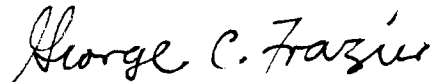


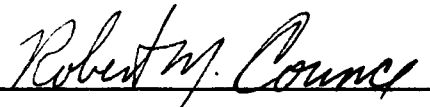
To the Graduate Council:

I am submitting herewith a thesis written by Richard W. Bone entitled "Computer Simulation and Design of Binary Distillation on a Personal Computer." I have examined the final copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Chemical Engineering.


Fred E. Weber, Major Professor

We have read this thesis
and recommend its acceptance:


George C. Frazier


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Accepted for the Council:


Vice Provost
and Dean of The Graduate School

COMPUTER SIMULATION AND DESIGN
OF BINARY DISTILLATION
ON A PERSONAL COMPUTER

A Thesis
Presented for the
Master of Science
Degree
The University of Tennessee, Knoxville

Richard W. Bone

March 1988

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ABSTRACT

A compiled BASIC computer code was developed for use on a personal computer with 256K random access memory to design a binary distillation column. The code ran successfully for seven test cases ranging from ideal and non-ideal systems. Execution times were less than two hours.

The computer code developed consisted of the following elements: Ponchon-Savarit for estimation of the number of theoretical stages; UNIFAC for vapor-liquid equilibrium prediction; choice of either Ideal, Yen-Alexander departure functions, Soave-Redlich-Kwong Equation of State to predict enthalpy; heat exchanger sizing; tower sizing and cost estimation. Optional routines included estimation of column heat loss and Murphree stage efficiencies.

Theoretical number of stages and minimum reflux estimation compared favorably with previous work for benzene-toluene systems. Stage estimates deviated less than 6% and minimum reflux varying between 4.3% and 29.1%. The methanol-water system varied 3% for the minimum reflux estimation with no deviation for stage estimation. The highly non-ideal systems of ethanol-water and n-propanol-water produced deviations in excess of 58% for both minimum reflux and stage estimations. The deviations were found to be due to the UNIFAC prediction of liquid phase activity coefficients.

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NOTATIONS

- a_{mk} = interaction parameter of functional group m with functional group k
- a_i = heat capacity coefficients
- Al = Antoine's Equation Coefficients
- a = volume correction coefficient in S-R-K equation of State
= temperature correction coefficient in S-R-K equation of State
- A = heat transfer area, ft^2
- B = bottoms flow rate, lbm/hr
- ΔB = bottoms difference point, Btu/lbm
- b = volume correction factor in S-R-K equation of state
- C_p = heat capacity, $\text{Btu/lbm}^\circ\text{F}$
- CF = flooding tray coefficient
- D = distillate flow rate, lbm/hr
- ΔD = distillate difference point, Btu/lbm
- D = diameter; D_o = outer diameter of tube/vessel, D_i = inside diameter of tube/vessel, ft
- D_e = eddy diffusion coefficient, ft^2/Hr
- DL = liquid diffusivity, ft^2/Hr
- E = joint efficiency
- E_{mv} = murphree stage efficiency
- E_{OG} = point gas-phase tray efficiency
- F = feed flow rate, lbm/Hr
- G' = vapor superficial mass velocity $\text{lbm/ft}^2\text{Hr}$
- G_m = molar flow rate, lbm/Hr

H = Enthalpy; HV = vapor enthalpy; HL = liquid enthalpy;
 HF = enthalpy of the feed stream; H_D = enthalpy of distillate stream; HB = enthalpy of bottoms stream; H^o = enthalpy of pure component; HS = enthalpy solution, Btu/lbm

Hw = Weir height, in

h = heat transfer coefficient; h_a = at surface of vessel;
 h_o = based on outside diameter; h_i = based on inside diameter,
 Btu/ft² hr °F/ft

K = thermal conductivity, Btu/ft²/ °F/in hr

k = boltzman constant, 1.3805×10^5 ergs/°k

L = liquid flow rate, lbm/HR

L' = liquid superficial mass velocity, lbm/ft² /Hr

m = mass flow rate, lbm/Hr

mw = molecular weight, lb/lbm

m = slope of equilibrium line, Btu/lbm

N_{pe} = peclet number, $Z/De\theta_L$

N_{RE} = Reynolds number, $DV\rho/\mu$

N_{SG} = Schmidt number $\mu/\rho D$

N_{pr} = Prandlt number, $C_p\mu/k$

N_o = Avogadro's Number, 6.023×10^{23} molecules/mole

N_L = Liquid phase transfer unit

N_g = gas phase transfer unit

N_{OL} = number of overall liquid transfer units

N_{OG} = number of overall gas transfer units

P = pressure; Pr = reduced pressure; P_c = critical pressure;
 P_{sat} = vapor pressure, lb/in²

Q = heat transferred; Q_c = heat transferred at the condenser;
 Q_L = heat loss; Q' = net flow of heat out of the enriching section; Q'' = net flow of heat into the stripping section,
 Btu/lbm

- Q_i = unifac area parameter of component i
 q = volumetric liquid flow rate, ft^3/hr
 R = ideal gas constant, $1.987 \text{ Btu}/\text{lbm}^\circ\text{R}$
 r = reflux rate
 R_i = unifac molecular volume parameter of component i
 S = maximum allowable stress for a given material of construction, lb_f/in^2
 T = Temperature; T_c = critical temperature; T_R = reduced temperature; T_{LM} = log mean temperature difference; T_{wall} = temperature at wall surface; T_{Bulk} = mean temperature of solution, $^\circ\text{F}$ or $^\circ\text{R}$
 T = wall thickness; T_{Pr} = wall thickness to withstand design pressure; T_w = wall thickness to withstand windloading; T_g = wall thickness to withstand internal pressure; T_{cr} = wall thickness for corrosion allowance, in
 T_{mk} = unifac group interaction parameter
 U = heat transfer coefficient, $\text{Btu}/\text{lb}^\circ\text{F}$
 V = vapor flow rate, lbm/hr
 V = volume, Ft^3
 VF = vapor velocity, ft/sec
 V_a = superficial gas velocity, ft/hr
 V_{air} = wind velocity, miles per hour
 V = molar volume, g/cm^3
 w = acentric factor
 W = width of liquid flow, in
 X = liquid composition, mole fraction
 y = vapor composition, mole fraction
 Y^* = vapor composition which would be in equilibrium with liquid leaving tray n

z = compressibility factor

z = unifac lattice coordination number, 10

Z = length of liquid flow on tray, in

z = height of tower, ft

GREEK

γ_i = liquid phase activity coefficient of component i;
 γ^c = combinational contribution; γ^r = residual contribution

Ψ = unifac segment fraction

Θ = unifac area fraction

$\checkmark$ = unifac number of functional groups of type in species i

Γ = unifac residual activity coefficient of functional group

Φ_i = gas phase activity coefficient of component i

λ = heat of vaporization, Btu/lbm

ρ = density, lb/ft³

μ = viscosity, lb/fthr

Θ_L = time of liquid residence on tray

σ = potential length constant

Ω_v = collision interval

σ = surface tension, dynes/cm³

$\delta = T^{1/6} / m^{1/2} p^{2/3}$

ECONOMIC

C_b = cost of the tower shell

C_{bt} = cost per tray

C_{PL} = cost of platforms and ladders

F_m = cost factor for the material of construction of the shell

F_{tm} = cost factor for the material of construction of trays

F_{tt} = cost factor for the tray type

F_{nt} = cost factor for number of trays

L = height of tower

N_t = number of trays

W_s = weight of shell

1.0 INTRODUCTION

In recent years, rapid fluctuations in the cost of energy and rising equipment cost have made accurate design a necessity. Companies are also faced with the expenses of not maximizing production and increased cost for environmental protection that may be caused by changes in feed conditions. Companies need to know how feed changes may affect product or effluent quality. Originally these questions had to be answered by laborious hand calculations. Today, these questions are answered quickly using digital computers.

The cost of mainframe computers has kept many firms from enjoying the benefit of quick answers to design or simulation problems. With the advent of personal computers, companies have available an inexpensive tool for solving these problems. Companies can now use the personal computer for either design or simulation, given the appropriate software and adequate random access memory (RAM). The execution time for a personal computer is many times longer; the RAM is considerably smaller than those of a mainframe computer. The lower initial cost offsets these disadvantages and makes them acceptable.

The purpose of this work was to develop software which could be used to design a major chemical processing step (e.g., distillation, extraction, etc.) using a personal computer with 256K RAM. Distillation was chosen as the thrust of this work. Results from the software would be compared with earlier work (Summer, 1986) on

distillation column design on the mainframe computer that had been performed at the University of Tennessee.

Distillation is a mass and energy transfer operation which uses heat and takes advantage of the relative volatility of the components of the liquid mixture to bring about a desired separation in the mixture. Heat is input into the bottom of the tower to produce a vapor, and as the vapor rises through the column it contacts liquid from the stage above. The contact of the liquid and vapor acts to enrich the vapor in the desired component while removing that component from the liquid. The degree of separation determines the total number of stages required. The amount of heat input to the column depends on the feed condition, the amount of reflux, and degree of separation.

The computer code developed for this work makes use of the Ponchon-Savarit graphical method for binary distillation. This method is rigorous, but it is limited by the lack of readily available enthalpy and concentration data. Where this data are unavailable they must be predicted, so the computer code for this work has several methods for estimating liquid and vapor enthalpy. Vapor and liquid enthalpies may be calculated by various methods, such as ideal, Yen-Alexander departure functions, or an equation of state such as Redlich-Soave-Kwong.

Each enthalpy prediction method does not work equally for all systems. For this reason, several estimation methods are included within the computer code for this work. The software user can choose the method which gives the best results for the specified binary system.

To improve the accuracy of the Ponchon-Savarit method, the program includes the option of estimating heat losses from the column and Murphree stage efficiencies. Other features of the computer code include reboiler and condenser sizing, tower sizing and cost analyses. The program sizes the tower and auxiliaries for a set reflux rate, or it will determine the optimum reflux ratio and size the tower for the lowest annual cost (where optimum reflux ratio is defined as the ratio where the yearly total of fixed and variable costs to operate the tower is minimized).

The program has been prepared so that the user interacts with the computer. It is equipped with a data bank of information for the following components: methanol, ethanol, acetone, n-propanol, water, benzene and toluene. The data bank contains information on critical properties, Antoine coefficients, heat capacity coefficients, molecular weight, eccentric factors, heat of vaporization, boiling point and molecular volumes. Normal inputs required by the program are the feed conditions, bottoms composition, distillate composition and tower operating pressure. VLE data for the Ponchon-Savarit method will be provided by the UNIFAC method. All data parameters required by UNIFAC (molecular volume and area, functional group interaction) are provided as part of the same data bank.

2.0 GENERAL BACKGROUND

The objective of this work was to develop a computer code to design a distillation column on a personal computer with 256K RAM. This was accomplished using subroutines to estimate the number of theoretical stages, the size of the distillation column and heat exchangers, and the cost.

The Ponchon-Savarit method was selected to perform the stage estimation because it is more general than other approaches. The Ponchon-Savarit method simultaneously solves material and energy (see Figure 2.1) balances to determine number of stages. The vapor-liquid equilibrium (VLE) data for material balances was obtained by the UNIFAC method. Four methods (Ideal, Ideal using Antoine's coefficients, Yen-Alexander departure functions, and Soave-Redlich-Kwong) are included to estimate enthalpy. The choice of methods provides greater flexibility and accuracy over a wide range of ideality. The Ponchon-Savarit method also provides estimates of vapor rates for column sizing and heat duty for sizing the heat exchangers. Physical data required to support the exchanger design are developed by separate subroutines. If desired, there are routines to correct for non-ideal column operation (heat loss and stage efficiency).

2.1 The Ponchon-Savarit Method

The Ponchon-Savarit graphical solution simultaneously solves material and energy balances. The solution divides the column into two

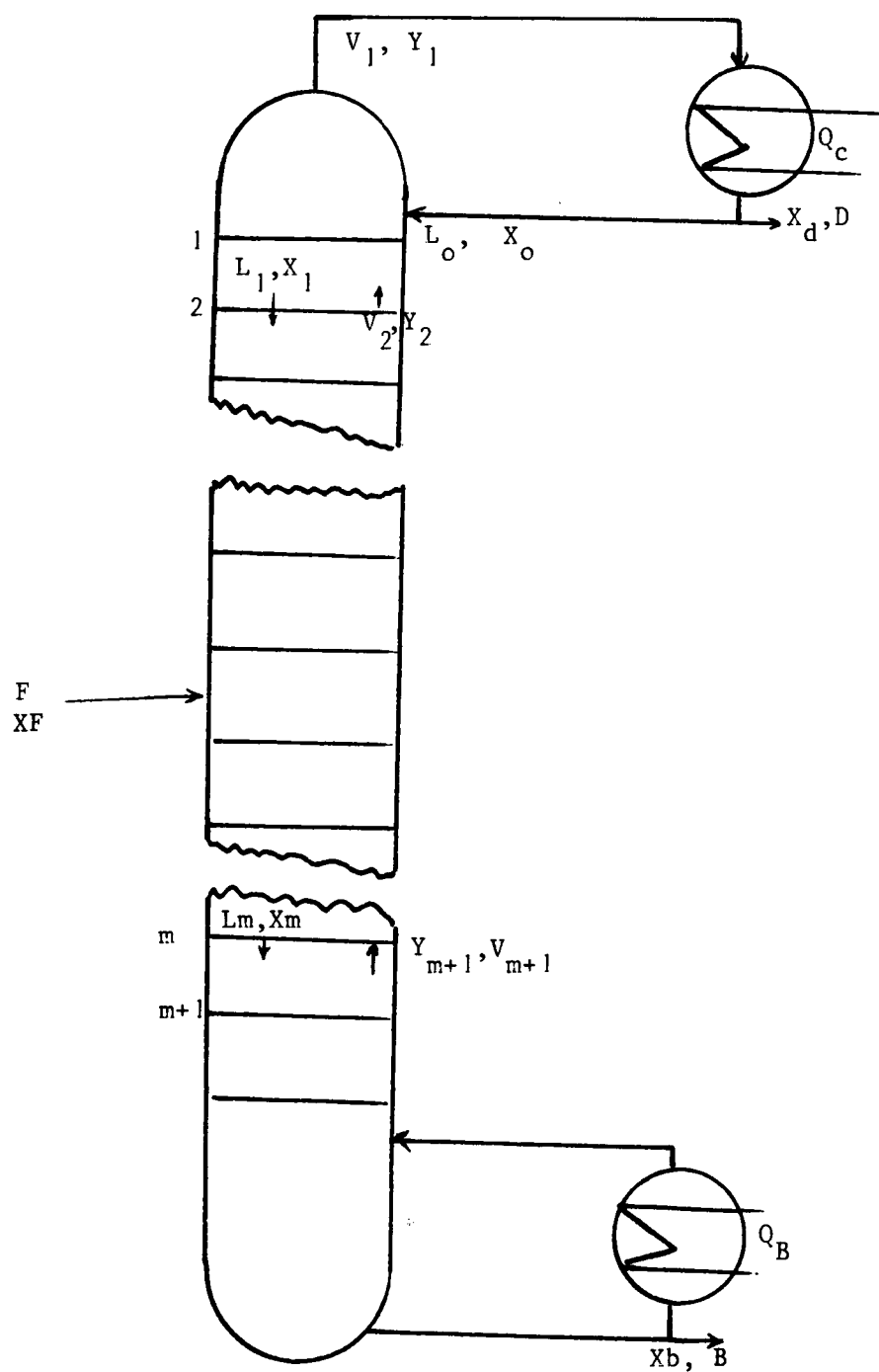


Figure 2.1. Distillation Column Material and Energy Balance.

sections centered around the feed point. The enriching section consists of the stages located above the feed line point. The stripping section consists of the stages located below. The distillation column is represented in Figure 2.2. The single stage mass and energy balances in the enriching section are written:

$$V_{n+1} = L_n + D \quad \text{single stage material balances} \quad (1)$$

$$V_{n+1} Y_{n+1,a} = L_n X_{n,a} + D X_{d,a} \quad \text{material balance for component a.} \quad (2)$$

The single stage enthalpy balances in the enriching sections are written:

$$V_{n+1} H_{V_{n+1}} = L_n H_{L_n} + Q_c + D H_d \quad (3)$$

$$V_{n+1} H_{V_{n+1}} Y_{n+1,a} = L_n H_{L_n} X_{n,a} + Q_c X_{n,a} + D H_d X_{d,a} \quad (4)$$

These equations do not take into account heat losses by conduction, convection or radiation from the column; instead they assume that either insulation or low state temperature results in negligible heat loss. However, some heat is removed from the column by the condenser and the distillate stream and is accounted for by the term Q' . This heat removal term, Q' is represented by:

$$Q' = (Q_c + D H_d) / D \quad (5)$$

$$Q' = (V_{n+1} H_{V_{n+1}} - L_n H_{L_n}) / D \quad (6)$$

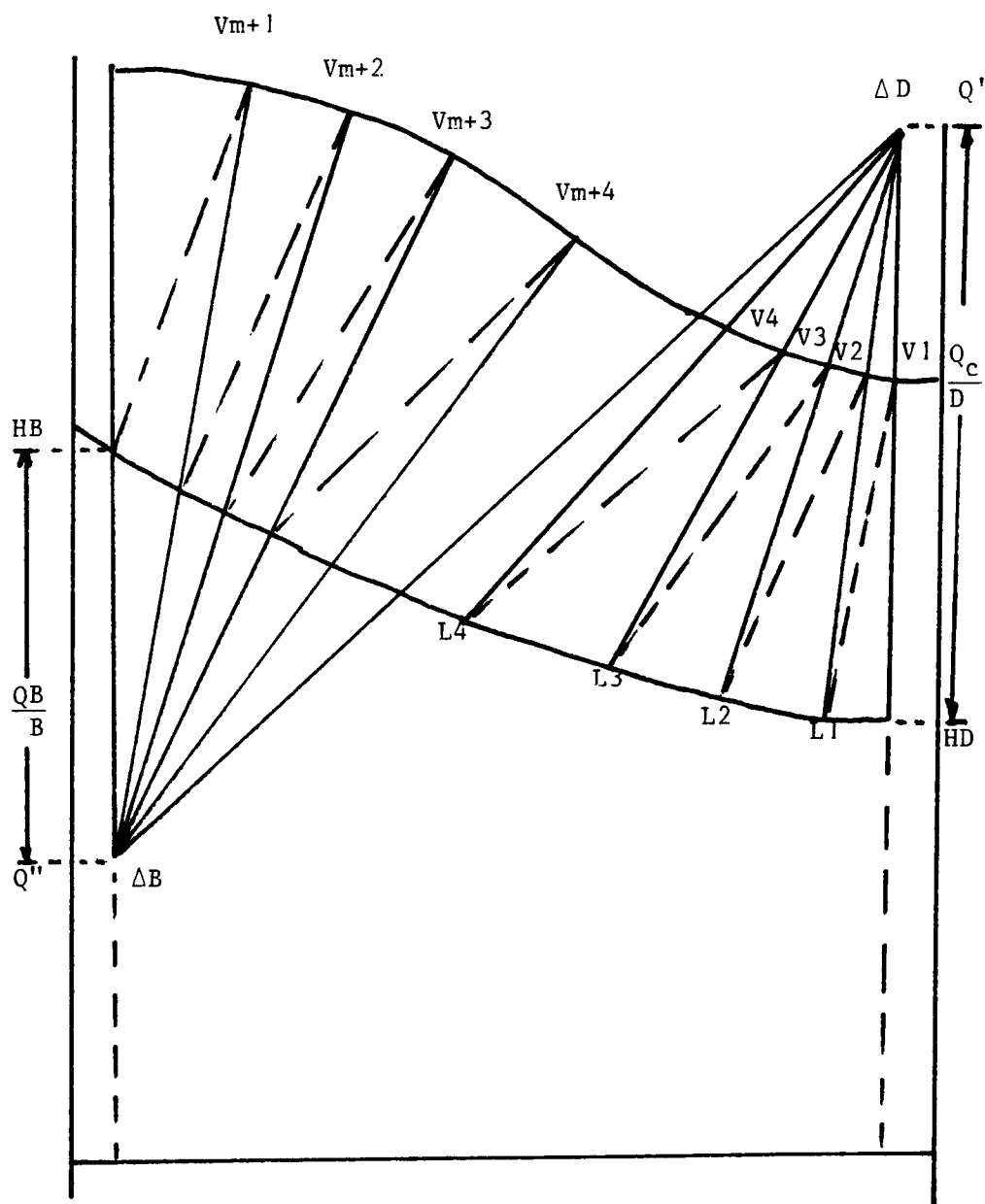


Figure 2.2. Illustration of the Ponchon-Savarit Method.

or combining equations 1, 2, 5 and 6.

$$L_n/V_{n+1} = (Z_d - Y_{n+1})/(X_d - X_n) \quad (7)$$

$$= (Q' - HV_{n+1})/(Q' - HL_n). \quad (8)$$

The ratio L_n/V_{n+1} is the internal reflux rate of the column. This ratio forms a family of straight lines on the enthalpy concentration diagram (see Figure 2.1). These lines pass through the points (HV_{n+1}, Y_{n+1}) at V_{n+1} , (HL_n, X_n) at L_n and (Q', X_d) at the point ΔD . ΔD is the difference point in the enriching section of the Ponchon-Savarit construction. This point represents the net flow of heat and material out of the distillation column from the condenser and distillate. Starting at the difference point, the operating lines in the enriching section are drawn to each tray. The equilibrium relationship between the liquid and vapor streams are used to indicate the location of the next tray. The lines that can be drawn from the vapor stream entering a stage and the liquid leaving that stage are called "tie" lines. These "tie" and operating lines are alternately drawn until the feed line is crossed.

A single stage mass and energy balances in the stripping section are represented by:

$$L_m = V_{m+1} + B \quad (9)$$

$$L_m X_{m,a} = V_{m+1} Y_{m+1,a} + BX_{b,a} \quad (10)$$

$$L_m HL_m + Q_b = V_{m+1} HV_{m+1} + BH_b \quad (11)$$

$$L_m HL_m X_{m,a} + Q_b X_{b,a} = V_{m+1} HV_{m+1} Y_{m+1,a} + BH_b X_{b,a} \quad (12)$$

Heat flows from the stripping with the bottoms as it does with the distillate in the enriching section. The net flow of heat from the stripping section, Q'' , is represented by:

$$Q'' = (BH_b - Q_b)/B \quad (13)$$

$$Q'' = (L_m HL_m - V_{m+1} HV_{m+1})/B. \quad (14)$$

When equations 10, 11, 14 and 15 are combined and terms are eliminated, the result is

$$L_m/V_{m+1} = (Y_{m+1} - X_b)/(X_m - X_b) \quad (15)$$

$$L_m/V_{m+1} - Q''/(HL_m - Q''). \quad (16)$$

Equations 15 and 16 form a family of straight lines representing the stripping section. The lines pass through (HL_m, X_m) at L_m , (HV_{m+1}, Y_{m+1}) at V_{m+1} and through (Q'', X_b) at ΔB . The point ΔB is the difference point for the stripping section, which represents the net flow of heat out of the column through the reboiler and bottoms flow. The stages in the stripping section are stepped off in a manner similar to those in the enriching section, starting from the bottoms and continuing past the feed point.

The two difference points are connected through the feed point. The relationship is developed through the column overall balances which follow:

$$F = D + B \quad (17)$$

$$FZ_f = DX_d + BX_b \quad (18)$$

$$FH_f = DQ' + BQ'' \quad (19)$$

Combining equation 17 and 18 to eliminate B and substituting into equation 15, results in

$$D/B = (Z_d - Z_f)/(Z_f - Z_b). \quad (20)$$

Substituting into equation 16, results in

$$D/B = (Q' - HF)/(HF - Q''). \quad (21)$$

The ΔD difference point is set by the choice of reflux rate and distillate condition. The column reflux rate is defined as:

$$R = L_o/D \quad (22)$$

$$R = (Q' - HV_1)/(HV_1 - HL_o). \quad (23)$$

The higher the reflux rate the higher the difference point ΔD and the more stages that are required.

Minimum reflux occurs at the lowest point of intersection of an enriching section "tie" line with an enriching section operating line or at the highest intersection of a stripping section "tie" line and

stripping section operating line. The usual starting point for finding the minimum reflux ratio is the intersection of the tie line that passes through the feed point and the line $X = Z_d$. When the minimum reflux ratio is found, it is used as the starting point for finding the optimum reflux ratio. Optimum reflux corresponds to the lowest annual column cost.

2.2 Unifac Model

The unifac group contribution method developed by Fred Enslund, Jones, and Prausnitz is used to provide the required equilibrium information. The unifac method functions by calculating the liquid phase activity coefficients for the mixture from the residual and combinatorial activities. For component i ,

$$\ln \gamma_i = \ln \gamma_{c_i} + \ln \gamma_{r_i}. \quad (24)$$

The combinatorial activity is estimated by

$$\begin{aligned} \ln \gamma_{c_i} = & \ln(\Psi_i/X_i) + Z/2(q_i)(1_n(\Theta_i/\Psi_i) + 1_i \\ & - (\Psi_i/X_i) \sum (X_j 1_j)) \end{aligned} \quad (25)$$

where Ψ_i is the segment fraction and Θ_i is the area fraction. The segment and area fractions are estimated by the following models

$$\Psi_i = X_i r_i / \sum_i X_i r_i \quad (26)$$

$$\Theta_i = X_i q_i / \sum_i X_i q_i. \quad (27)$$

The molecular volume r_i and area parameters q_i are estimated by:

$$r_i = \sum_k \sqrt{k} R_k. \quad (28)$$

$$q_i = \sum_k \sqrt{k} Q_k \quad (29)$$

The term $\sqrt{k}$ is the number of functional groups of type K in species i, and R_k and Q_k are the area and volume parameters for each functional group. The last term in the estimation of the combinatorial activity, l_i , is estimation from:

$$l_i = \left(\frac{Z}{2} \right) (r_i - q_i) - (r_i - 1) \text{ where } Z = 10. \quad (30)$$

The residual activity contribution is estimation using:

$$\ln \gamma_i R = \sum_K \sqrt{K}^{(i)} (\ln \Gamma_K - \ln \Gamma_K^{(i)}) \quad (31)$$

where γ_i is the residual activity of the functional group K. The functional group activity is estimated using:

$$\ln \Gamma_K = Q_K [1 - \ln(\sum_m \Theta_m T_{mk}) - \sum_m \Theta_m T_{mK} / \sum_n \Theta_n T_{nm}] \quad (32)$$

$$\Theta_m = X_m Q_m / \sum_n X_n Q_n \quad (33)$$

$$X_m = \sum_j \sqrt{j}^{(j)} X_j / \sum_j \sum_n (\sqrt{j}^{(j)} X_j) \quad (34)$$

$$T_{mk} = \exp(-a_{mk}/T). \quad (35)$$

The term a_{mk} is the interaction parameter between the functional groups.

After the liquid phase activity coefficient has been calculated at a given composition and temperature, the composition of the saturated vapor in equilibrium with the liquid is determined from the equation

$$Y_i \phi_i P = X_i P_i^S \gamma_i \quad (36)$$

Normally the vapor phase activity coefficient ϕ_i is assumed to behave as an ideal gas so ϕ_i is set equal to 1.0. Equation 36 reduces to

$$Y_i = X_i P_i^S \gamma_i / P. \quad (37)$$

The saturation pressure is estimated by Antoine's Equation, which is

$$P_i^S = P_c \exp (A1 - A2/(T+A3)). \quad (38)$$

2.3 Enthalpy Calculations

Component enthalpy is estimated for the saturated liquid and vapor, and for the superheated vapor and supercooled liquid. To improve accuracy the data is generated by several different methods. Saturated vapor enthalpy is estimated using one of the following methods: the Ideal Vapor method, Yen and Alexander Enthalpy Departure Equations or the Soave-Redlich-Kwong Equation of State.

When the binary mixture is thought to behave ideally in the vapor state the vapor enthalpy may be estimated by

$$H_V = \sum_{i=1}^2 Y_i C_{p_i} + \sum_{i=1}^2 Y_i \lambda_i. \quad (39)$$

The heat capacity of the vapor will be represented as

$$C_{p_i} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \quad (40)$$

and is given in Btu/lbmole °F. The heat of vaporization, λ_i , can be estimated by any of four models; the Watson relation, Antoine's equation, Fish and Lielmez's relations or the method of Reid, Prausnitz and Sherwood.

The Watson equation estimates the heat of vaporization at temperature T_2 given the heat of vaporization at a given temperature T_1 by the equation

$$\Delta H_2 = \Delta H_1 (1-T_{r2}/1-T_{r1})^{.38}. \quad (41)$$

The Fish and Lielmez's equation relates the heat of vaporization at some temperature to the heat of vaporization at the boiling point ΔH_{bp} of each component. The equation is

$$\Delta H = \Delta H_{bp} (T_r/T_{br}) [X + X^{.35298}] / [1 + X^{.13856}] \quad (42)$$

$$X = (T_{br}/T_r) [1 - T_r / 1 - T_{br}]. \quad (43)$$

Antoine's equation is a correlation utilizing the coefficients from the vapor pressure equation. The heat of vaporization is estimated by

$$\Delta H = A_2/T_c [T_r/(T_r - A_3/T_c)]^2. \quad (44)$$

The final correlation for heat of vaporization is one proposed by Ried, Prausnitz, and Sherwood. The correlation is

$$\Delta H = T_c (7.08(1-T_r)^{.354} + 10W(1-T_r)^{.456}). \quad (45)$$

For ideal or nonideal gas behavior, enthalpy may be estimated by either Soave-Redlich-Kwong Equation of State or the Yen and Alexander Departure Equations. The Soave-Redlich-Kwong Equation is a modification with improved accuracy of the Redlich-Kwong Equation. The S-R-K Equation of State is of the form:

$$P = RT/(V-b) - Aa/V(V+b) \quad (46)$$

$$a = [1+m(1-T_r)^{.5}]^2 \quad (47)$$

$$m = 0.48 + 1.574W - 0.176W^2 \quad (48)$$

$$T_r = T/T_c. \quad (49)$$

The S-R-K Equation of State is solved by finding the solution of the cubic relationship for the compressibility factor, Z. The cubic relationship for the compressibility factor is

$$Z^3 - Z^2 + Z(A-B-B^2) - AB = 0 \quad (50)$$

where

$$A = \sum_{i=1}^2 \sum_{j=1}^2 Y_i Y_j A_{ij} \quad (51)$$

$$A_{ij} = (A_i A_j)^{.5} \quad (52)$$

$$A_i = 0.42747 a_i (P_{ri}/T_{ri}^2) \quad (53)$$

$$B = \sum_{i=1}^2 Y_i B_i \quad (54)$$

and $B_i = 0.08664 P_{ri}/T_{ri}$.

After the compressibility factor has been estimated, the enthalpy is estimated from

$$H = H_v^0 + RT [Z - 1 - (1/B) \ln(Z + B/Z) [\sum_{i=1}^2 \sum_{j=1}^2 Y_i Y_j A_{ij} [1 - (m_i T_{ri}^{.5} / 2 a_i^{.5}) - (m_j T_{rj}^{.5} / 2 a_j^{.5})]]] \quad (55)$$

and

$$H_v^0 = T_o^{TH} [C_p dT] = \sum_{K=1}^5 a_K [(T^k - T^{ko})/K]. \quad (56)$$

The terms a_K are the constants used to estimate the vapor phase heat capacity.

The final method available for estimating vapor phase enthalpy is the Yen and Alexander Enthalpy Departure Equations. These functions are only applicable for components with critical compressibility factors in the range of $Z_c = 0.23$ to $Z_c = 0.29$. The saturated vapor enthalpy is estimated from

$$\frac{H^0 - H}{T_c} = \frac{A Pr^B}{1 + C(-\ln Pv)^D}. \quad (57)$$

The terms A, B, C and D are constants that vary at different compressibility factors (.23, .25, .27, .29). The superheated vapor enthalpy is estimated from

$$\frac{H^0 - H}{T_c} = \frac{m Pr (1 - Pr/X_o)}{\exp[-C_1 (Pr)^2] [1 + C_4 C_5 Pr + C_6 Pr^2]} \quad (58)$$

where $[] = 1 - C_2 - C_4 - C_5 \text{Pr} + C_2(1/\pi)[\arctan(C_3 - C_3 \text{Pr}) + 0.5]^2$.

The constants m , X_o , C_1 , C_2 , C_3 , C_4 , C_5 , and C_6 are functions of T_r that change with the critical compressibility.

The liquid enthalpy may be estimated through any of three methods: Yen and Alexander Departure Functions, the heat of solution of the mixture method presented by Treybal⁽¹⁸⁾ or the ideal liquid mixture enthalpy method.

For a saturated liquid the Yen and Alexander Departure Function is

$$\frac{H^o - H}{T} = \frac{A + B(-\ln \text{Pr})^C}{1 + D \ln \text{Pr}} \quad (59)$$

where A-D are constants that change with Z_c . The form of the equation for the supercooled enthalpy is

$$\begin{aligned} \frac{H^o - H}{T_c} = & A(\text{Pr} - 4.2) - B(T_r - 0.77) - C(T_r - .77)^2 \\ & D(P_r - 4.2)(T_r - 0.77) + E \ln P_r + \\ & F(\ln P_r)(\ln T_r) + G(\ln P_r)(\ln T_r)^2 + H \end{aligned} \quad (60)$$

where the constants A-H vary with critical compressibility factor.

For the ideal liquid mixture enthalpy is estimated from

$$\begin{aligned} H_L = & [H_{iv}^o - 1.0695RT_p \frac{p_i^s}{p_{ci}} \frac{p_i^s}{T_{ri}} \frac{TA_2}{(T + A_3)} [RT/p_i^s - 0.4278RT_{ci} - V_{iL}] \\ & + 5.7E_i(p - p_i^s)]. \end{aligned} \quad (61)$$

The molar volume of the liquid, V_{il} , is estimated by $V_i = E_i (5.7 + 3.0T_r)$ but E_i is a constant that must be back estimated for each species using a known molar volume at a reference temperature. The constants A_2 and A_3 are from Antoine's Equation for calculating vapor pressure.

The final method of liquid enthalpy approximation comes from Mass Transfer Operations by Treybal. This method uses the heat of solution of one component in another along with the liquid phase heat capacities of both components to estimate enthalpy. The equation is

$$HL = C_{pL} (t_c - t_o) MW_{avg} + \Delta H_s \quad (62)$$

where ΔH_s is the heat of solution at temperature t_o , and C_{pL} is the liquid heat capacity in terms of Btu/lb_m^oF.

2.4 Column Design

The distillation column is sized by limiting the vapor velocity to 80% of the velocity necessary to flood the column. The vapor velocity can be estimated from

$$VF = CF(\rho_L - \rho_v)^{.5} / g \quad (63)$$

where CF is the flooding constant which is dependent upon tray design. For this work CF will be represented as

$$CF = [\log(1/(L'/G')(\rho_g/\rho_L)^{.5}) +](\sigma/.02)^{.2}. \quad (64)$$

In this equation L' and G' are the superficial mass velocities and are empirical tray constants defined as

$$\alpha = 0.0062 (\text{Tray Spacing}) + .0385 \quad (65)$$

$$\beta = 0.00253 (\text{Tray Spacing}) = .05. \quad (66)$$

When the vapor mold flow rate has been estimated utilizing the Ponchon-Savarit material balances, the tower diameter is

$$\text{Diameter} = 2(\text{vapor flow}) / (0.8(VF)(\pi))^{.5}. \quad (67)$$

The outside diameter of the tower can be estimated after considering requirements for wind loading, corrosion, design pressure and the girth seam. Thickness of the tower is estimated by

$$T_{PR} = (P_g)(\text{DIAM}) / (E)(S) - .6P_g \quad (68)$$

$$T_w = P_{air} V_{air}^2 (D_o + Z_1 (T_i^2 / (S D_o^2))) \quad (69)$$

$$T_g = (P_g R) / (2SE + .4P_g) \quad (70)$$

where S is the maximum allowable stress for a given material of construction and E is the joint efficiency. The three thicknesses are T_{PR} , the thickness needed to withstand design pressure P_g , T_w , the thickness to withstand wind loading at a wind velocity V_{air} , and T_g , the thickness to withstand internal pressure are totalled with a tolerance for corrosion to estimate the outside diameter of the tower.

2.5 Non-Ideal Operation

The Ponchon-Savarit method is rigorous in its assumptions, but accuracy can be improved by considering heat losses from the column and stage efficiency. Heat loss affects column behavior by increasing the

amount of heat removed from either the stripping and enriching sections. This affects the terms Q' and Q'' , raising the difference point in the stripping section and can result in more stages, depending upon the magnitude of the heat loss. Heat loss can be estimated as

$$QL = (T_{col_n} - 70)(\ln D_i / D_o) / (h_a \pi K_p + 1/2 D_o) \quad (71)$$

where T_{col} is the temperature of the column at stage n , h_a is the heat transfer coefficient at the surface of the column, and D_i and D_o are the inside and outside diameters of the tower.

Stage efficiency also affects the number of trays required for a given separation. In stepping off the number of stages in the column, equilibrium relationships from one stage to another are represented by the "tie" lines. In an actual column the ideal relationship represented by the "tie" line is only approached. The percentage of mass transfer that occurs at each stage is estimated by the Murphree Stage efficiency, Emv . This efficiency is defined as

$$Emv = (Y_n - Y_{n-1}) / (Y_n^* - Y_{n-1}) \quad (72)$$

where Y_n^* is composition of vapor which would be in equilibrium with the liquid leaving tray n . Emv estimation is accomplished using the method outlined in A.I.Ch.E Tray Design and in Treybal's Mass Transfer Operations. This approach estimates the stage efficiency, Emv , by using

$$Emv/Eog = \frac{1 - e^{-(n' + NPE)}}{(n' + NPE)[1 + \{[n' + NPE]/n'\}]} + \frac{e^{n'} - 1}{[1 + \{[n' + NPE]\}n']} \quad (73)$$

where

$$n' = \frac{Npe \left((1+4 EOG/NPE)^{.5} - 1 \right)}{2} \quad (74)$$

$$\text{and } Npe = Z_1^2 / D_{col}.$$

The Peclet number, NPE, is estimated from length of liquid transfer, Z_1 , and the eddy diffusion coefficient, De . The diffusion coefficient is calculated by

$$De = (3.93 \times 10^{-3} + 0.0171 V_a + 3.678/W + 0.18hw)^2 \quad (75)$$

where q_1 = liquid flow rate, ft^3/min

and w = width of flow path, ft.

The other terms, Nog , the number of overall gas transfer units and λ , the stripping factor are estimated from

$$Eog = 1 - e^{-Nog} \quad (76)$$

$$Nog = \frac{1}{1/Ng + \lambda/Nl} \quad (77)$$

$$\lambda = mG_m / L_m \quad (78)$$

where m is equal to the slope of the equilibrium curve and G_m and L_m are the gas and liquid molar flow rate. The gas and liquid transfer units, N_g and Nl , are estimated by

$$N_g = (0.776 + 0.116hw - 0.298V_a \rho_g^{.5} + 9.72q/Z)NSG^{.5} \quad (79)$$

$$N_L = (7.31 \times 10^5 D_L^{.5} (0.26 V_a \rho_L^{.5} + 0.15) \Theta_L) \quad (80)$$

$$\text{where } D_L = (3.93 \times 10^{-3} + 0.017 V_a + 3.67 q / Z + 0.18 h_w)^2 \quad (81)$$

$$\text{and } \Theta_L = h_1 z Z / q \quad (82)$$

$$\text{with } NSG = \mu / \rho D. \quad (83)$$

The remaining terms, Z , W , h_w and h_1 , are dependent upon the particular design of each tray.

2.6 Heat Exchanger Design

Heat exchanger designs must be accomplished for both the condenser and reboilers. For both designs it is necessary to calculate the Reynolds and Prandtl number first. These dimensionless numbers are

$$N_{RE} = (do)(\text{Fluid Velocity})(p)/u \quad (84)$$

$$N_{PR} = (Cp)(u)/k. \quad (85)$$

The basic design equation for the condenser is

$$Q = U A \Delta T_{LM} \quad (86)$$

where

$$\Delta T_{LM} = \Delta T_2 - \Delta T_1 / \ln(\Delta T_2 / \Delta T_1). \quad (87)$$

The overall heat transfer coefficient, U , is dependent on the tube-side and shell side individual heat transfer coefficients as well as fouling coefficients. The tube-side heat transfer coefficient varies with the Reynolds number and is

$$N_{RE} < 2100 \text{ Laminar Flow Region } Hi = 0.116 \quad (88)$$

$$\begin{aligned} & (N_{RE})^{2/3} (N_{PR})^{1/3} \\ & ((1+Di)/Tlen)^{2/3} \\ & (\mu/\mu_{wall})^{.14} (k/Di) \end{aligned}$$

$$2100 < N_{RE} < 3000 \text{ Transition Flow Region } Hi = \quad (89)$$

$$1.86(N_{RE})^{1/3} (N_{PR})^{1/3} (\mu/\mu_{wall})^{.14} (k/D_i)$$

$$N_{RE} > \text{Turbulent Flow Region } Hi = 0.023(N_{RE})^{1/3} (N_{PR})^{1/3} \quad (90)$$

$$(\mu/\mu_{wall})^{0.14} (k/D_1)$$

where μ_{wall} is the viscosity of the solution in the tubes estimated at the wall temperature.

The heat transfer coefficient on the outside of the tubes is estimated using

$$h_o = 0.815((K^3 \rho_L (\rho_L - \rho_g) 4.18E8) / (u D_o (T_{wall} - T_{Bulk})))^{.25}. \quad (91)$$

The overall coefficient U_o is estimated by

$$U_o = \frac{(1/h_o + Do-D_1 + 0.005 Do/Di + Do/HiDi + .001)^{-1}}{KwA_{avg}} \quad (92)$$

where

$$A_{avg} = \pi(Do-Di) / \log(D_o/D_i). \quad (93)$$

The design equation for the reboiler is the same as the condenser in that

$$Q = U A \Delta T_{LM} \quad (86)$$

$$\text{and } \Delta T_{LM} = \Delta T_2 = \Delta T_1 / 1_n (\Delta T_2 / \Delta T_1). \quad (87)$$

The tube-side individual heat transfer coefficient for steam flowing through the tubes is estimated using the Reynold Number which is estimated as

$$N_{RE} = 4 M / (D_i u) \quad (94)$$

where M is the mass flow rate of the steam in lbs per hour. The individual heat transfer coefficient for steam flowing through the horizontal tubes is

$$h_1 = 0.02 N_{RE}^{.6} / (M^2 / (4.18E8 K^3 P_L (P_L - P_g)))^{1/3}. \quad (95)$$

The heat transfer coefficient for the solution on the external surface of the horizontal tubes is

$$h_o = .62(4.18E8 P_L (P_L - P_g) K^3 / DoM(T_{wall} - T_{Bulk}))^{1/4}. \quad (96)$$

Once the reboiler individual heat transfer coefficients have been estimated, the overall coefficient, U_o , is found using

$$U_o = (1/h_o + 0.005 Do/Di + .001 + O^{Do - D1}) / DiKw + Do/HiDi). \quad (92)$$

2.7 Physical Properties

In order to design the heat exchangers and to size the column, physical property data is required. The physical properties needed are the density, viscosity, thermal conductivity of the surface tension of the liquid mixture.

The vapor mixture viscosity is estimated using Wilke's Approximations for a binary system. The mixture viscosity μ_m is estimated by

$$\mu_m = \frac{Y_1 \mu_1}{Y_1 + Y_2 \Theta_{12}} + \frac{Y_2 \mu_2}{Y_2 + Y_1 \Theta_{21}} \quad (97)$$

where μ_1 and μ_2 are the individual vapor viscosities estimated by the Chapman-Enskog viscosity equation. Viscosity in this form is estimated using

$$\mu = 26.69 M_w^{1/2} T^{1/2} / \sigma^2 \Omega_v \quad (98)$$

The potential length constant, σ , and the term E/k are estimated by

$$\sigma = 2.3551 - \frac{0.874 w}{(P_c/T_c)^{1/3}} \quad (99)$$

$$E/k = T_c [0.715 + .1693w] \quad (100)$$

The collision interval, Ω_v , is estimated by an empirical equation suggested by Neufeld

$$\Omega_v = A/T^*B + C/\exp(D/T^*) + E/\exp(FT^*) \quad (101)$$

$$\text{where } T^* = T/(E/k) \quad (102)$$

The constants in the equation are $A = 1.116145$, $B = 0.14874$, $C = 0.52487$, $D = 0.7732$, $E = 2.16178$, and $F = 2.43787$. The terms Θ_{12} and Θ_{21} are estimated by

$$\Theta_{12} = [1 + (\mu_1/\mu_2)^{.5} (M_{w2}/M_{w1})^{.25}]^2 / [8(1 + \mu_1/\mu_2)]^{.5} \quad (103)$$

and

$$\Theta_{21} = \mu_{2Mw1} \Theta_{12} / \mu_{1Mw2}. \quad (104)$$

The liquid mixture viscosity is estimated using a correction suggested by Letsou and Stiel. The viscosity of the mixture μ_{LM} is

$$\mu_{LM} = \mu_L \delta / E \quad (105)$$

$$\delta = T_{cm}^{1/6} / M_w^{1/2} P_{cm}^{2/3} \quad (106)$$

and

$$\mu \delta = (\mu_L \delta)^0 + w_m (\mu_L \delta)^1. \quad (107)$$

The constants $(\mu \delta)^0$ and $(\mu \delta)^1$ are estimated by

$$(\mu \delta)^0 = 0.015174 - 0.02135 T_{rm} + 0.894 T_{rm}^2 \quad (108)$$

$$(\mu \delta)^1 = 0.042552 - 0.042552 T_{rm} - 0.07674 T_{rm} + 0.034 T_{rm}^2 \quad (109)$$

The terms T_{cm} , W_{cm} , P_{cm} and T_{rm} are the mixture physical properties which are estimated using the following mixing rules:

$$T_{cm} = \sum Y_i T_{ci} \quad (110)$$

$$P_{cm} = \sum P_{ci} Y_i \quad (111)$$

$$W_{cm} = \sum w_i Y_i \quad (112)$$

$$T_{rm} = \sum Y_i T_{ri} \quad (113)$$

where

$$T_{ri} = T / T_{ci}. \quad (114)$$

Vapor mixture density is estimated using the compressibility factor for each component as shown in Section 2.3. After the compressibility factor, Z , has been estimated then vapor density of each component is:

$$\rho_i = M_{wi} P / Z_i T. \quad (115)$$

The vapor density of the mixture is:

$$\rho_m = \sum Y_i \rho_i. \quad (116)$$

The density of the liquid is estimated by the method of Gunn and Yamada,

$$\frac{V}{VR} = \frac{V_r^{(o)} T_r (1-w(T_r))}{V_r^{(o)} T_r^R (1-w(T_r))} \quad (117)$$

where VR and T_r^R are the liquid molar volume and reduced temperature at same reference point.

The terms $V_r^{(o)}$ and w are functions of reduced temperature, T/T_c , and are described as

$$\begin{aligned} V_r^{(o)} = & 0.33593 - 0.33953 T_r + 1.51941 T_r^2 - 2.02512 T_r^3 \\ & + 1.11422 T_r^4 \end{aligned} \quad (118)$$

and

$$w = 0.29607 - 0.09045 T_r - 0.03842 T_r^2. \quad (119)$$

The thermal conductivity of the vapor mixture is estimated using the Wassiljewa Equation,

$$k_m = \sum Y_i k_i / \sum Y_i A_{ij}. \quad (120)$$

The term A_{ij} is a function of viscosity, molecular weight, temperature and pure gas viscosity. This function is represented by Lindsay and Bromley as

$$A_{ij} = \frac{1}{4} \left[1 + \left[\frac{\mu_i}{\mu_j} \left(\frac{\mu_j}{\mu_i} \right)^{3/4} T + S_i \right]^{1/2} \right]^2 \frac{T + S_j}{T + S_i} \quad (121)$$

where

$$S_i = 1.5 T_B \quad (122)$$

and

$$S_{ij} = (S_i S_j)^{.5}. \quad (123)$$

The liquid conductivity of the mixture is estimated using the Method of Robbins and Kingrea to find the pure liquid conductivity and then by the L_i Equation to find the mixture conductivity. The L_i equation is

$$k_m = \sum \sum \Theta_i \Theta_j k_{ij} = \Theta_i^2 k_i + 2 \Theta_i \Theta_j K_{ij} + \Theta_j^2 k_j \quad (124)$$

where

$$K_{ij} = 2(K_i^{-1} + K_j^{-1})^{-1} \quad (125)$$

and

$$\Theta_i = X_i V_i / \sum X_j V_j. \quad (126)$$

The term V is the molar volume of the pure liquid. This value can be estimated for the required temperature as presented in Section 2.2.

The pure liquid conductivity is estimated by

$$k_L = \frac{(88.0 - 4.94H)(10^{-3})}{\Delta S^*} \frac{(0.55)^{N_{C_P}}}{T_r^{4/3}} \quad (127)$$

where

$$\Delta S^* = \Delta H_{vb}/T_b + R \ln (273/T_b) \quad (128)$$

and C_p , the heat capacity, and ρ , the density can be estimated as discussed earlier. The constants H and N can be obtained from Table 2.1 below.

Table 2.1
Functional Group for H and N Values

Functional Group	H
Paraffins	0
Olefins	0
Rings	0
CH ₃ Branches 1	1
2	2
3	3
Cl Substitutions	1
OH Substitutions 1 (iso)	1
1 (normal)	-1
2	0
1 (tertiary)	5
Ketones, aldehydes -C=O	0
acids, esters O=C-O	0
ethers -O-	2
NH ₂ Substitutions 1	1
<u>Liquid Density</u>	<u>N</u>
> 1g/cm ³	1
< 1g/cm ³	0

The surface tension of a pure liquid is estimated using a correlation suggested by Miller, which relates the three terms Q, A and α . These terms are estimated as

$$\sigma_i = p^{2/3} T_c^{1/3} Q (1 - Tr)^{11/9} \quad (129)$$

where

$$Q = 0.1207 \left(1 + \frac{T_{br}^{1.5} P_c}{1 - T_{br}} \right) - 0.281. \quad (130)$$

The mixture surface tension is found from

$$\sigma_m = X_i \sigma_i + X_j \sigma_j - \frac{A}{2RT} (\sigma_i - \sigma_j)^2 X_i X_j \quad (131)$$

where A is a surface area term represented as

$$A = (A_i + A_j) / 2 \quad (132)$$

and

$$A_i = (M_{wi} / \rho_i)^{2/3} (No)^{1/3}. \quad (133)$$

The term No is Avogadro's Number.

2.8 Economics

The distillation tower is designed for either an optimum or a set reflux ratio. For optimum reflux, the lowest annual cost must be established. Cost data is required for both cooling water and steam. In this research cost for steam data was established at \$0.5/1000 lbs. This information was taken from Plant Design and Economics for Chemical Engineers by Peter and Timmerhaus. The data was adjusted for today's

date using the ratio of the Chemical Plant Indexes found in Chemical Engineering Magazine. Cost data for cooling water was provided by Erwin Utility Company and established at \$1.295/1,000 gallons.

The cost of the distillation tower is calculated using cost estimates taken from Chemical Engineering Magazine. Cost of the tower is estimated using

$$\text{Tower Cost} = C_b F_m + N_t C_{bt} F_{tm} F_{tt} F_{nt} + C_{PL} \quad (134)$$

where

$$C_b = \exp (6823 + 0.14178 \ln W_a + 0.02468 (1_n W_a)^2 + 0.0158 (L/Di) 1_n (T_b/T_p)). \quad (135)$$

The weight of the tower, W_2 , is

$$W_a = Di(L + -.8116 Di) T_3 \quad (136)$$

where

$$L = 1.5 N_t \quad (137)$$

$$T_a = 1/2 (T_p + T_w + T_g + T_c) \quad (138)$$

$$T_p = 15 Di / (0.855 - 18). \quad (139)$$

The thickness of the tower is calculated to allow for stress, corrosion and internal pressure. This was discussed in Section 2.4. The cost factors F_m and F_{tt} are listed in Tables 2.2 and 2.3.

Table 2.2
Tower Material of Construction Cost Factor

Material	Cost Factor, F_m
304 Stainless Steel	1.7
316 Stainless Steel	2.1
Monel 400	3.6
Inconel 600	3.9
Titianium	7.7

Table 2.3
Cost Factors for Tray Type

Tray Type	Cost Factor, F_{tt}
Valve Tray	1.00
Grid	0.80
Bubble Cap	1.59
Sieve Tray	0.85

Auxiliary tower costs are estimated using

$$C_{bt} = 278.38 \exp (0.1739 D_i) \quad (140)$$

$$F_{tm} = 1.489 + 0.0577 D_i \quad (141)$$

$$F_{nt} = 2.25 / (1.0414) N_t \quad (142)$$

$$C_{pl} = 151.85 D_i^{0.63316} L^{0.08016} \quad (143)$$

The cost estimation for both the reboiler and condenser were also adapted from information taken from Chemical Engineering Magazine.

These correlations are

$$\text{Heat Exchanger Cost} = \text{Base} (F_d + F_p) F_m (\text{CP Index 1984/CP Index 1969}) \quad (144)$$

where

$$\text{Base} = 623.8 + 11.27 \text{ Area} \quad (145)$$

and the area is estimated as described in Section 2.6. The cost factors for the heat exchanger are listed in Tables 2.4 and 2.5. The additional cost for piping, insulation and instrumentation is estimated at 60% of the installed equipment cost. The sum of the tower, heat exchangers and auxiliaries is the fixed capital investment. The life of the investment is assumed to be 10 years. Each year of the equipment life is apportioned to the annual cost dependent upon the current ACRS rate.

Table 2.4
Cost Adjustment Factors

Design Type	Fd Design Pressure		Fp
Kettle, Reboiler	1.35	150 psi	1.0
Floating Head	1.00	300 psi	1.10
V Tube	0.85	400 psi	1.25
Fixed Tube Sheet	0.80	500 psi	1.52

Table 2.5
Cost Factor of Construction, F_m (Shell/Tube)

Surface Area	CS/CS	CS/Brass	CS/SS	SS/SS	Monel/Monel
100 Ft. ²	1.0	1.05	1.54	2.50	3.20
100 to 500 Ft. ²	1.0	1.10	1.78	3.10	3.50
500 to 1000 Ft. ²	1.0	1.15	2.25	3.28	3.65

3.0 PROGRAM DEVELOPMENT

The program code was developed so that a personal computer could be used to design a distillation column, condenser and reboiler. Program development utilized an IBM Model PC-XT personal computer with 256K RAM running at 4.77 MHz. The IBM comes equipped with a Microsoft BASIC interpreter. This software, however, is limited to 60,891 bytes (59.4k) of available memory for programming. To eliminate this, Microsoft BASIC compiler software version 1.0 was used. In order to accomplish this goal, the design equations outlined in the general background section were developed into coherent subprograms that would later be combined through the program flow sheet (Figure 3.1) to form an operating program. As each subprogram was developed, it was tested for accuracy prior to integration into the main program. Since success of the column design depends upon the enthalpy and equilibrium information, the accuracy of these subprograms is especially important. For the reboiler and condenser, physical properties of the liquid and vapor mixtures were important for design accuracy.

After each section had been tested, the overall program was compiled and tested. Testing utilized several different binary systems, in particular benzene-toluene, ethanol-water, methanol-water and finally n-propanol-water. The behavior of these systems varied from the ideal behavior of benzene-toluene, to the n-propanol-water system which exhibits extremely non-ideal enthalpy behavior. After the

various systems were tested, the results were compared with previous work, or where available, existing column performance.

3.1 Program Flow Sheet

The program development was split into three main areas of concern: data input and initialization, minimum reflux calculation, optimum reflux or total stage calculation. The program is described in more detail below.

Data is input to the program interactively through the terminal. Initial data specifically relates to column parameters of pressure, components, feed rate, feed concentration and quality, distillate concentration and bottoms concentration. If the components chosen are not listed among the seven available in the program (water, methanol, ethanol, n-propanol, acetone, benzene, and toluene), then the additional physical property data must be input. This data includes unifac molecular volume, area, and interaction parameters, critical properties of temperature, volume and compressibility, molecular weight, boiling point temperature, Antoine constants and five constants for heat capacity calculation.

After data is input, the program proceeds to the minimum reflux calculation. Minimum reflux is modeled by a tie line from the equilibrium interaction passing through the feedpoint. The subprograms locate the tie line by comparing the feed point to the saturated vapor points. When all three of these points lie along a straight line, as determined by the slope of the line between the points, then the tie line has been found. When the slopes of the lines are not equal, the

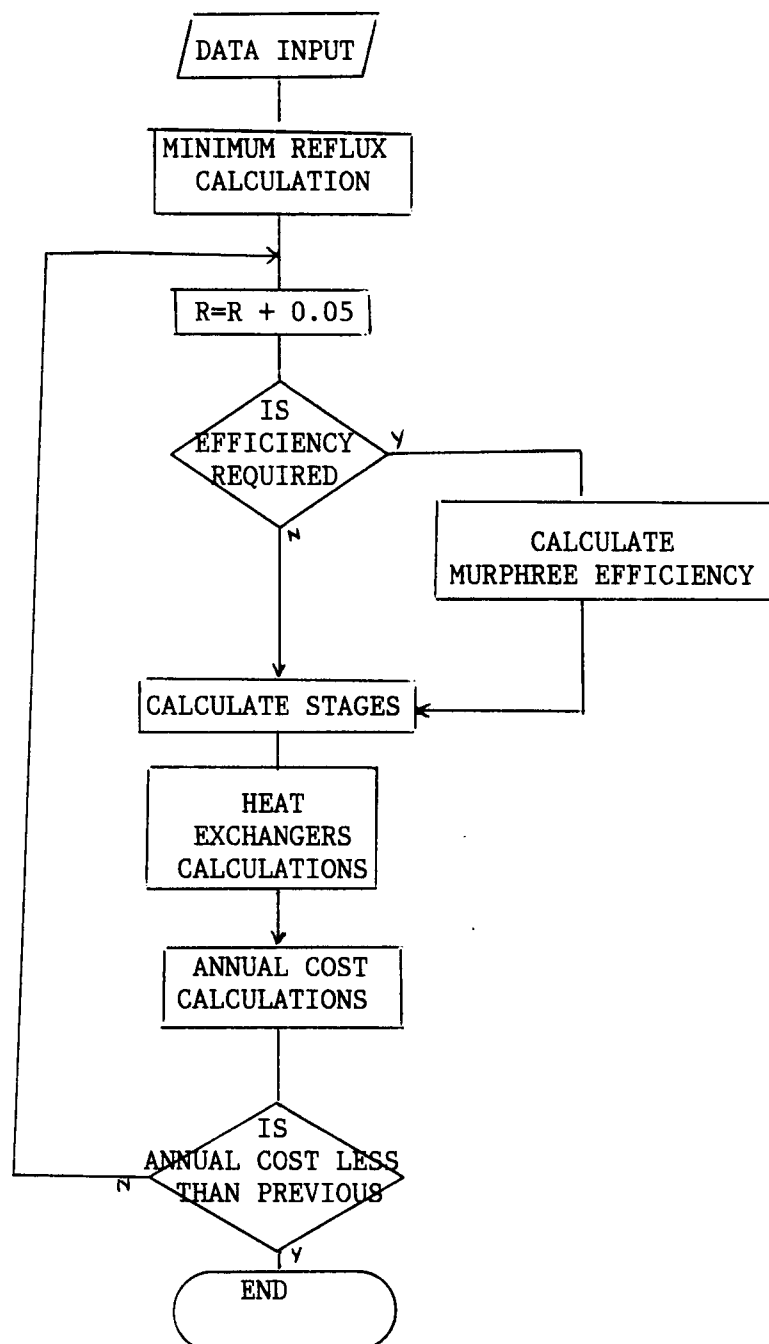


Figure 3.1. Program Flow Sheet.

program adjusts the saturated liquid concentration and repeats the procedure (see Figures 3.2, 3.3, and 3.4). After the slope of the tie line is computed, the intercept with the X axis is found. The intercept and slope are used in calculating the difference points ΔD and ΔB . These points are located at the intersection of the tie line with XB. Next, the enthalpy of the saturated vapor at XD is calculated and finally the minimum reflux is calculated from the relationship

$$R_{\min} = (Q_{\text{DIST}} - HV \text{ at XD}) / (HV \text{ at XD} - HL \text{ at XD})$$

Following the calculation of $r_{\min}$ the program starts the stage-by-stage calculation for tower design. The user must decide for a set reflux rate or for optimum reflux. For the optimum reflux calculation the reflux rate is increased above the minimum amount and then the tower and heat exchangers are sized and costed. The annual cost is calculated and the reflux rate is increased again. This pattern is repeated until the lowest annual cost of the tower system is found. Column design for a set reflux rate is accomplished by bypassing the optimum reflux calculation.

The first part of the stage-by-stage calculations begins with the enriching section. The enriching section calculation determines the number of trays in this section as well as the liquid and vapor flows and concentrations at each tray. To accomplish this the equilibrium relationship is used to determine when the liquid concentration is in equilibrium with the vapor leaving that tray. Different values of vapor concentration are then tested to find the point that will lie on

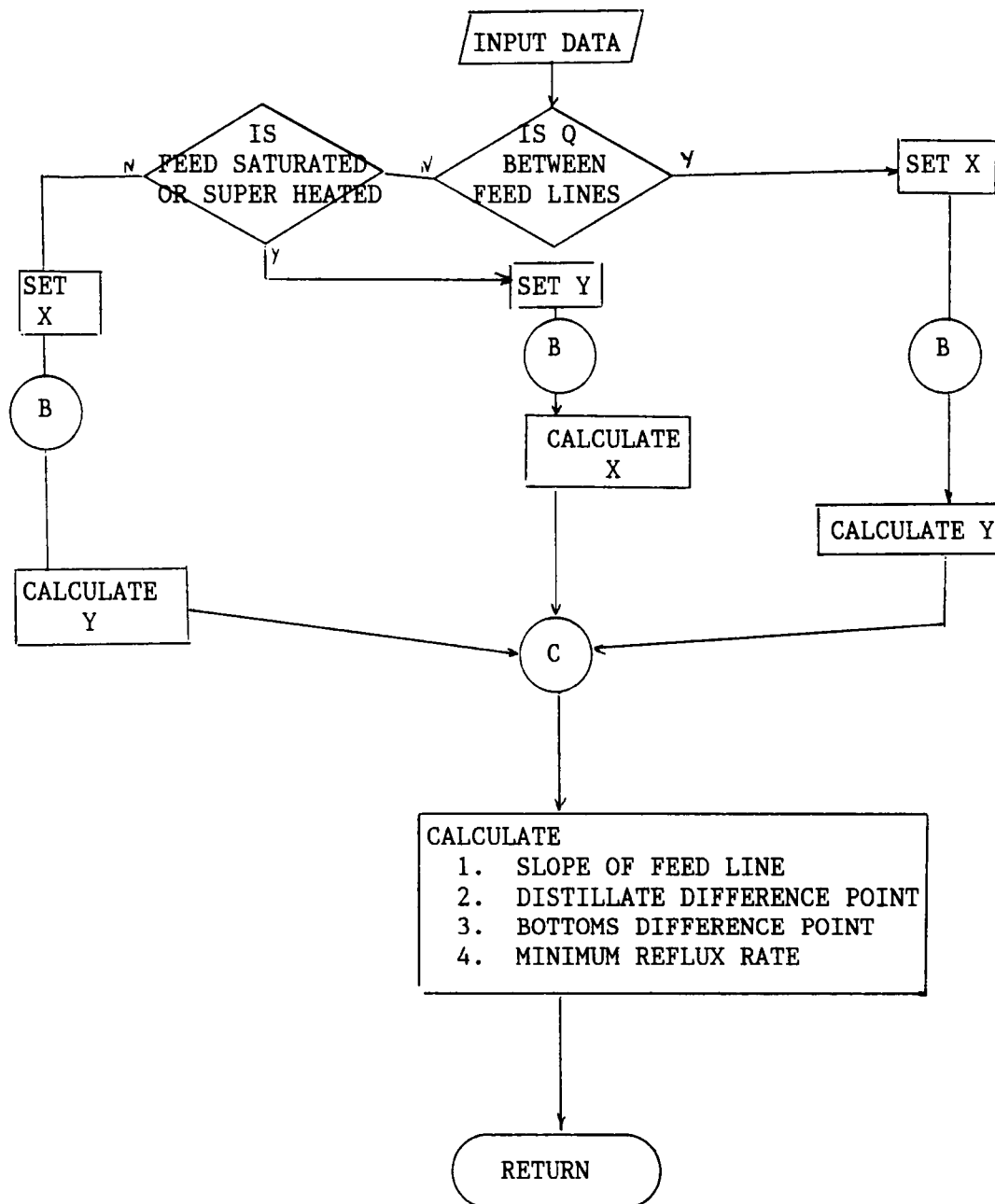


Figure 3.2. Minimum Reflux Flow Sheet.

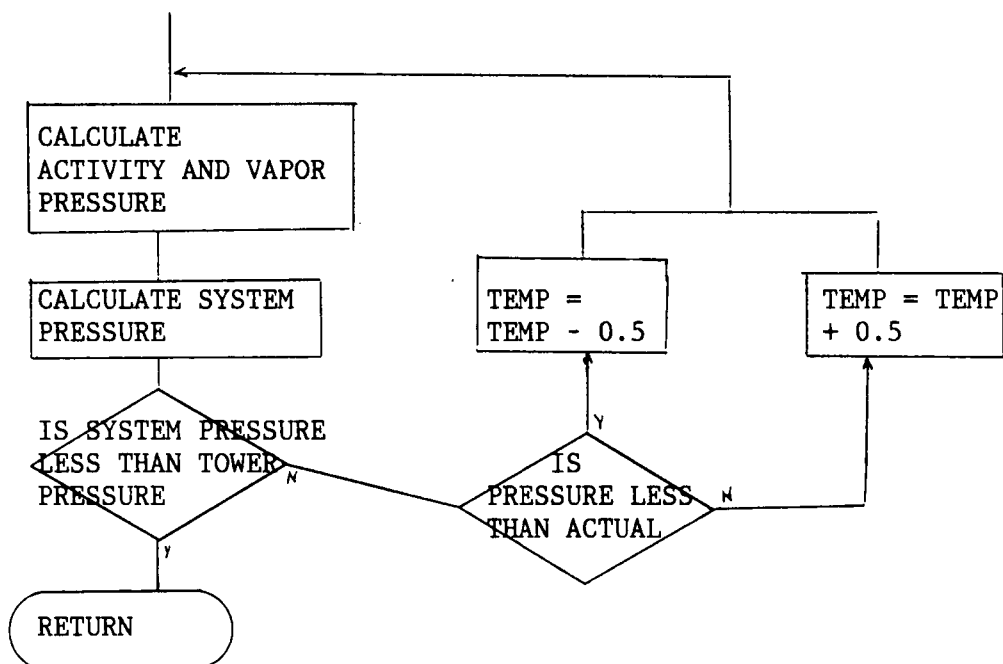


Figure 3.3. Temperature Correction. Loop B.

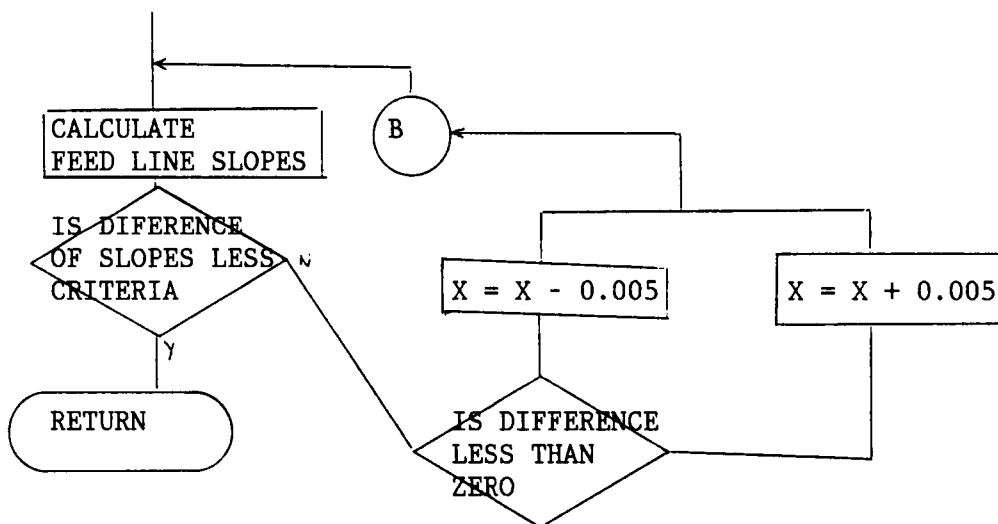


Figure 3.4. Slope Test. Loop C.

a straight line with the distillate difference point, ΔD , which is a function of the reflux rate, and the liquid and vapor concentrations. This determines the vapor concentration entering the tray. The equilibrium relationship determines the concentration of the liquid leaving the tray. The liquid flow rate entering from the tray above and the vapor flow entering from the tray below are then calculated. This procedure is repeated until the concentration of a liquid stream leaving the tray is less than the saturated liquid enthalpy curve. (See Figure 3.5).

All of the subprogram listed so far are dependent upon the temperature correction loop (Figure 3.3). This loop centers on the equilibrium relationship

$$Y_i \phi_{iv} P = X_i \gamma_{il} P^{lsat}$$

By assuming that the vapor phase activity coefficient, ϕ_{iv} , is equal to 1.0, this relationship is simplified to

$$Y_i P = X_i \gamma_{il} P^{sat}$$

For two binary components,

$$Y_i P + Y_j P = X_i \gamma_{il} P^{sat}_i + X_j \gamma_{jl} P^{sat}_j$$

The program loop then varies the temperature until the sum of the partial pressures above equals the system pressure.

The stripping section functions slightly different from the enriching section (see Figures 3.5 and 3.6). In the stripping section,

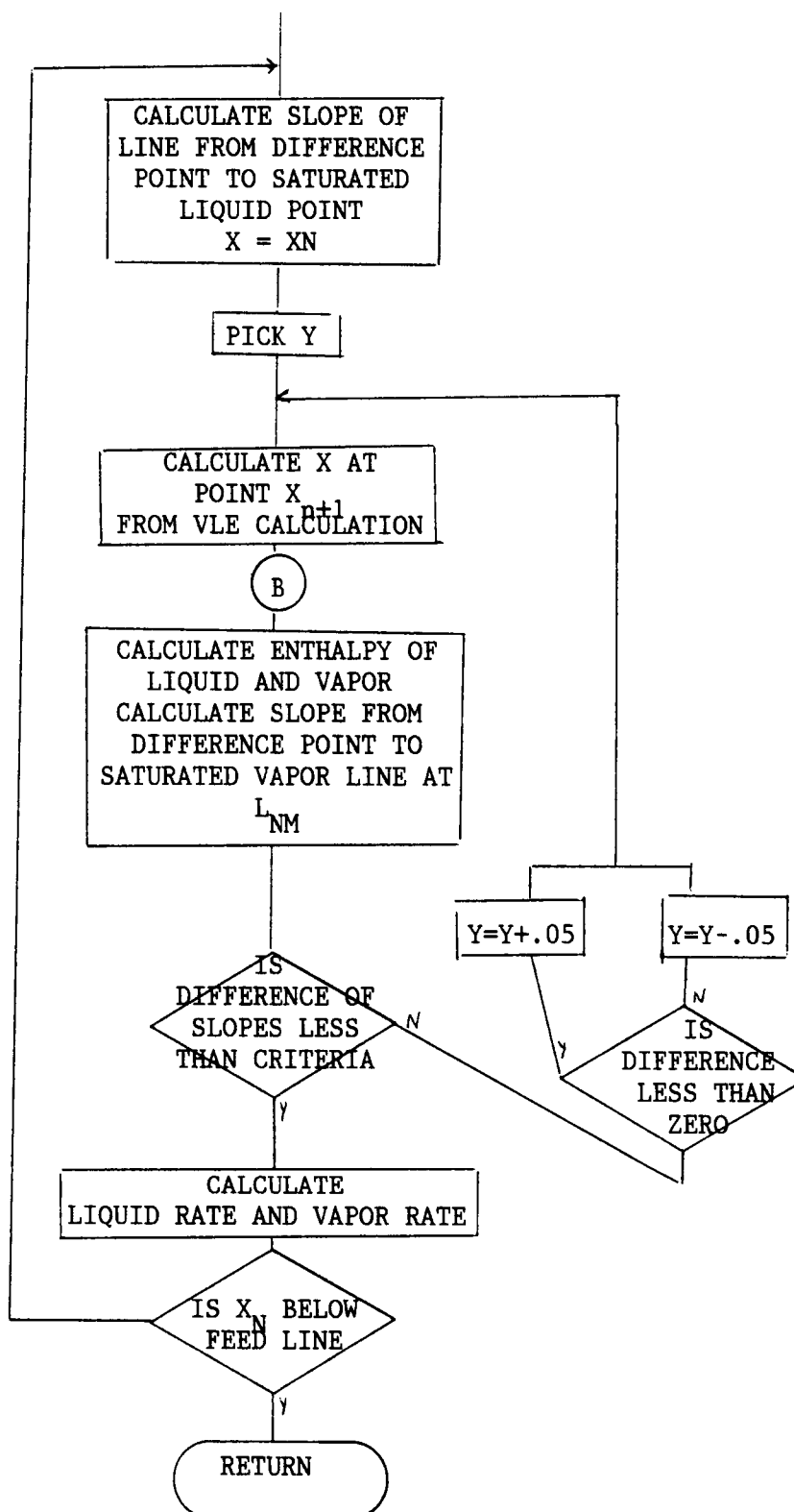


Figure 3.5. Enriching Section Flow Sheet.

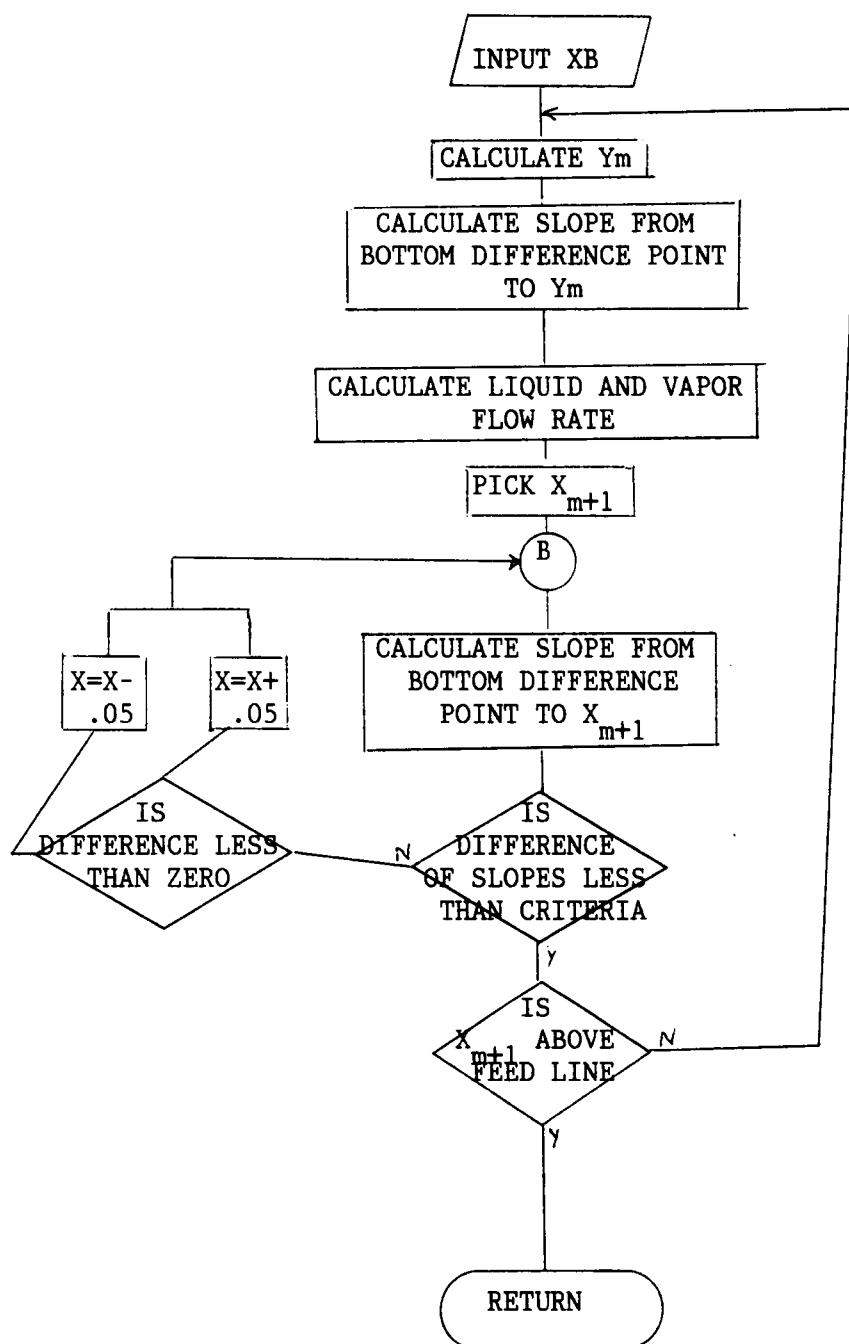


Figure 3.6. Stripping Section Flow Sheet.

the equilibrium relationship is used to calculate the concentration of the vapor leaving a tray from the concentration of liquid leaving the tray. This information is used to calculate the respective liquid and vapor flows. Then the intersection of the line from the bottom differences point, ΔB , to the saturated vapor curve at the saturated liquid curve is found. This is done by varying the liquid concentration until the slope of the line from the saturated liquid curve to the difference point is equal to the slope from the saturated vapor curve to the difference point. The intersection point on the saturated liquid curve determines the concentration of the liquid stream entering the tray. The equilibrium relationship then determines the vapor concentration leaving the tray. This procedure is repeated until the liquid concentration entering a tray is greater than the concentration of the liquid at the point where the tie line crosses the saturated liquid enthalpy line.

The heat exchanger calculations (see Figures 3.7 and 3.8) follow in straightforward manner. From the input information the Reynolds number and Prandlt numbers are calculated for the heating or cooling sides and the process side. From the heat balances, the inlet and outlet stream temperatures are determined and the log temperature difference for the exchanger is calculated. The temperature at the wall and the bulk temperature of the process fluid is found. Then the film temperature T_f , defined as $TF = THI - .75 (THI - T_{wall})$ is determined. With this information, the inside and outside tube individual heat transfer coefficients are calculated. An overall heat

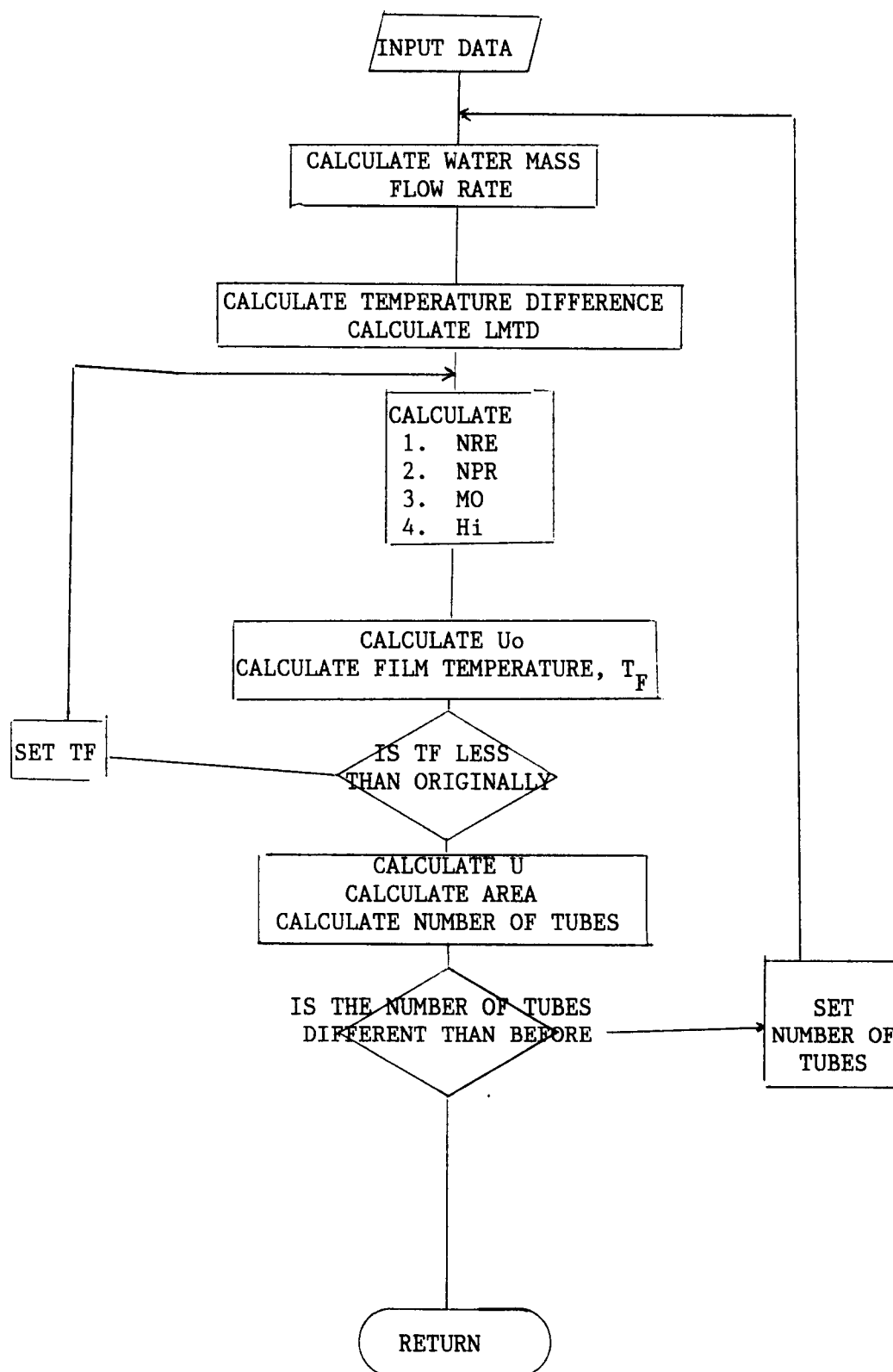


Figure 3.7. Heat Exchanger Flow Sheet (Condenser).

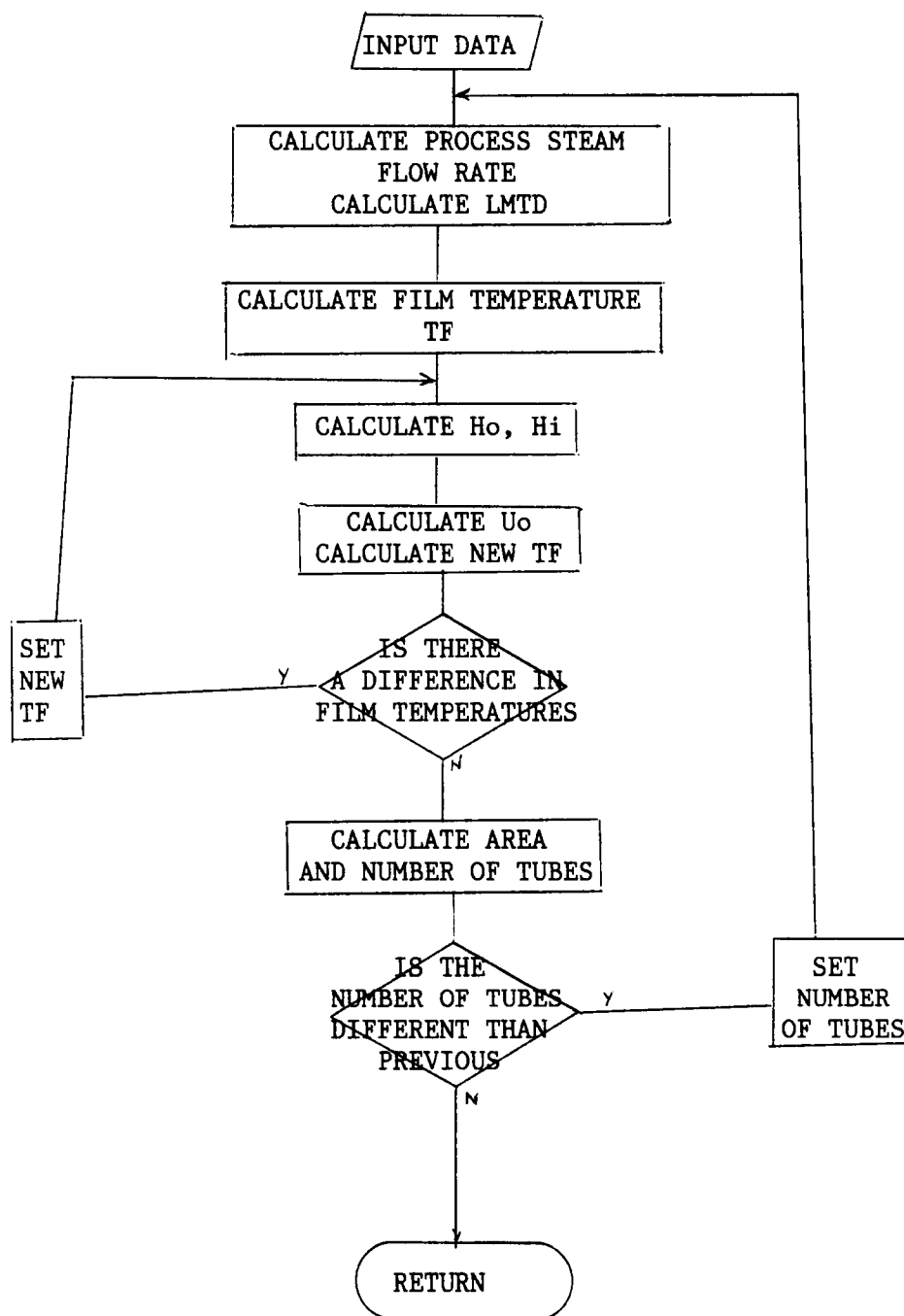


Figure 3.8. Heat Exchanger Flow Sheet (Reboiler).

transfer coefficient is then calculated. The water or steam side resistance and the process side resistance are found, and a new ΔT is estimated. From ΔT the wall temperature is then compared with the original and if they are less than 5°F then the calculation continues. If the temperature difference is greater than 5°F , then the calculations are repeated starting from the individual heat transfer coefficient calculation. When the temperature difference is less than 5°C the calculation for the heat exchanger area and number of tubes is conducted. If the number of tubes is the same as originally specified, then the exchanger has been sized. If the number of tubes is different, then the number of tubes is adjusted and the entire calculation series is repeated starting with the recalculation of the Reynolds number. All calculations are now complete.

3.2 Subprogram Testing

To assure that the overall program functioned properly, the enthalpy, unifac, and physical property subroutines were tested for accuracy. This was accomplished by isolating these routines from the main program and varying the concentration of the saturated liquid from 0 to 1.

The temperature correction feature is integral to the entire procedure as all of the calculations are temperature dependent. As the concentration is changed, the temperature at this concentration is found. The unifac routine then calculates the liquid phase activity and the vapor concentration in equilibrium with the liquid by the relationship $Y_i = X_i \gamma_i p^s / p$. After the vapor concentration is found

both the liquid and vapor enthalpies are calculated. Following enthalpy calculation the physical properties (thermal conductivity, density, and viscosity) are calculated for both saturated liquid and vapor streams.

3.3 Test Case Description

The main program was tested by imposing varying operating conditions for different binary systems. Initially the system was tested with the benzene-toluene system. The feed condition, feed composition, bottoms composition and distillate composition were varied to correspond with examples in Peters and Timmerhaus⁽¹⁷⁾ and in McCabe and Smith⁽¹⁵⁾. After benzene-toluene system was used to validate the program, code addition checking was done with increasingly non-ideal binary systems. First an example using the methanol-water binary system from Treybal⁽²²⁾ was used. Two additional cases using ethanol-water and n-propanol-water binary systems were attempted. The details of the test cases are listed in Table 3.1.

Table 3.1

Test Cases

Binary System	Feed Condition	Feed Composition	Feed Rate(lbm/hr)	Distillate Composition	Bottoms Composition	Reflux Rate
1. Benzene/Toluene	1.000	0.44	350	0.974	0.0235	3.5
2. Benzene/Toluene	1.365	0.44	350	0.974	0.0235	3.5
3. Benzene/Toluene	0.330	0.44	350	0.974	0.0235	3.5
4. Benzene/Toluene	1.000	0.45	700	0.920	0.0500	*1
5. Methanol/Water	1.040	0.36	98.6	0.915	0.00565	*2
6. Ethanol/Water	1.000	0.30	100	0.700	0.0240	*1
7. n-Propanol/Water	1.000	0.20	100	0.420	0.0500	*1

*1 Rate set at 1.5 times minimum reflux rate.

*2 Rate set at optimum reflux rate.

4.0 RESULTS AND DISCUSSION

The main objective of this work was to develop a computer code that would design a distillation column on a personal computer with 256K of RAM. The code was written for the BASIC computer language. Due to the amount of memory required for the code (~70K) the buffer space allocated for use with the IBM BASIC (59K) was insufficient to operate the code. It was necessary to divide the program into several parts and then use Microsoft's Quickbasic 1.0 compiler to link the parts together. When compiled, the program required between 1 1/2 and 2 hours of operating time to execute.

Evaluation of the accuracy of the program required testing with several different operating conditions. The test cases used in this work are described in Table 3.1. The results, page 62, for the benzene-toluene and methanol-water binary systems were within 6% of the results obtained by Summers⁽²¹⁾ and Manzoor⁽¹³⁾. However, the accuracy of the program deteriorated when highly non-ideal systems (ethanol-water and n-propanol-water) were tested. The calculation of number of stages deviated by 58.3% when the ethanol-water system was tested. No result was obtained with n-propanol when the minimum reflux rate estimated was negative!

To determine why the program failed for the non-ideal systems, equilibrium data were developed and compared with experimental results (see Tables 4.1 through 4.4). The average deviation was 4.2% for the

Table 4.1
Equilibrium Data for the Benzene-Toluene System^a

<u>X</u>	YCALCULATED	Y EXPERIMENTAL	% ERROR
0.1	0.203	0.21	3.3
0.2	0.369	0.372	0.8
0.3	0.505	0.51	1.0
0.4	0.618	0.62	0.3
0.5	0.712	0.72	1.1
0.6	0.79	0.79	0.0
0.7	0.857	0.85	0.8
0.8	0.911	0.91	0.1
0.9	.96	0.96	0.0
Average deviation 0.8%			

^aData Source (Kojima and Tochngi, 1979)

Table 4.2
Equilibrium Data for the Methanol-Water System^a

<u>X</u>	YCALCULATED	Y EXPERIMENTAL	% ERROR
0.1	0.432	0.418	3.3
0.2	0.538	0.579	1.7
0.3	0.678	0.665	1.9
0.4	0.743	0.729	1.7
0.5	0.194	0.779	1.9
0.6	0.839	0.825	1.7
0.7	0.881	0.870	1.3
0.8	0.923	0.915	0.8
0.9	0.969	0.958	0.2
Average deviation 1.6			
Average deviation using experimental temperature 0.6%			

^aData Source (Perry's Handbook, 4th Ed., 1963)

Table 4.3
Equilibrium Data for the Ethanol-Water System^a

$\underline{X}$	Y _{CALCULATED}	Y _{EXPERIMENTAL}	% ERROR
.019	0.246	0.170	44.7
.072	0.478	0.389	22.8
.097	0.521	0.438	18.9
.124	0.552	0.470	17.4
.166	0.555	0.500	14.9
.234	0.615	0.545	13.4
.261	0.618	0.558	12.7
.327	0.655	0.583	12.3
.397	0.684	0.612	11.2
.508	0.725	0.656	10.5
.520	0.739	0.660	10.5
.573	0.753	0.684	10
.676	0.804	0.739	8.4
.747	0.836	0.782	6.9
.894	0.921	0.894	3.0

Average deviation 14.5%
Average deviation using experimental temperature 4.4%

^aData Source (Jones et al., 1943)

Table 4.4
Equilibrium Data for the n-Propanol-Water System^a

<u>X</u>	Y _{CALCULATED}	Y _{EXPERIMENTAL}	% ERROR
0.003	0.069	0.071	-2.8
0.013	0.226	0.215	5.1
0.072	0.455	0.375	21.3
0.139	0.488	0.393	24.2
0.275	0.503	0.407	23.6
0.327	0.511	0.415	23.1
0.396	0.527	0.421	25.2
0.515	0.569	0.456	24.7
0.721	0.683	0.561	21.7
0.766	0.716	0.596	20.1
0.867	0.810	0.710	14.1
0.913	0.864	0.785	10.1
0.955	0.921	0.878	5.4
Average deviation 17.0%			
Average deviation using experimental temperature 4.5%			

^aData Source (Morti and Van Winkle, 1958)

ideal benzene-toluene system and 1.6% for the slightly non-ideal methanol-water system. However, equilibrium estimates for the other two binary systems resulted in 14.5% and 17% average deviation for ethanol-water and n-propanol-water, respectively.

In order to determine if the deviations in stage calculations were the result of inaccurate equilibrium data or a combination of poor equilibrium and enthalpy data, the saturated liquid and vapor enthalpy data were estimated. The data were then compared with experimental data for benzene-toluene and methanol-water systems. The benzene system had a maximum deviation of less than 1% for the vapor enthalpy and less than 5% for the saturated liquid enthalpy. The methanol system had a maximum error of 1.5% for saturated vapor enthalpy and an average error of 19.8% for the saturated liquid. Results for both systems are described in Tables 4.5 through 4.7.

To evaluate the cause of the deviations between the predicted and experimental equilibrium data for the highly non-ideal systems, the method of estimation must be considered. At a given liquid concentration, the vapor phase in equilibrium with the liquid is estimated by $y_i = x_i \gamma_i P_i^S / P \phi_i$. Normally the vapor phase is assumed to behave ideally ($\phi=1.0$). Therefore only the vapor pressure, P_i^S and liquid activity coefficient, γ_i , need to be estimated. Since Antoine's equation accurately predicts vapor pressure at the temperature and pressure the column is operating, the deviation is most likely caused by the UNIFAC estimation of liquid phase activity. The three parameters (molecular area, molecular volume, and interaction) used by

Table 4.5

Comparison of Experimental and Calculated Vapor Enthalpies for the Benzene-Toluene System^a

X	HV ^{exp} (Btu/lbm)	HV Ideal Method (Btu/lbm)	HV SRK Method (Btu/lbm)	HV Yen Alex. (Btu/lbm)	% Error Ideal Method	% Error SRK Method	% Error Yen-Alex.
.1	21465	21500	21493	21580	0.16	-0.13	1.0
.2	21095	21079	21073	21246	-0.070	-0.10	.72
.3	20725	20698	20682	20858	0.13	-0.16	.64
.4	20355	20333	20327	20488	-0.110	-0.14	.76
.5	19980	19973	19967	20124	0.04	-0.07	.72
.6	19610	19616	19610	19765	0.03	0	.79
.7	18865	18877	18872	18706	0.05	0.02	.82
.8	18865	18877	18872	18706	0.06	0.04	.84
.9	18500	18503	18498	18515	0.02	0.01	.08
Average Deviation					+0.03%	-0.06%	0.71%

^aData Source (Henley and Seady, 1981)

Table 4.6

Comparison of Experimental and Calculated Liquid Enthalpies for the Benzene-Toluene System^a

X	HL Experimental (Btu/lbm)	HL Heat of Solution (Btu/lbm)	HL Yen Alex. (Btu/lbm)	HL Antoine Coef. (Btu/lbm)	% Error Heat of Solution	% Error Yen-Alexander	% Error Antoine Coef.
.1	7620	6483	7702	7287	-14.9	1.1	-4.3
.2	7180	5966	7319	7015	-16.9	1.9	-2.3
.3	6785	5576	6911	6756	-17.8	1.9	-0.4
.4	6460	5265	6481	6497	-18.5	-0.3	0.6
.5	6165	5007	6034	6235	-18.8	-2.1	1.1
.6	5890	4786	5571	5967	-18.7	-5.4	1.3
.7	5630	4586	5097	5692	-18.5	-9.5	1.1
.8	5380	4402	7846	5409	-18.2	45.8	0.5
.9	5135	4236	7424	5117	-17.5	44.	0.3
	Average Deviation				-17.8%	8.6	-0.23%

^aData Source (Henley Seady, 1981)

Table 4.7

Comparison of Experimental and Calculated Liquid and Vapor Enthalpies for the Methanol-Water System^a

X	HV ϕ_{HP} (Btu/lbm)	HL ϕ_{HP} (Btu/lbm)	HL Yen-Alex. Method (Btu/lbm)	HL Antoine Coef. (Btu/lbm)	% Error HV	% Error HL
0.1	20,340	2950	20641	3584	1.5	21.5
0.2	20,000	2760	20171	3511	0.9	27.2
0.3	19,640	2620	19754	3319	0.6	26.7
0.4	19,310	2540	19356	3072	0.2	20.9
0.5	18,970	2470	18970	2793	0	13.1
0.6	18,650	2410	18595	2491	-0.3	3.4
0.7	18,310	2370	18215	2178	-0.5	8.1
0.8	17,980	2330	17841	1851	-0.8	20.6
0.9	17,680	2290	17602	1516	-0.4	33.8
Average Deviation					0.6%	19.5%

^aData Source (Henley and Seady, 1981)

UNIFAC are not sufficient to accurately predict activity for highly non-ideal azeotropic systems. The deviation in the VLE data is also reflected in the estimation of bubble point temperature. Bubble point temperature is estimated by calculating the sum of the partial pressures of the binary components. When the sum of the partial pressure equals the system pressure, the bubble point temperature has been estimated. When the saturation temperature from the experimental data was substituted for the calculated bubble point temperature, the error in the VLE data was reduced from 17% to 4.5% for n-propanol-water and from 14.5% to 4.4% for ethanol-water.

The saturated vapor enthalpy data was estimated using three different methods: Ideal, Soave-Redlich-Kwong, and Yen-Alexander Departure functions. For the two systems tested the saturated vapor enthalpy could be estimated by any of the methods with relatively little deviation. The best results, however, were obtained using the Yen-Alexander Departure functions. For the saturated liquid enthalpy the best results were obtained by the ideal enthalpy method using Antoine's Coefficients. The benzene system had an average deviation of 2.3% while the methanol system deviation was 19.8%. While this constitutes a large percentage deviation, the absolute value of the deviation (~ 400 Btu/lbm) is small compared to the vapor enthalpy (17,600-20,600 Btu/lbm). The deviation is also consistent and parallels the experimental saturated liquid enthalpy curve. Considering the excellent equilibrium and stage results obtained with

the methanol system and the considerably higher deviation in liquid enthalpy estimation, the deviation must not be very significant.

Table 4.8

Comparison of Previous and Calculated Column Design Data^a

Test Case	Calculated Minimum Reflux	Minimum ^m Reflux	% Error	Calculated Number of Stages	Number ^m of Stages	% Error
1	1.53	1.45	5.52	11	11	0
2	1.51	1.17	29.06	10	10	0
3	2.37	2.16	9.72	12	12	0
4	0.658	0.658	3	8	8	0
5	1.19	1.14	4.38	17	18	5.5
6	0.18	0.40	-55	5	12	58.3
7	-.21	.04	-62.5	N/A	4	N/A

N/A No stage calculation was conducted due to negative Rmin.

^aData source (Summer, 1986)

5.0 CONCLUSIONS AND RECOMMENDATIONS

The objective of this work was to develop a computer code that could be used to optimize the design of a distillation column on a personal computer with 256K RAM. This was accomplished for seven test cases (Table 3.1) ranging from ideal to non-ideal systems. The following conclusions have been made:

1. The distillation code gave results within 6% (e.g., theoretical number of stage for a specified separation) of previous results for the ideal benzene-toluene system and the moderately non-ideal methanol-water system. This validated the code for systems that are no more than moderately non-ideal.

2. The highly non-ideal systems of n-propanol-water and ethanol-water yielded results that were less than satisfactory. The deviation for minimum reflux and theoretical number of stages ranged from 55% to 62.5%. The principle reasons for these deviations were due to the prediction of VLE data as by UNIFAC. The data predicted by UNIFAC were not in agreement with experimental data (average deviation ranged from 14.5% to 17%).

3. For purposes of distillation design by the Ponchon-Savarit method, the UNIFAC method of estimating VLE and enthalpy data for highly non-ideal binary system appeared to be inadequate at this time.

4. Enthalpy calculations for the saturated vapor in moderately non-ideal systems were excellent using the Yen-Alexander departure functions (average deviation less than 0.71%). Best results with the

saturated liquid enthalpy estimation were obtained by ideal method with Antoine's coefficients (0.23% deviation for benzene-toluene and 19.8% with methanol-water.) While the methanol-water system deviation is large, the value is small compared to the value for saturated vapor enthalpy.

5. Although the run times (1.5 to 2.0 hours) were long, this is acceptable for a personal computer.

To improve the computer code, the following recommendations are suggested:

1. Replace the UNIFAC method with either the Wilson or the UNIQUAC method to improve the accuracy of liquid phase activity coefficients. This will improve the accuracy of the bubble point temperature and VLE prediction estimations.
2. Update the economic data (e.g., tax depreciation schedule, cost for steam and water service, Chemical Plant Indexes) to reflect current conditions.
3. Incorporate most of the required input data into a data base accessed by a component's name to simplify the user interface.

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