALL LIQEPY(X,TEMP,HL,CP)
      HLO=HL
      GO TO 14
* Enthalpy calculation of saturated liquid distillate of non-ideal system
10    TOPS=0
      CALL NONIDL(X,TEMP,TOPS,HL,CP)
      HLO=HL
* Enthalpy calculation of ideal vapors from top of the column
11    X=0.005
      DO 12 I=1,1000
          CALL UNIQAC (X,TEMP,Y)
          IF(ABS(Y-XD).LE.0.001)GO TO 13
          X=X+0.001
12    CONTINUE
      WRITE(5,*)' CONVERGENCE CRITERIA IS NOT MET AT STMT:11'
      GO TO 56
13    Y=XD
      CALL NONIDV(Y,TEMP,TOPS,HV,CP)
      HV1=HV
      GO TO 17
* Enthalpy calculation of non-ideal vapors from top of the column
14    X=0.005
      DO 15 I=1,1000
          CALL UNIQAC(X,TEMP,Y)
          IF(ABS(Y-XD).LE.0.001)GO TO 16
          X=X+0.001
15    CONTINUE
      WRITE(5,*)' CONVERGENCE CRITERIA IS NOT MET AT STMT:14'
      GO TO 56
16    Y=XD
      CALL IENTPY(Y,TEMP,HV,LAMDA,CP)
      HV1=HV
* Feed enthalpy calculation starts
17    XF=XT(2)
      CALL FEED(SO,HF,QM)
* Enthalpy calculation of bottom stream starts
      X=XT(3)
      XB=X
      CALL UNIQAC(X,TEMP,Y)
      IF(SO.EQ.1)GO TO 18
      CALL LIQEPY(X,TEMP,HL,CP)
      CALL IENTPY(Y,TEMP,HV,LAMDA,CP)

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      HLB=HL
      GO TO 19
18     TOPS=0
      CALL NONIDL(X,TEMP,TOPS,HL,CP)
      HLB=HL
* Material & Energy balance starts
19     DD=FR*(XT(2)-XT(3))/(XT(1)-XT(3))
      BB=FR-DD
      RM=(QM-HV1)/(HV1-HLO)
      RRO=RM*RR
      QBAR=(RRO*(HV1-HLO))+HV1
      QDBAR=(HF-(((XT(2)-XT(3))/(XT(1)-XT(2)))*(QBAR-HF)))
      QC=(QBAR-HLO)*DD
      QB=(HLB-QDBAR)*BB
      CALL SWITCH(SO,QBAR,QDBAR,XP)
* The program now starts stepping down in the rectification section from
* the top of the column
      KFLAG=1
20     X=0.005
      DO 21 I=1,1000
          CALL UNIQAC(X,TEMP,Y)
          IF(ABS(Y-YT).LE.0.001)GO TO 22
          X=X+0.001
21     CONTINUE
      WRITE(5,*)' CONVERGENCE CRITERIA FOR VAPOR MOLE FRACTION IN
1 RECTIFICATION SECTION IS NOT MET'
      GO TO 56
22     IF(X.LT.XP)GO TO 23
      CALL YNRECT(SO,X,TEMP,QBAR,YT)
      KFLAG=KFLAG+1
      GO TO 20
23     WRITE(5,24)KFLAG,KFLAG
      WRITE(23,24)KFLAG,KFLAG
24     FORMAT(' NUMBER OF PLATES IN RECTIFICATION SECTION IS',I5,' AND
1 FEED PLATE IS',I5)
* Stepping down in the stripping section starts
      IFLAG=1
      CALL IDLSTP(SO,X,TEMP,QDBAR,YT)
25     X=0.005
      DO 26 I=1,1000
          CALL UNIQAC(X,TEMP,Y)
          IF(ABS(Y-YT).LE.0.005)GO TO 27
          X=X+0.001
26     CONTINUE
      WRITE(5,*)' CONVERGENCE CRITERIA FOR VAPOR MOLE FRACTION IN
1 STRIPPING SECTION IS NOT MET'
      GO TO 56
27     IF(X.LT.XB)GO TO 29
      IF(X.EQ.XB)GO TO 28
      CALL IDLSTP(SO,X,TEMP,QDBAR,YT)
      IFLAG=IFLAG+1
      GO TO 25
28     JFLAG=KFLAG+IFLAG
      GO TO 30
29     JFLAG=KFLAG+IFLAG+1
30     WRITE(5,31)IFLAG,JFLAG
      WRITE(23,31)IFLAG,JFLAG
31     FORMAT(' NUMBER OF PLATES IN THE STRIPPING SECTION IS',I5,
1 ' AND TOTAL NUMBER OF PLATES IS',I5)
      WRITE(23,32)QC,QB,RM
      WRITE(5,32)QC,QB,RM

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32   FORMAT(' HEAT TAKEN OUT AT THE CONDENSER IS',F20.5/ ' HEAT
    1   ADDED AT THEREBOILER IS',F20.5/ ' MINIMUM REFLUX RATIO IS'
    2   ,F20.5)
* Tower diameter calculation starts
    MD=(FR*(XT(2)-XT(3)))/(XT(1)-XT(3))
    MB=FR-MD
    VD=MD*(RRO+1.0)
    QT=(VD*22.41*(TEMPT))/(273.0*3600.0)
    TD=((4.0*QT)/(VMAX*3.1416))**0.5
    DO 42 I=1,1000
        IF(TD.LE.1.0)GO TO 33
        IF(TD.LE.3.0)GO TO 34
        IF(TD.LE.4.0)GO TO 35
        IF(TD.LE.8.0)GO TO 36
        GO TO 54
33     SMT=0.5
        GO TO 37
34     SMT=0.6
        GO TO 37
35     SMT=0.75
        GO TO 37
36     SMT=0.9
37     IF(RA.GE.0.1)GO TO 38
        ALFA=(0.0744*SMT+0.01173)*((5.*RA)+0.5)
        BETA=(0.0304*SMT+0.015)*((5.*RA)+0.5)
        GO TO 39
38     ALFA=0.0744*SMT+0.01173
        BETA=0.0304*SMT+0.015
39     AMWG=(XD*MG)+((1.0-XD)*ML)
        AMWL=(XB*MG)+((1.-XB)*ML)
        DG=(AMWG*273.)/(22.41*(TEMPT))
        VR=(MD*22.41*(TEMPT))/(273.*3600.0)
        LR=(MB*AMWL)/(DL*3600.0)
        DEN=((LR*DL)/(VR*DG))*((DG/DL)**0.5)
        IF(DEN.GT.0.1)GO TO 40
        DEN=0.1
40     CF=(ALFA*(ALOG10(1./DEN))+BETA)*((SIGMA/0.02)**0.2)
        VF=CF*(((DL-DG)/DG)**0.5)
        V=VF*(VFL/100.)
        AREA=QT/V
        DIA=((4.*AREA)/3.1416)**0.5
        ERR=0.05
        WRITE(5,41)TD,DIA
        WRITE(23,41)TD,DIA
41     FORMAT(' TD AND DIA ARE',2F10.2)
        IF(ABS(TD-DIA).LE.ERR)GO TO 43
        DELTD=0.01
        TD=TD+DELTD
42     CONTINUE
43     IF(I.EQ.1000)GO TO 45
        WRITE(5,44)DIA
        WRITE(23,44)DIA
44     FORMAT(' THE DIAMETER OF TOWER IS',F10.2)
        GO TO 47
45     WRITE(5,46)
        WRITE(23,46)
46     FORMAT(' THE VALUES OF ASSUMED AND CALCULATED DIAMETER DO NOT
    1   CONVERGE')
        GO TO 56
* Cost estimation starts
47     DIAIN=DIA*39.36

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      COST=EXP(5.16474-0.06366*(ALOG(DIAIN))+0.1755*((ALOG(DIAIN))
1  **2.)-0.004*((ALOG(DIAIN))**3.))
      SLOPE=RRO/(RRO+1.)
      TL=(JFLAG-1.)/(PE/100.)
      ACOST=COST*TL*(1.+SLOPE)*(PFC/100.)
      WRITE(5,48)ACOST
      WRITE(23,48)ACOST
48  FORMAT(' ANNUAL COST FOR DISTILLATION COLUMN IS',F10.2)
      HAC=QC/(UC*(TEMPT-TEMPCW))
      CC=4741.43+(59.94*HAC)+(0.1873*(HAC**2.))-(0.0008824*(HAC**3.))
      ACC=(CC/HAC)*HAC*(1.+SLOPE)*(PFC/100.)
      WRITE(5,49)ACC
      WRITE(23,49)ACC
49  FORMAT(' ANNUAL COST OF CONDENSER IS',F10.2)
      HAR=QB/(UR*(TEMPS-TEMPB))
      CR=9712.681+(79.99*HAR)+(0.118*(HAR**2.))-(0.0003663*(HAR**3.))
      AR=(CR/HAR)*HAR*(1.+SLOPE)*(PFC/100.)
      WRITE(5,50)AR
      WRITE(23,50)AR
50  FORMAT(' ANNUAL COST OF REBOILER IS',F10.2)
      AW=(QC*CW*OPT)/(LAMW*DELTW)
      WRITE(5,51)AW
      WRITE(23,51)AW
51  FORMAT(' ANNUAL COST OF COOLING WATER IS',F15.2)
      AS=(QB*CS*OPT)/HC
      WRITE(5,52)AS
      WRITE(23,52)AS
52  FORMAT(' ANNUAL COST OF STEAM IS',F10.2)
      TAC=ACOST+ACC+AR+AW+AS
      WRITE(5,53)TAC
      WRITE(23,53)TAC
53  FORMAT(' TOTAL ANNUAL COST IS',F15.2)
      GO TO 56
54  WRITE(5,55)
55  FORMAT(' ESTIMATED TOWER DIAMETER IS GREATER THAN 8 METERS
1  THEREFORE TRAY SPACING ESTIMATION FOR CONSTANTS ALPHA AND BETA
2  CANNOT BE MADE')
56  STOP
      END

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VITA

Shabbir Khurshid Hussain was born in Karachi, Pakistan on May 12, 1956. He attended elementary school in that city and graduated from B.V.S. Parsi High School in July 1974. After going through a two-year Junior College he entered the N.E.D. University of Engineering and Technology in Karachi, in December 1976. In December 1981 he was awarded a Bachelor of Engineering degree in Chemical Engineering. In October 1982, he accepted a full-time position with a petroleum company, as a Trainee Engineer. He entered the graduate school of The University of Tennessee, Knoxville, in September 1983. He received the Master of Science degree with a major in Chemical Engineering in March 1985.