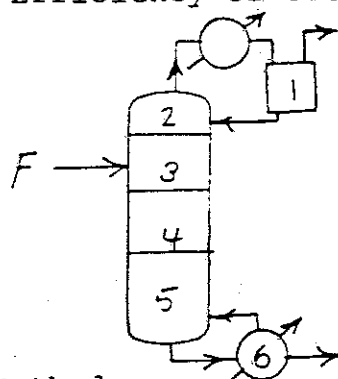


Example Problem 4: For the column shown below, construct
 A assuming that each stage operation with a Murphree
 Vapor Efficiency of 85%



A=

-1	1	.15	0	0	0
0	-1	.85	.15	0	0
0	0	-1	.85	0	0
0	0	0	-1	.15	.15
0	0	0	0	.85	.85
0	0	0	0	-1	-1

Short Cut Method

In order to use the previously presented matrix methods it is useful to have some means of estimating the number of stages to approximate a separation as a starting point for more rigorous calculations. The method presented here is as follows:

1. Determine the minimum reflux R_m by the Underwood equation
2. Determine the minimum number of plates P_m
3. Determine a real reflux ratio, R
4. Use Gilliland correlation to get the approximate plates using R , R_m and P_m .

Step 1. Determining minimum reflux R_m by the Underwood equation.

- a. Define a light and heavy key as the most and least volatile component present in appreciable amounts in both products.
- b. Define relative volatilities, α_j , based upon the heavy key component where

$$\alpha_j = K_j / K_{hk} \quad (47)$$

Total Reflux plus 1

Step 2. Determine the minimum number of trays¹, P_m , using
The Fenske equation

$$P_{m+1} = \frac{\ln \left[\left(\frac{X_{1k}^D}{X_{hk}^D} \right) \left(\frac{X_{hk}^B}{X_{1k}^B} \right) \right]}{\ln \alpha_{1k \text{ av}}} \quad (50)$$

where D = distillate

B = bottoms

$$\alpha_{1k \text{ av}} = \left(\alpha_{1k}^{\text{top}} \alpha_{1k}^{\text{bott}} \right)^{0.5}$$

Step 3. Estimate a realistic reflux ratio. Gilliland (1940)

Suggests 1.2 to 1.5 times the minimum reflux.

Step 4. Use Gilliland's Correlation (Figure 5) to estimate
an actual number of plates.

From Figure 5 a reflux ratio of 1.2 to 1.5 R_m corresponds
to $P - P_m / P + 1 = 0.4$ to 0.6. If 0.5 is taken as a nominal
value and if $P \gg 1$

$$\text{then } P - P_m / P = 0.5$$

or $P = 2P_m$ as a rough rule of thumb.

Example Problem 5. A column is fed a four component mixture

as shown below. The benzene in the distillate has a purity
specification of .9895 mole fraction. Give $q = 1.4$.

Assume the bottoms percentage of benzene is .000155 mole
fraction. Estimate the number of plates required for
the separation. Use Raoult's Law and

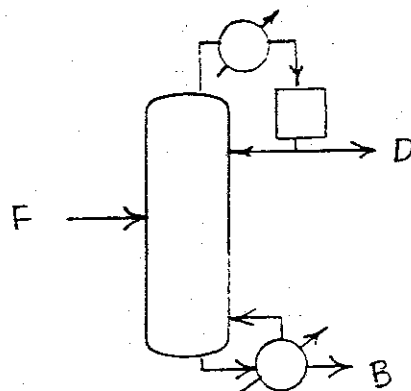
$$\log P^{\circ} = A - B / (t + C)$$

where

P° = vapor pressure, mm Hg

t = temperature, °C

Component	Feed Mole Fract.	Feed	A	B	C
78 1) C_6H_6	0.931	9.602	6.90565	1211.033	220.79
112 2) C_6H_5Cl (MCB)	.5631	58.08	6.94504	1413.12	216.0
146 3) $P-C_6H_4Cl_2$ (DCB)	.2292	23.638	6.89797	1507.3	201.0
4) $O-C_6H_4Cl_2$ (DCB)	.1146	11.819	6.92400	1538.3	200.0
		103.139			



$P = 15$ psia

Assume there is no DCB in the distillate. Then the light key = C_6H_6 and the heavy key = C_6H_5Cl

From purity specifications for the distillate and bottoms combined with a mass balance one can calculate for the distillate

$$\frac{(4.265)(9.602)}{4.265 - \phi} + \frac{1(58.08)}{1 - \phi} + \frac{0.2790(23.64)}{0.2790 - \phi} + \frac{0.2274(11.819)}{0.2274 - \phi} = 103.139 \quad (1-1.4)$$

Since there are no components between the light and heavy keys there is only one value of ϕ . Solving $\phi = 2.062$

$$\text{Using } \sum_{j=1}^{hk} \frac{\alpha_j X_j D^D}{\alpha_j - \phi} = D (R_m + 1) \quad (49)$$

$$\frac{4.265(.98954)(9.689)}{4.265 - 2.062} + \frac{1(.01046)(9.689)}{1 - 2.062} = 9.689 (R_m + 1)$$

$$R_m = 0.906$$

Step 2.	$K_{C_6H_6}$	K_{MCB}	α_{1k}
T			
81°C	1.007	.198	5.079
143°C	4.866	1.316	3.698

$$P_{m+1} = \frac{\ln \left[\left(\frac{.98954}{.01046} \right) \left(\frac{.620425}{.000155} \right) \right]}{\ln \left[(5.079)(3.698)^{0.5} \right]}$$

$$P_m = 7.759$$

$$\text{Step 3. } R = 1.5 \times R_m = 1.36$$

$$\text{Step 4. } \frac{R - R_m}{R + 1} = \frac{1.36 - 0.906}{2.36} = .1923$$

Table 7-2 Feed and products for depropanizer example (data from Edmister, 1948)

Component	mol %			mol/100 mol feed		α_i (rel. to C_3)
	Feed	Distillate	Bottoms	Distillate	Bottoms	
Methane (C_1)	26	43.5	26	10.00
Ethane (C_2)	9	15.0	9	2.47
Propane (C_3)	25	41.0	10	24.6	0.4	1.0
n-Butane (C_4)	17	0.5	41.7	0.3	16.7	0.49
n-Pentane (C_5)	11	27.4	11	0.21
n-Hexane (C_6)	12	29.9	12	0.10
	100	100	100	59.9	40.1	

326 SEPARATION PROCESSES

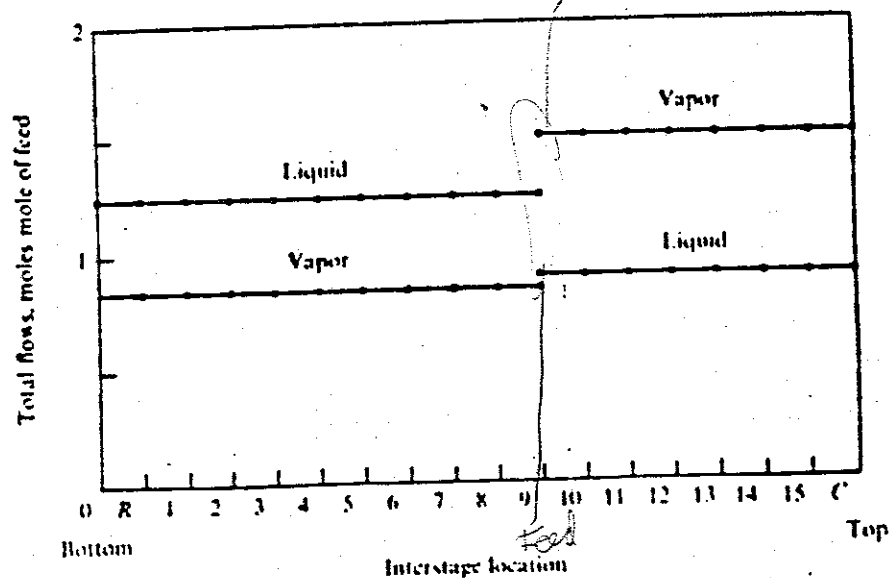


Figure 7-10 Total vapor and liquid flows in depropanizer. (Results from Edmister, 1948.)

PATTERNS OF CHANGE 331

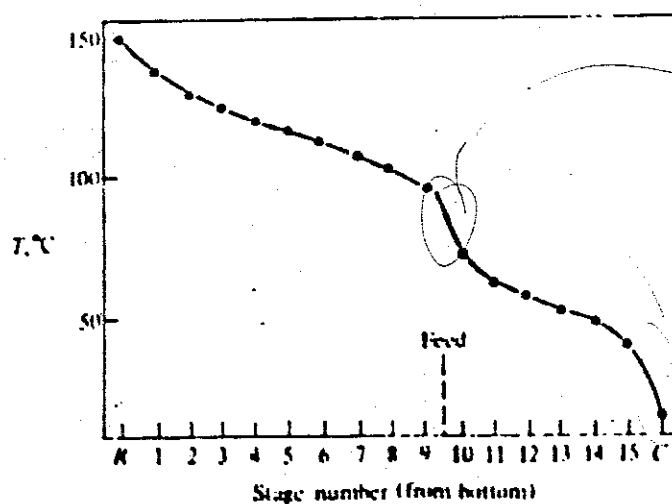


Figure 7-13 Temperature profile for depropanizer. (Results from Edmister, 1948.)

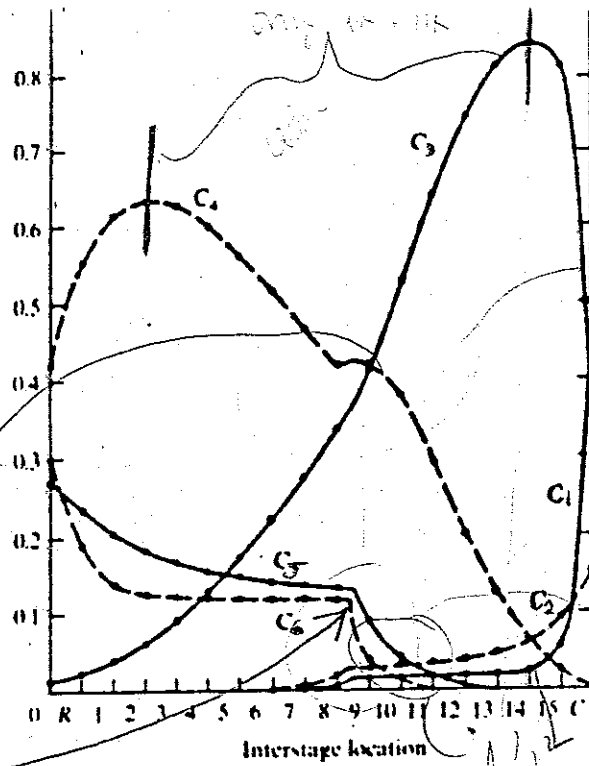


Figure 7-12 Liquid-composition profile in depropanizer. (Results from Edmister, 1948.)

HK vs. LK

Thru max corresponds to
 Since heavy key components are dropping rapidly a new max is in C₄
 keep not frac.

don't go to zero because of feed

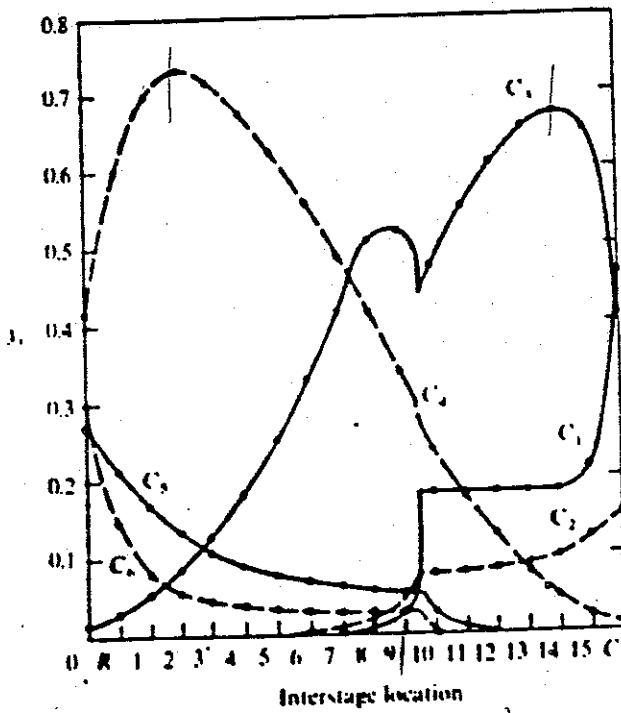
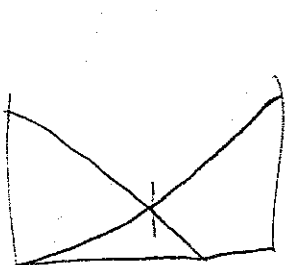


Figure 7-11 Vapor-composition profile in depropanizer. (Results from Edmister, 1948.)

Big temp changes
 Feed, top, Bottom

K_{av} find K values at different temperatures for



Steps to Calculating Multicomponent Distillation Constant Molar Overflow Case

One must first specify enough variables in a column to enable a single calculation to be made. If the results of the calculation are unsuitable, then one of the initial specifications may be changed to enable another calculation, with better results. Typically one might specify the following:

1. The feed flow rate, composition, and quality
2. The number of stages in the Column
3. The feed stage number
4. A distillate specification (e.g. D , x_{D1} , or one fractional distillate recovery [how much of one component in the feed goes to the distillate])
5. A reflux flow specification (e.g. L/D , \bar{V}/B , or Q_R)
6. An enthalpy specification for the reflux (e.g. bubble point liquid for D , or T_{reflux})
7. The operating pressure

With the above variables specified the solution to the column (temperatures and mol fractions of each component in each phase on each stage) may be calculated by the technique:

1. From the Column Specification and Mass Balances, determine the traffic (L, V, \bar{L}, \bar{V}) in the column
2. Determine a temperature at the top and the bottom of the column (e.g. by assuming a split of the feed and performing a bubble point calculation on the distillate and bottoms)
3. Linearly interpolate the temperature on each stage from the top and the bottom temperature. (We'll correct this assumption of temperature later in the calculation)
4. With the temperature and pressure on each stage, calculate the K_i value for each component on each stage (assuming the K_i is only a function of T and P)
5. Write a component mass balance on each stage in the column
6. Express each y_i in terms of x_i using $y_i = K_i x_i$.
7. At this point in the calculation for a given component you have one mass balance equation for each stage in the column. Fortunately the number of unknown (x_i values) also equal the number of stages. Simultaneously solve the set of equations for the x_i value on each stage.
8. Repeat Step 7 for each component in the column. At this point you have a value of x_i for each component on each stage. Also solve for y_i on each stages using $y_i = K_i x_i$.
9. Find some logical error function for each stage. For example one might use $\sum y_i = 1.0$, $\sum x_i = 1.0$, or $\sum y_i - \sum x_i = 0.0$ on each stage, where the summation is over all components.
10. Use the error function to determine a better temperature on each stage (see following method for T corrections)
11. With the better estimate of temperature on each stage, return to Step 4 and do the calculation again. Stop when the error function on each stage is within an acceptable tolerance.
12. At the conclusion of the calculation the compositions of each component on each stage in each phase and the temperature on each stage is obtained.

MULTICOMPONENT CONSTANT MOLAR OVERFLOW DISTILLATION

In the last chapter binary distillation was considered for the case of constant molal overflow. The binary CMAO case is a tool for determining as a qualitative basis how changes will affect the distillation process. For example, the effect of loss of cooling water to the condenser is easier to determine by considering the binary CMO case than by considering the multicomponent case with varying vapor and liquid flows in the column.

In industrial practice, however, binary distillation is seldom encountered and is regarded as a laboratory curiosity. The constant molar overflow assumption is still a good assumption in many cases due to the fact that similar substances are frequently distilled, such as the normal paraffins, isomers, or other substances whose vapor pressures do not vary widely. For this reason, the present chapter is concerned with the development of a (CMO) program for distillation.

In the initial portion of this chapter, a multicomponent CMO method is developed for a simple column. The method is then extended to encompass more complicated flows, even inter-connecting columns, in the next section. The third section

The approach to solving multicomponent CMO distillation problem is iterative and is normally done on a computer. For simplicity we assume K to be a function of T and P only in these calculations.

In this solution method, unlike the binary method of the previous chapter, one assumes that a column with a set number of theoretical stages is available, and the exiting product concentrations are calculated. If the exiting products do not meet specifications, the number of stages is changed until the desired product specifications are obtained. The steps in the approach to the problem are as follows:

1. Vapor and liquid flows are determined in each part of the column using overall mass balances as done in the previous chapter.
2. A temperature is guessed for each stage in the column.
3. For a given component the mass balance equation is written and K_i value is calculated for each stage in the column. The combined mass balances and K_i values are solved for the entire column for the components, resulting in the liquid mass fraction of that component on each stage.
4. Step 3 is repeated for each component until all of the liquid mole fractions on each stage have been determined.

For a single tray, j as shown in Figure 1b.

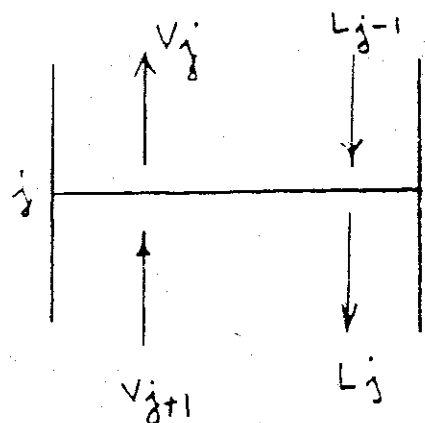


Figure 1b. Single Tray

By a Mass Balances on component i :

$$\underbrace{Y_{j+1} V_{j+1} + X_{j-1} L_{j-1}}_{\text{IN}} - \underbrace{Y_j V_j + X_j L_j}_{\text{OUT}} = 0 \quad \text{For all stages except feed stage} \quad (1)$$

$$Y_{F+1} V_{F+1} + X_{F-1} L_{F-1} - Y_F V_F - X_F L_F = -F X_{\text{in feed}} \quad \text{Feed Stage}$$

We can write a set of equations like (1) for the entire column for each component distilled. For each component, the set looks like the one below:

$$\left. \begin{array}{l} y_2 V_2 + \overbrace{X_0 L_0}^O - \overbrace{y_1 V_1}^D - X_1 L_1 = 0 \quad \text{Partial Condenser} \\ y_3 V_3 + X_1 L_1 - y_2 V_2 - X_2 L_2 = 0 \quad \text{Stage 2} \\ \vdots \\ y_{F+1} V_{F+1} + X_{F-1} L_{F-1} - y_F V_F - X_F L_F = -F X_{\text{in feed}} \quad \text{Feed Stage} \\ \vdots \\ y_N V_N + X_{N-2} L_{N-2} - y_{N-1} V_{N-1} - X_{N-1} L_{N-1} = 0 \quad \text{Stage N-1} \\ \underbrace{y_{N+1} V_{N+1} + X_{N-1} L_{N-1}}_0 - y_N V_N - \underbrace{X_N L_N}_B = 0 \quad \text{reboiler} \end{array} \right\} \quad (2)$$

This set of equations was obtained solely from mass balances (individual and total) and equilibrium relations with the known variables: F, x in feed, D and B and the unknown variables: all K 's and x 's.

Since we have N equations (1 for each stage) and $2N$ unknowns (K 's and x 's) we need to specify N unknowns. We do this by assuming that K 's are only a function of T and P . If we can guess a T on each stage, given the column pressure:

1. We can compute all the K values on each stage.
2. We can solve the equations for all x unknowns.
3. We can use the resulting x values to obtain better estimates of T 's on each stage, after the x 's are obtained for all components. Then $y_i = K_i x_i$
4. When $\sum_i y_i = 1.0$ on each stage, the problem is solved.

Solving for x Values

Once the T 's are guessed for each stage and the K values are calculated on each stage for component i we solve for x_i on each stage in the following manner

Rearranging Equations (7) we get

We may write equation (8) in matrix form as

$$\begin{bmatrix}
 B_1 & C_1 & 0 & 0 & \dots & 0 \\
 A_2 & B_2 & C_2 & 0 & 0 & \dots & 0 \\
 0 & \dots & A_F & B_F & C_F & 0 & 0 \\
 \vdots & & & & & & \\
 0 & 0 & 0 & \dots & A_{N-1} & B_{N-1} & C_{N-1} \\
 0 & 0 & 0 & 0 & \dots & A_N & B_N
 \end{bmatrix}
 \begin{bmatrix}
 x_1 \\
 x_2 \\
 \vdots \\
 x_F \\
 \vdots \\
 x_{N-1} \\
 x_N
 \end{bmatrix}
 =
 \begin{bmatrix}
 D_1 \\
 D_2 \\
 \vdots \\
 D_F \\
 \vdots \\
 D_{N-1} \\
 D_N
 \end{bmatrix}
 \quad (10)$$

This large matrix is called a tridiagonal matrix, because it only has B elements along the main diagonal and A and C elements along the adjacent diagonals; all other matrix elements are 0. This type of matrix has a very fast, efficient method of solution called the Thomas Algorithm as used by J.C. Wange and G.C. Henke (1966).

This involves the calculation of three different quantities (β_j and γ_j) for each row, going forward through the matrix

$$\beta_j = B_j - A_j C_{j-1} / \beta_{j-1} \text{ with } \beta_1 = B_1 \quad (11)$$

$$\text{and } \gamma_j = (D_j - A_j \gamma_{j-1}) / \beta_j \text{ with } \gamma_1 = D_1 / B_1 \quad (12)$$

Values of x_j are then obtained by working backwards up the rows:

$$x_N = \gamma_N \text{ and } x_j = \gamma_j - C_j x_{j+1} / \beta_j \quad (13)$$

$$\text{then } de/dT = - \sum_i x_i dK_i/dT \quad (16)$$

$$\text{It has been determined that } e = \sum_i x_i - \sum_i x_i K_i \quad (17)$$

works better than Eqn. (15). For the new temperature on each stage then

$$T_{v+1} = T_v - \frac{[\sum x_i - \sum x_i K_i]}{-\sum x_i dK_i/dT} \quad (18)$$

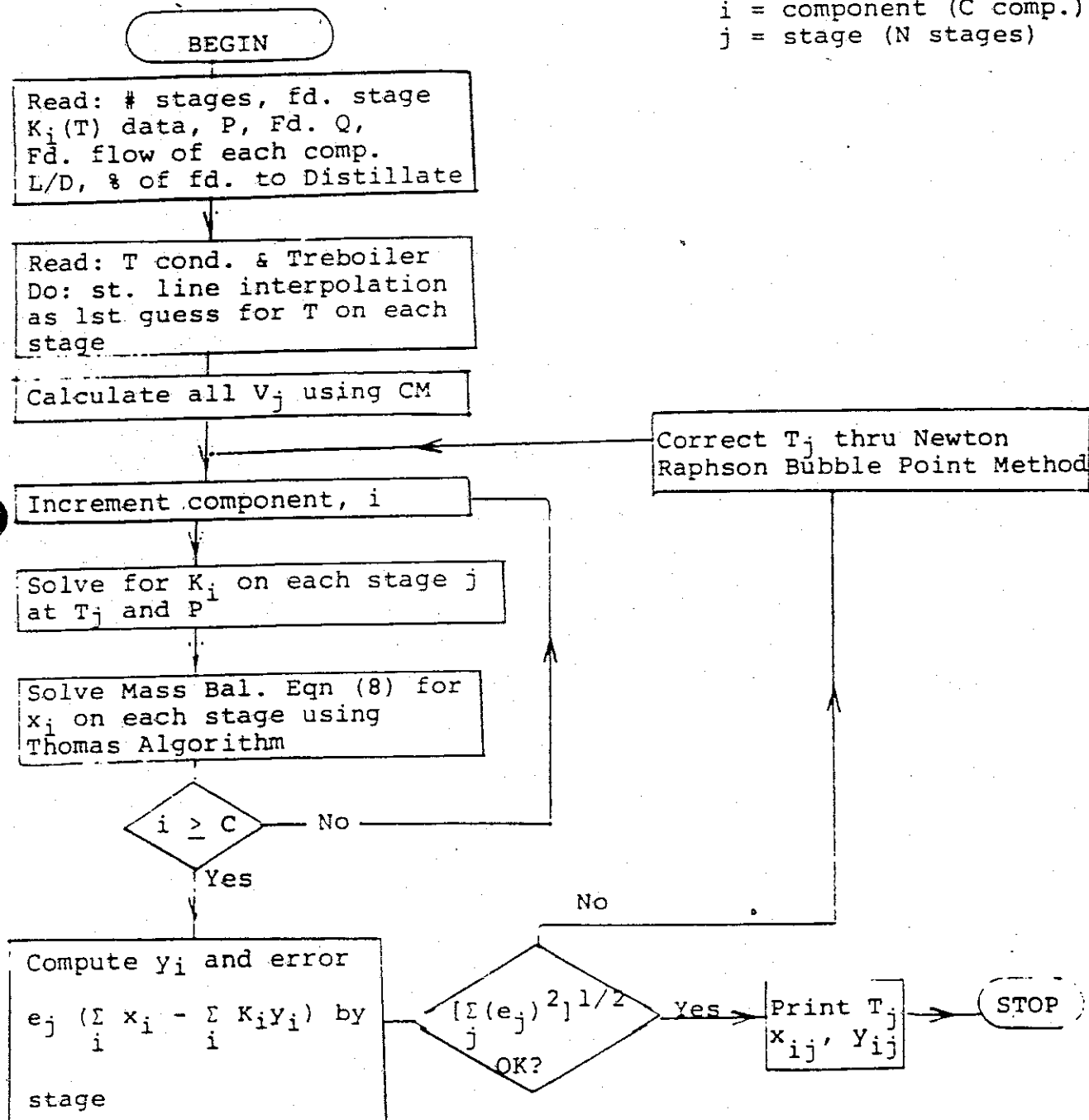
Note in equations (16) and (18) that the quantity dx_i/dT has been set equal to zero. This is not true and causes the Newton-Raphson scheme to give slower convergence than is normally obtained with Newton-Raphson schemes. The above derivative has been arbitrarily neglected for ease of computation, if the derivative was considered the matrices would no longer be tridiagonal and the rapid computer solution due to the Thomas Algorithm could no longer be employed. In the rigorous matrix solution of the next section, the derivative dx_i/dT is given full consideration.

A computer program may be constructed so that the temperature of each stage in the column is corrected at once. This is done using matrices as follows:

$$\begin{pmatrix} S \\ -v \end{pmatrix} (T_{v+1} - T_v) = -E_v \quad (19)$$

Figure 3. Algorithm for Constant Molal Overflow DistillationCalculation

i = component (C comp.)
 j = stage (N stages)



Step 1: Calculate vapor and liquid flows in the column assuming CMO.

$$V_1 = D_V = 100/5 = 20 \text{ lb moles}$$

$$L_1 = 2.25 \times 20 = 45 \text{ lb moles}$$

$$L_2 = 100 + 45 = 145 \text{ lb moles}$$

$$L_3 = F - D_V = 100 - 20 = 80 \text{ lb moles}$$

$$V_2 = V_3 = L_2 - B = 145 - 80 = 65 \text{ lb moles}$$

Step 2. Guess the middle stage temperature

$$T_2 = (T_1 + T_3)/2 = (175 + 250)/2 = 212.5^\circ\text{F}$$

Step 3. Write the mass balance equations for a given component on each stage, including the K_i values.

From equations (8)

$$\text{Condenser } (D_V - V_2 - K_1 D_V) x_1 + (K_2 V_2) x_2 = 0$$

$$\text{Feed } (V_2 - D) x_1 + (-L_3 - V_3 - K_2 V_2) x_F + (K_3 V_3) x_3 = -F x_{\text{Feed}}$$

$$\text{Reboiler } (V_3 + B) x_2 + (-L_3 - K_3 V_3) x_3 = 0$$

Step 4. Calculate coefficients for Thomas Algorithm for component 1 (ethane)

$$K_1 = 3.729$$

$$K_2 = 4.664$$

$$K_3 = 5.752$$

Step 7: Do Steps 4, 5, and 6 for n-C₄ and n-C₆.

The x's and y's from these calculations are given below.

Component	Stage →	Liquid Mole Fraction			Vapor Mole Fraction		
		1	2	3	1	2	3
↓ C ₂		0.118	0.04659	0.01488	0.4404	0.2173	0.0856
n - C ₄		0.7887	0.7899	0.7408	0.5372	0.7113	0.8504
n - C ₆		0.0519	0.1739	0.2483	0.00689	0.0381	0.0823

Step 8: Calculate errors on each stage and Euclidean norm

$$\text{from (22) } e_j = \sum x_i - \sum y_i$$

$$e_1 = -0.0258; e_2 = +0.0437; e_3 = -0.01432$$

$$\text{from (23) } \sigma = [\sum_j e_j^2]^{1/2}$$

$$\sigma = .05273$$

Step 9: Determine if σ is greater than convergence. σ is greater than our convergence criteria of 0.001.

Step 10: correct Temperatures using Newton-Raphson method

$$dK/dT = \beta + 2\gamma t + 3\delta t^2$$

Table of dK/dT values

Stage Comp. →	1	2	3
↓ 1	2.2819×10^{-2}	5.5371×10^{-3}	1.944×10^{-3}
2	2.702×10^{-2}	6.1937×10^{-3}	2.654×10^{-3}
3	3.0975×10^{-2}	7.0375×10^{-3}	3.348×10^{-3}

It is apparent from the preceeding example that the calculations are very tedious without a digital computer, and this becomes more apparent as the number of stages and the number of components are increased. Accordingly, a multi-component multistage computer program DISTIL.FOR is described and is presented on pages to . This program is written in compliance with the flow algorithm presented in Figure 3. As in all Newton-Raphson techniques, convergence is not guaranteed, especially when the initial guesses are far away from the true answer.