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A computer program for the optimization of binary distillation in a dual-column system

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A COMPUTER PROGRAM FOR THE OPTIMIZATION OF BINARY DISTILLATION IN A DUAL-COLUMN SYSTEM

BY

RICHARD VINCENT O'LENICK

A THESIS

PRESENTED IN PARTIAL FULFILLMENT OF

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ABSTRACT

A computer program is presented for the optimization of a two-column distillation system involving a two-component mixture. The economic reflux ratios in each column are determined using the McCabe-Thiele Method. Activity coefficients are computed by either the Wilson equation, the Margules equation, or both. The program is general and may be used for any binary system where the assumption of constant molal overflow is valid.

Options in the program permit use of either column in separate calculation schemes.

While the optimization effort was prepared in general terms, the initial work was directed toward the acetone-water system. Full data for this system are included in the program, but this specialty can be bypassed.

APPROVAL OF THESIS

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OPTIMIZATION OF BINARY DISTILLATION

IN A DUAL-COLUMN SYSTEM

BY

RICHARD VINCENT O'LENICK

FOR

DEPARTMENT OF CHEMICAL ENGINEERING

NEWARK COLLEGE OF ENGINEERING

BY

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APPROVED: _____

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NEWARK, NEW JERSEY

MAY, 1970

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MAY 1970 RICHARD O'LENICK

TABLE OF CONTENTS

LIST OF FIGURES

I INTRODUCTION

Distillation of binary mixtures is a common problem in chemical engineering. However, problems can arise when the more volatile component must be obtained at high purity levels. In the acetone-water system, for example, the shape of the vapor-liquid equilibrium curve is such that separations are very easy for modest purity levels, but the separation becomes very difficult for high-purity product. One possibility for such separations is the use of two columns in series. The problem then becomes one of coupling together two separate designs in the most advantageous way. This "most advantageous way" is open to many choices: minimum trays, equal trays in each column, proportioned external reflux conditions, minimum cost per pound of products, etc.

In this thesis this criterion will be economic minimization of cost per pound of product. This optimization is done by computer and the thesis work included development of the computer programs, development of suitable convergence procedures, development of cost criteria, development of options, and print-out forms so as to permit general use of the program with many binary systems. The systems that can be used must be reducible to McCabe-Thiele conditions.

The method of fictitious molecular weights proposed by Peters[14] is a procedure to extend the applicability of the McCabe-Thiele

method to systems where the assumption of constant molal overflow is invalid. This technique has not been included in the present work but should be kept in mind for future modification of the program.

The flow scheme understudy is shown in Figure 1. An example run is included in Appendix I. Appendix II contains a listing of the program. The flow chart for the program appears in Appendix III along with a dictionary of program variables.

FIGURE 1 SYSTEM FLOW DIAGRAM

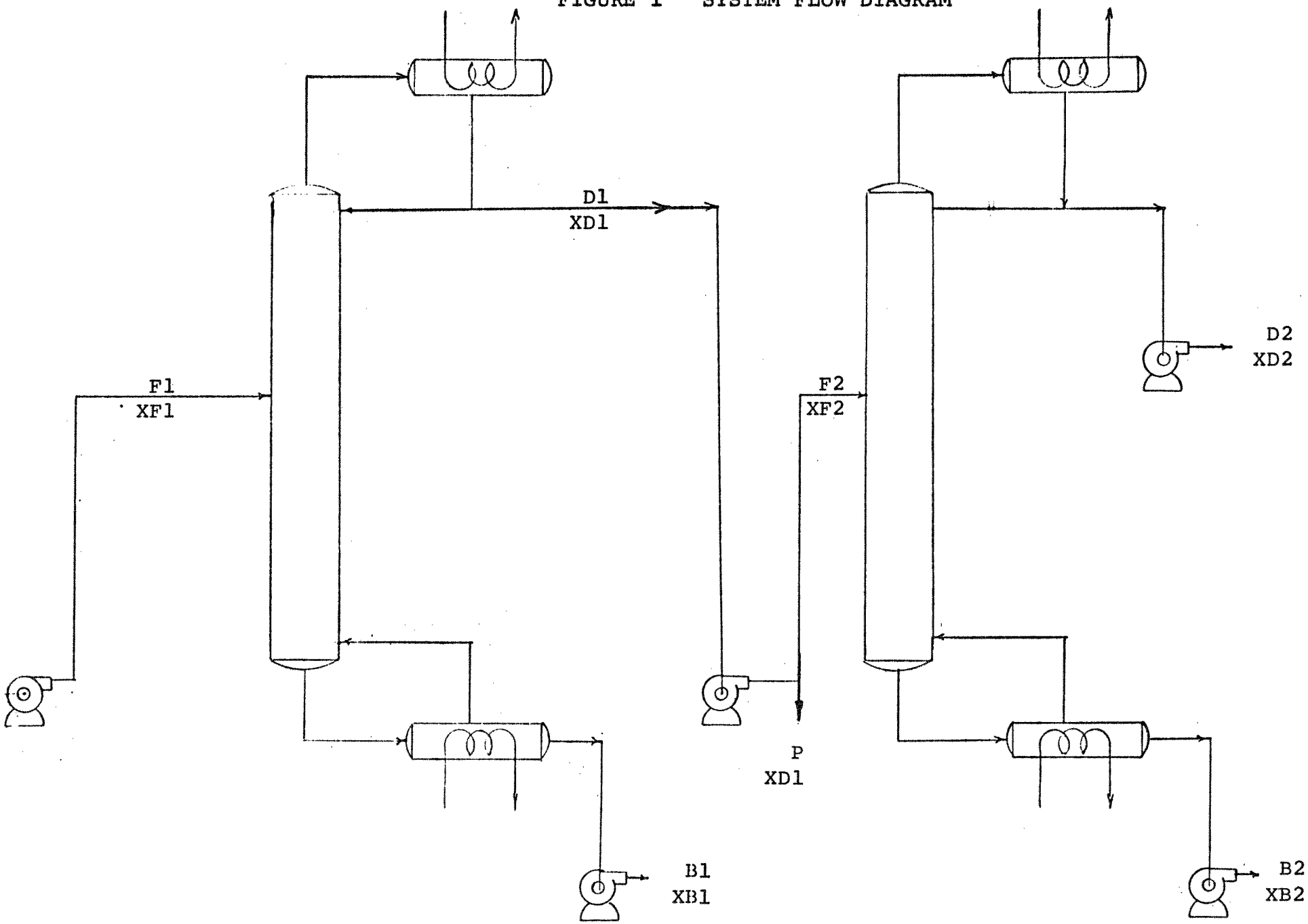
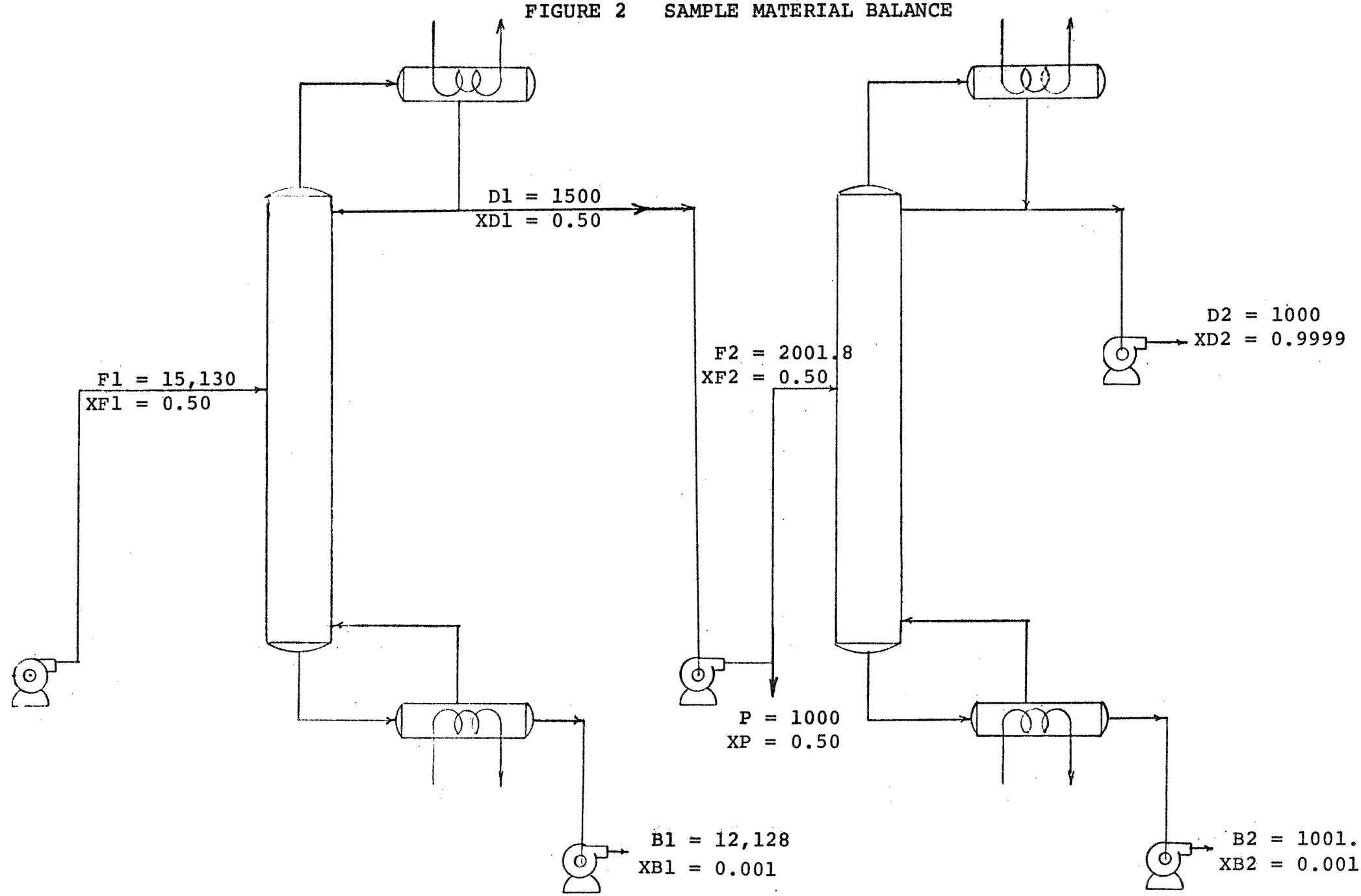


FIGURE 2 SAMPLE MATERIAL BALANCE



II THERMODYNAMIC RELATIONSHIPS FOR VAPOR-LIQUID EQUILIBRIA

The thermodynamic study of vapor-liquid equilibria has continued over many years. The aim of these studies was to predict vapor-liquid equilibria from minimal experimental data. The most common equations in use are: Van Laar, Margules, Redlich-Kister, and Wilson.

The system of initial interest in the present work was acetone-water. This is a relatively non-ideal system which caused some difficulty in applying the above equations. The equations have the following form:

1. Van Laar:

$$\log \gamma_1 = \frac{A_{12}}{(1 + A_{12}X_1/A_{21}X_2)^2}$$

$$\log \gamma_2 = \frac{A_{21}}{(1 + A_{21}X_2/A_{12}X_1)^2}$$

2. Margules:

$$\log \gamma_1 = (2A_{21} - A_{12})X_2^2 + 2(A_{12} - A_{21})X_2^3$$

$$\log \gamma_2 = (2A_{12} - A_{21})X_1^2 + 2(A_{21} - A_{12})X_1^3$$

3. Redlich-Kister:

$$\log \frac{\gamma_1}{\gamma_2} = B_{12}(1 - 2X_1) + C(6X_1X_2 - 1) + D(1 - 2X_1)(1 - 8X_1X_2) + \ldots$$

4. Wilson:

$$\text{Ln}\gamma_1 = -\text{Ln}(1 - A_{21}X_2) + X_2\left[\frac{X_2A_{12}}{1 - A_{12}X_1} - \frac{X_1A_{21}}{1 - A_{21}X_2}\right]$$

$$\text{Ln}\gamma_2 = -\text{Ln}(1 - A_{12}X_1) - X_1\left[\frac{X_2A_{12}}{1 - A_{12}X_1} - \frac{X_1A_{21}}{1 - A_{21}X_2}\right]$$

The data used in this study were those of Brunjes and Bogart.[7] Attempts were made to fit these data by various equations to predict activity coefficients for this unusual system over the entire composition range. These efforts were only partially successful.

The acetone-water equilibrium diagram becomes concave upward at high acetone concentrations. This means that where high purity acetone is desired (say 99.99 percent) a high reflux ratio accompanied by a large number of stages is required. Because of the asymptotic nature of the diagram, the number of calculated stages is very sensitive to the position of the equilibrium curve and its extrapolation to high concentrations becomes extremely critical.

The curve fitting technique for determining the Margules constants indicated that it was manifestly impossible to fit the equilibrium curve with a single Margules Equation. A plot of $\text{Log}\,\gamma_1/X_2^2$ vs X_2 is normally a straight line whose intersection with the Line $X_2 = 1$ is the Margules constant A12. For the acetone-water system, however, a plot of these parameters yields two straight lines which intersect at a 100-degree angle at about 90 percent acetone. The best Wilson equation tried yielded an equilibrium curve which fit well above 40 percent and below

2 percent but had a marked negative deviation in between.

In view of these factors, it was decided to use two equations to fit the X-Y diagram rather than compromise accuracy at the higher concentrations in order to fit the curve with a single equation.

Excellent results were obtained using the Wilson Equation above 40 percent acetone and the Margules Equation for the lower concentration ranges. The constants are:

Wilson Equation	$A_{12} = 0.597754$
	$A_{21} = 0.767919$
Margules Equation	$A_{12} = 0.9400$
	$A_{21} = 0.7293$

The equilibrium curve calculated by this procedure appears in Figure 3. Tabulation of the computer generated equilibrium points appears in Table I.

FIGURE 3: COMPARISON OF COMPUTER GENERATED X-Y DIAGRAM WITH EXPERIMENTAL CURVE

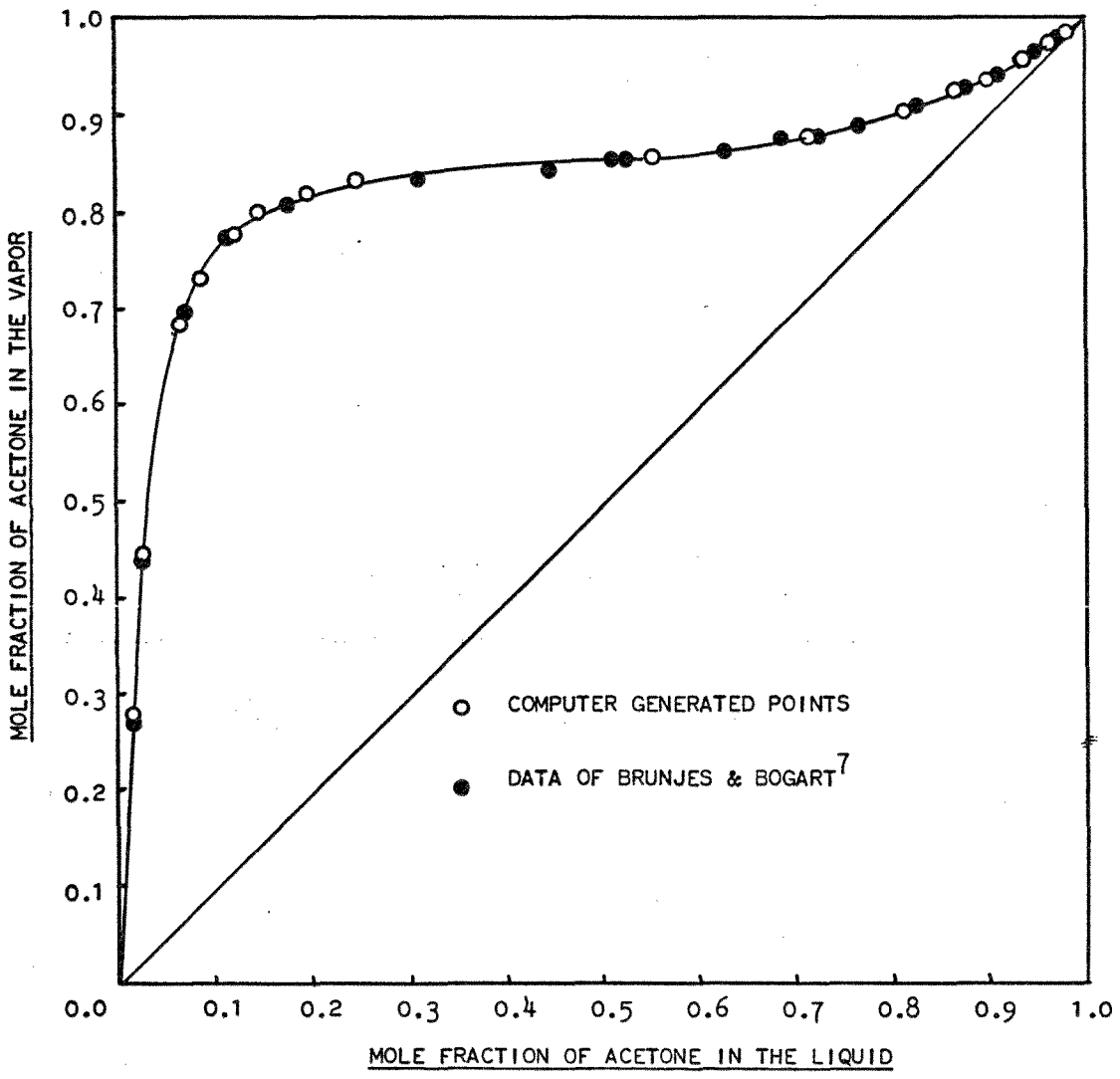


TABLE I : EQUILIBRIUM RELATIONSHIPS FOR THE ACETONE-WATER SYSTEM

TRIAL			X1	Y1	GAMMA1	GAMMA2	TEMP (C)	
1	13	12	.981275	.984400	1.00067	4.98731	56.1094	0
2	11	12	.973462	.979300	1.00135	4.84487	56.1562	0
3	11	12	.963306	.971500	1.00255	4.66947	56.2031	0
4	8	11	.937525	.956200	1.00725	4.26842	56.3906	0
5	11	14	.921900	.947200	1.01121	4.05241	56.5078	0
6	8	11	.897681	.935300	1.01897	3.75186	56.6953	0
7	10	13	.863306	.920800	1.03327	3.38534	56.9766	0
8	10	11	.813306	.903700	1.06096	2.95106	57.3984	0
9	11	11	.713306	.879000	1.14218	2.32498	58.2891	0
10	10	15	.550806	.851200	1.36725	1.70663	59.6953	0
11	1	13	.246118	.830900	2.98740	1.15723	59.6953	1
12	7	17	.192603	.820000	3.62963	1.09566	60.8203	1
13	9	11	.166821	.810000	4.01546	1.07168	61.7578	1
14	11	14	.162524	.807300	4.08553	1.06804	61.9453	1
15	5	14	.148071	.800000	4.33460	1.05648	62.6953	1
16	9	14	.133423	.790000	4.60974	1.04583	63.6328	1
17	10	15	.122290	.730000	4.33562	1.03858	64.4766	1
18	8	12	.119946	.777700	4.88515	1.03712	64.6641	1
19	10	14	.351306E-01	.730000	5.71006	1.01880	68.6016	1
20	8	16	.846728E-01	.680900	6.28789	1.01088	72.1641	1
21	11	19	.243408E-01	.448800	7.67419	1.00156	84.7266	1
22	11	21	.118396E-01	.279100	8.18255	1.00037	91.3828	1

A ZERO IN THE RIGHTMOST COLUMN INDICATES THE WILSON EQ WAS USED

A ONE IN THE RIGHTMOST COLUMN INDICATES THE MARGULES EQ WAS USED

III SYNOPSIS OF THE PROGRAM

A computer program is presented for the calculation of the optimum distillation conditions for a binary mixture in a dual column process. Figure 1 depicts the flow scheme. The program is entirely general and may be used for any two component system where the assumption of constant molal overflow is acceptable. The Wilson Equation, the Margules Equation, or both are employed for the calculation of activity coefficients. An option is available which calculates one portion of the equilibrium diagram via the Wilson Equation; then switches to the Margules Equation for the remainder of the curve. Either equation, however, could be used for the entire X-Y diagram. Since the program calculates equilibrium relationships internally, no K values need be supplied. The program is written in General Electric, Mark II, Timesharing Fortran and uses the McCabe-Thiele method for calculating the number of stages. Some salient features are itemized below.

1. Activity Coefficients: These are calculated by either the Wilson Equation or the Margules Equation as described previously. The appropriate constants for these equations must appear in the input data.
2. Cost Equations: Methods suggested by Aries and Newton[1] were used to develop the cost relationships. Multiple regression analysis was used, where necessary, to curve fit the equipment cost data presented by Page.[2] Costs

were developed based upon carbon steel equipment. A material factor multiplier is included, however, to account for the additional cost of materials other than carbon steel. A cost index multiplier is supplied to account for inflation.

3. Tower Option: A single column system, rather than a dual column process can be analyzed by a simple adjustment of the input variables.

4. Feed Quality: The degree of saturation of the feeds to both columns may be specified through the "q" variable. This allows either a partial or total condenser to be used on either column.

5. Process Variables: The process variables which must be specified in the input are:

   a. Feed composition to Column 1, XF1
   b. Overhead composition from Column 2, XD2
   c. Bottoms composition from Column 1, XB1
   d. Bottoms composition from Column 2, XB2
   e. Overhead product rate from Column 2, D2
   f. Intermediate product rate, P
   g. Overhead composition from Column 1, XD1

   These variables are sufficient to define the material balances for the entire system. Note that reflux ratios are not required to fix the material balance for the process. That is, the reflux ratios may be varied

independently of the material balance. This important point allows each column to be optimized separately and coupled to each other by means of the Column 1 overhead composition, XD1. This discussion is expanded in a subsequent section.

The process variables which are calculated by the computer to complete the material balance are:

a. Feed rate to Column 1, F1
b. Bottoms rate from Column 1, B1
c. Overhead rate from Column 1, D1
d. Feed rate to Column 2, F2
e. Intermediate product composition (same as XD1)

6. Vapor Pressure: Vapor pressures are calculated by the Antoine Equation. The constants must be supplied in the input. Since the acetone-water system was chosen as an example, there are special vapor pressure equations.[3,4] For these two components and the Antoine constants need not be supplied for this case.

7. Tray Efficiency: An overall tray efficiency may be supplied in the input data to account for the imperfect equilibrium on the trays. Values of overall tray efficiencies are readily obtained from the literature.[5,6]

8. Column Design: The Souders-Brown Equation is used to determine the maximum allowable velocity for the top and the bottom tray. The smaller value is chosen and a safety

factor (specified by the programmer) is applied. The Souders-Brown Equation is valid for sieve trays as well as for bubble caps. Consequently, the program is suited for the optimization of either column type. The constant for this equation must be supplied in the input data. These values are tabulated in the literature[6] for both sieve tray and bubble cap columns.

This is a brief treatment. Specific details are considered more fully as part of the "Discussion of the Program" in a later section of this thesis.

IV BASIC EQUATIONS USED IN THE PROGRAM

The equations used in the equilibrium and optimization calculations of the program include vapor pressure, cost, design, material balance, McCabe-Thiele and activity coefficient equations. These are described in the following sections.

A. Vapor Pressure Equations

Three vapor pressure equations are available in the program. If the system components are neither water nor acetone, the Antoine Equation may be used for both components. If the components are water and/or acetone special equations[3,4] may be used for vapor pressure. The three equations are:

1. Antoine Equation:

$$\text{Log } P = A - \frac{B}{t + C}$$

where $P = \text{mmH}_g$

$t = {}^{o}C$

An excellent source for the Antoine constants is Dreisbach.[8] They may also be readily determined by an appropriate plot of vapor pressure data.

2. Water Equation:[3]

$$\text{Log } \frac{Pc}{P} = \frac{X}{T} \frac{a' + b'X + c'X^3}{1 + d'X}$$

where P = vapor pressure in Int atm

$P_c = 218.167$ Int atm

$T = t^{o}C + 273.16$

$X = (T_c - T)$

$a' = 3.2437814$

$b' = 5.86826 \times 10^{-3}$

$c' = 1.1702379 \times 10^{-8}$

$d' = 2.1878462 \times 10^{-3}$

$T_c = 647.27$

3. Acetone Equation[4]

$$\text{Log } P = A - \frac{B}{(273.2 + t^{\circ}C)} - C \text{ Log}(273.2 + t^{\circ}C)$$

where $A = 22.57411$

$B = 2312.5$

$C = 5.0325$

B. Cost Equations

The equation used for the determination of unit product cost is:

(A) $C = 0.595\ P/r + 1.4M' + 3.05L' + 1.22(U' + R')$

where c = total cost of overhead product ($/#)

L' = direct labor cost ($/# product)

M' = direct maintenance cost ($/# product)

U' = utilities cost ($/# product)

P = purchased equipment cost ($)

r = annual overhead production (# product/yr)

R' = raw materials cost ($/# product)

The program is set up to calculate the cost/# of overhead product from Column I and use this value as the raw materials

cost for Column II. Derivation of the terms used in the equation presented above will now be discussed.

Step One is the determination of Fixed Capital Expenses. These are based upon purchased equipment cost curves presented by Page.[2] Fixed Capital Expenses are broken down as follows:

Purchased Equipment	P	($)
Instrumentation	0.2P	
Foundations	0.07P	
Platforms and Supports	0.11P	
Installation	0.25P	
Piping	0.5P	
Electrical	0.1P	
Insulation	0.08P	
Total Physical Plant Cost	2.31P	($)
Engineering (30 percent of Physical Plant Cost)	0.693P	($)
Total Direct Cost	3.003P	($)
Contractor's Fee (10 percent of Direct Cost)	0.30P	
Contingency (15 percent of Direct Cost)	0.45P	
Total Fixed Capital (F)	3.754P	($)

Step Two is the computation of operating cost:

a. Fixed Capital Related Costs

Depreciation	0.10F	($/Yr)
Property Taxes	0.02F	
Insurance	0.01F	
Total Fixed Capital Related Costs	0.13F	($/Yr)

Conversion to $/# product is accomplished by dividing by r the annual overhead production (#/Yr)

Total Fixed Capital Related Cost = 0.13 F/r ($/#)

b. Labor Related Costs

Direct Labor	L	($/Hr)
Supervision	0.10L	
Payroll Overhead	0.20L	
Laboratory	0.20L	
Plant Overhead	L	
Total Labor Related Cost	2.5L	($/Hr)

Conversion to $/# product is accomplished by dividing by the hourly overhead product rate L' = L - product rate in #/Hr

c. Maintenance Related Costs

Direct Maintenance Cost	M'	($/#)
Plant Supplies	0.15M'	
Total Maintenance Related Costs	1.15M'	($/#)

The program computes the maintenance cost for each piece of equipment by methods suggested on Page 165 of Aries and Newton.[1]

d. Utilities; U'

These are steam, cooling water, and electricity costs in ($/#)

e. Raw Material Costs in ($/# of Product); R'

Combination of a, b, c, d, and e leads to the following equation for Operating Cost:

(B) $O = 2.5L' + 1.15M' + 0.13F/r + U' + R'$

In addition to the above operating expenses are General Expenses which include costs for Administration, Sales, Research, and Finance. Aries and Newton suggests that these expenses be taken as 22 percent of the operation cost. Multiplying equation (B) by 1.22 and substituting 3.754P for F leads to equation (A).

It is appropriate to note at this point that the equation for bubble cap column diameter vs cost was obtained by a least squares fit of the curve presented in Page.[2] The equation has the form:

$$\text{Log (Total Column Cost per Tray)} = A + B \text{ Log } (D) + C \text{ Log } (D)^2$$

where A, B, and C are constants and D is the column diameter This function plots as a parabola on Logarithmic paper. The constants for the above equation have been included in the program for bubble cap columns. A column diameter vs cost curve could not be located for a sieve tray column. If it is desired to optimize sieve tray columns, the operator has two choices:

1. A factor has been included in the program which allows the sieve tray column cost to be computed as a percentage

of a bubble cap column cost. Chilton[9] recommends a value of 0.6 to 0.7 for this factor.

2. When a sieve tray cost curve becomes available, it may be fit with an equation of the above form and a set of constants determined. The program is designed to accept these constants should they become available.

C. Design Equations

The column is sized by use of the Souders-Brown Equation for maximum velocity. The reboiler and condenser are sized in the standard manner with the heat transfer coefficients being obtained from input data. The Souders-Brown Equation states:

$$U_{max} = K_V \sqrt{\frac{\rho_L - \rho_V}{\rho_V}}$$

The value for the constant is obtained from the input data. The maximum velocity is determined for the top and bottom trays and the lesser value is used as a design basis. The ideal gas law, as recommended by Perry,[10] is used to calculate the vapor densities. A safety factor, obtained from input data, is applied to U max and the column is sized based upon this reduced velocity.

D. Material Balances

The following equations are used to determine the material balances for the dual column system, illustrated in Figure 1. The equations were obtained by simultaneous solution of the individual balances.

$$(1) \quad B2 = \frac{D2(XD2-XF2)}{(XF2-XB2)}$$

$$(2) \quad F2 = B2 + D2$$

$$(3) \quad F1 = \frac{XB1(B2+P+D2)-(XB2)(B2)-(XD1)(P)-(XD2)(D2)}{(XB1)-(XF1)}$$

$$(4) \quad B1 = \frac{(XF1)(F1)-(XB2)(B2)-(XD1)(P)-(XD2)(D2)}{(XB1)}$$

$$(5) \quad D1 = F1-B1$$

$$(6) \quad V1 = \frac{D1}{1-\left[\frac{L}{V}\right]_1}$$

$$(7) \quad V2 = \frac{D2}{1-\left[\frac{L}{V}\right]_2}$$

$$(8) \quad L1 = \left[\frac{L}{V}\right]_1 (V1)$$

$$(9) \quad L2 = \left[\frac{L}{V}\right]_2 (V2)$$

Values for XF1, XD1, XD2, XB1, XB2, D2, and P are obtained from input data and the preceding equations are applied sequentially to complete the material balance. Note that if all Column 2 variables are set equal to zero, the equations will reduce to those of a single column.

E. McCabe-Thiele Equations

The program is set up for a single feed stream to each column. The standard operating line equations were used for the stripping and enriching sections. The intersection of the "q" line with the operating line was used to determine the optimum feed location.

These equations are described below.

1. Operating Line Enriching Section:

$$Yn = \frac{L}{V} Xn+1 + DX_D/V$$

2. Operating Line Stripping Section:

$$Ym = \frac{L'}{V'} Xm+1 - BX_B/V'$$

3. "q" Line Equation:

$$Y = \frac{q}{q-1} X - \frac{X_F}{q-1}$$

where $V' = V - (1-q)F$

$L' = L + qF$

$$q = \frac{\text{heat to convert 1 mole of feed to saturated vapor}}{\text{molar heat of vaporization}}$$

The "q" line equation and the operating line equation are solved simultaneously to find the optimum point to switch operating lines.

F. Activity Coefficients

The Wilson Equation, the Margules Equation, or both, may be used to calculate activity coefficients. These equations have been described previously in the section of this thesis entitled "THERMODYNAMIC RELATIONSHIPS FOR VAPOR-LIQUID EQUILIBRIA".

V DISCUSSION

Two different convergence procedures were used in the calculations. The procedure used in the computation of equilibrium relationships was developed especially for this thesis. The procedure used to converge the economic optimization, on the other hand, is a modification of the classical half-interval search technique. Both methods are described in the succeeding sections along with the general approach to the optimization.

A. General

Inspection of the material balance equations previously listed indicates that the material balance can be completely defined by the specification of XF1, XD1, XD2, XB1, XB2, D2, and P without specifying the internal reflux ratio in either column. (See Figure 1.) That is, the external stream rates are completely independent of the internal reflux ratios in either column. Let us look at a typical industrial problem for a moment in order to gain some insight into the nature of the variables which must be specified. We shall return to the subject of the independence of reflux ratios later.

Assume we have a production quota and a product specification to meet. Two product streams are involved: the intermediate product stream, (P), and the overhead product from Column 2, (D2). These restrictions fix P, XP, D2, and XD2. However, since Stream

P has the same composition as the overhead from Column 1 we have fixed XD1. Now assume that the recovery of the more volatile component has been specified by setting XB1 and XB2. Lastly, assume that the feed concentration, (XF1), has been fixed by a previous unit in the production train. Now a sufficient number of variables have been fixed or specified to allow the calculation of B2, F2, F1, B1, and D1 via the material balance equations on page 20. The only process variables remaining to be specified for the optimization procedure are the internal reflux ratios for each column. This being the case, we can optimize each column independently since the L/V ratios will not affect the material balance. We can find the optimum L/V for Column 1 using the variables F1, XF1, B1, XB1, D1, and XD1. Then using XD1 as the feed composition to the second column, along with the additional variables F2, B2, XB2, D2, and XD2 the optimum L/V may be found for Column 2. It should be emphasized that by splitting up the two columns we do not sacrifice rigor. The optimum reflux ratios obtained by this procedure will be the true optimum values for the combined system.

The computer program is set up to calculate the optimum reflux ratios for the situation stated above. The program in part requires input data consisting of the compositions XF1, XB1, XD1, XD2, and the flow rates B1, P, and D2. An estimate of the minimum L/V is desirable, although not essential, in order to avoid wasting computer time. The program calculates the remaining

variables, and finds the optimum reflux ratios in each column. Note that the two columns are coupled through the XD1 variable.

Although the program calls for XF1, B1, XB1, P, XD1, D2, and XD2 as input, the programmer can specify any process variables he wishes (as long as he specifies a sufficient number of variables to define the system), and can hand calculate the remaining variables required for the input data. Consider the following example.

Assume that a production rate of 1000 #/hr of 99.99 percent acetone has been specified by the sales department. This fixes the overhead rate, (D2), and the overhead composition, (XD2), for Column 2. Since the bottoms product is being discharged into a nearby stream the maximum concentration of acetone in the bottoms has been set at 0.1 mole percent. This specifies XB1 and XB2. Suppose that 15,130 #/hr of a byproduct stream is available as feed and has a 10 percent acetone concentration. F1 and XF1 have now been specified. The engineer realizes that he needs a value for the flow rate of Stream P in order to use the computer program so he refers back to the material balance equations given on page 20. The variables D2, XD2, F1, XF1, XB1, and XB2 have been fixed at this point. A total of seven process variables are necessary to define the system and we thus far have only six, so the Column 1 overhead composition, (XD1), is arbitrarily specified as 50 percent. (Note that this is not necessarily the most advantageous choice for

XD1 and that the system must be analyzed for several values of this variable.)

B2 can now be calculated from Equation (1) on page 20 noting that XF2 = XD1. F2 can be calculated from Equation (2) on page 20. Since F1 was specified, Equation (3) on page 20 may be solved for P. Once P is determined, no other hand calculations are required, since the computer will calculate the remaining variables. The required variables (XF1, B1, XB1, P, XD1, D2, and XD2) are now known and a computer run may be made.

Recall that XD1 was chosen arbitrarily. In order to truly optimize the system, that value of XD1 must be found which yields the lowest cost per pound for the product. This is accomplished by feeding in several values of XD1 to the computer. In a single run, the computer will calculate optimum reflux ratios for the dual column system, for as many values of XD1 as desired. The computer will yield a cost per pound for each value of XD1 fed in. The programmer need only choose the XD1 which gives the least cost per pound. This is best accomplished by plotting cost/# against XD1 and taking the minimum.

Thus in this example, instead of inputting a single value of XD1, many values, say, 20 percent, 30 percent, 40 percent, 60 percent, etc, could have been fed in at one time.

When the optimum is determined, it will represent the optimized cost for the intermediate product P as well as for the D2 stream. This is true because the columns were optimized individually.

A complete material balance for this example is shown in Figure 2. A summary of the important points covered in this section appears below.

1. Any seven process variables may be specified to define the system. The programmer must, however, hand calculate values for XF1, B1, XB1, P, XD1, D2, and XD2 if not specified.
2. If XD1 has not been fixed by process conditions, several values must be fed in as input. The correct value of XD1 is the one which yields the minimum cost per pound.
3. When an optimum has been computed, it will be the optimum cost per pound for both the intermediate product P and the Column 2 overhead product.

B. Iteration Schemes

1.) Equilibrium calculations No K values are required to use the program. Each X-Y point is calculated as the stages are stepped off. This might seem, at first, to be a rather extravagant approach but bear in mind the following points:

a. The program was formulated around the acetone-water system where the extrapolation of equilibrium data is extremely critical. It was desired to extrapolate the data to extremely high acetone concentrations, ie, 99.99 percent. Decent data was available only up to 97 percent.

b. The program is designed for general application. This eliminates curve fitting of a specific equilibrium curve.

c. The program is workable with knowledge of only a single X-Y point. From one point the Wilson or Margules constants may be determined and the optimization run using these constants.

The starting point in any McCabe-Thiele calculation is the vapor composition leaving the top stage, Y_N. Since a vapor composition is supplied to the computer, rather than a liquid composition, the calculation of the activity coefficient is a trial and error. The calculation of a single X-Y point would proceed as follows.

1. Assume a bubble point temperature.
2. Calculate P_1^o, the vapor pressure of Component 1 at this temperature.
3. Specify $Y_{n,1}$, the liquid composition on Tray n, for Component 1.
4. Guess an $X_{n,1}$, the liquid composition on Tray n, for Component 1.
5. Compute the activity coefficient for Component 1 using the trial value of $X_{n,1}$.
6. Compute $Y_{n,1}$ for Component 1 from

$$Y_{n,1} = \frac{\gamma_1 X_{n,1} P_1^o}{P_T}$$

7. Check to see if $Y_{n,1}$ computed in Step 6 agrees with the value of $Y_{n,1}$ specified in Step 3. If not, guess a new $X_{n,1}$ and repeat Step 4. If $Y_{n,1}$ specified = $Y_{n,1}$ computed, go onto Step 8.

8. Compute $X_{n,2} = (1 - X_{n,1})$

9. Compute γ_2

10. Compute $Y_{n,2}$ from

$$Y_{n,2} = \frac{\gamma_2 X_{n,2} P_1^o}{PT}$$

11. Check to see if $Y_{n,1} + Y_{n,2} = 1.0$. If not, guess a new temperature and repeat Step 1.

In the McCabe-Thiele calculation a new $Y_{n+1,2}$ would be computed via the operating line and the entire procedure repeated until the bottoms product specification was met.

The convergence procedure for the two loops shown above is rather unique. Let us look at the inner loop. A Function ϕ is defined as: (Y specified - Y calculated). An initial guess for X is used to compute a value for Y calculated. ϕ is determined and its sign is noted. The computer next increments X by an arbitrary amount: TOL. Thus, the new guess for X is X new = X old + TOL. A new value of Y calculated is computed and a new value of ϕ determined. The object of the convergence, of course, is to have $\phi = 0$. The computer now checks two things:

1. Do ϕ old and ϕ new have the same sign.
2. Is the absolute value of ϕ new greater or less than ϕ old.

If ϕ old and ϕ new both have the same sign, and ϕ new is less than ϕ old, this means we are heading in the correct direction, toward $\phi = 0$. That is, Y calculated is closer to Y specified for trial two than it was for trial one. For the next trial X is again incremented by +TOL.

If $\emptyset$ old and $\emptyset$ new both have the same sign but $\emptyset$ new is greater than $\emptyset$ old, this means we are heading in the wrong direction, away from $\emptyset = 0$. That is, Y calculated is further away from Y specified for trial two than it was for trial one. For the next trial we want to decrease the guess for X. In order to avoid repeating the previous trial, X is incremented by -2*TOL. If we incremented by -TOL, we would be using the same guess for X that was used for trial one.

If $\emptyset$ new has a different sign from $\emptyset$ old, this means that we have overshot the goal of $\emptyset = 0$. In this case we reverse direction and proceed half the distance in the opposite direction. That is, X new = X old - 0.5*TOL.

The process is continued from trial to trial. Each time there is an overshoot the direction is reversed and one half the distance is traversed in the opposite direction.

The advantages of this convergence procedure are:

1. It is mathematically impossible for this procedure to diverge for unimodal, real systems.
2. The method is relatively insensitive to the initial guess. Convergence is assured regardless of the initial choice of sign for the variable TOL. The choice of the magnitude of TOL will, of course, affect the number of iterations required. However, TOL may be chosen as large as desired in order to attain rapid convergence without inducing instability.

This convergence scheme is the extension of a suggestion by Dr John McCormick.

2.) Optimization calculations The convergence scheme used to locate the optimum reflux ratio is the half-interval search (sequential dichotomous search) described by Kuo.[11] The technique is limited to unimodal functions and the solution must be known to lie between two extremes. The method has been modified to calculate slopes rather than points on a curve. The initial reflux ratios specified in the input, say A and B, must be chosen such that they bracket the optimum L/V. For the latter to be true the slope of the cost versus L/V curve must be negative at A (the smaller initial L/V), and positive at B (the larger initial L/V). (See Figure 4.) If this condition is satisfied, a new L/V, (C), is chosen by the computer halfway between A and B and the slope determined at this point. If the slope at C is positive as in Figure 4, the optimum must lie between A and C. A new L/V, (D), is chosen halfway between A and C. If the slope ad D is negative as in Figure 4, the optimum must lie between C and D. This procedure is continued until the interval has been narrowed to that specified by the programmer. The computer will print the optimum L/V and other design information and then move on to a new case.

Boas[12] shows that if the solution is known to lie within a given span, then after 14 trials the interval will have been narrowed to 1 percent of the original span.

3.) General convergence discussion Many methods have been developed in chemical engineering which are so convenient and simple to use that they are applied mechanically with little, if any, thought given to the principles upon which they are based. The McCabe-Thiele diagram is such a method. Consider the situation represented in Figure 5. At first glance it appears that the overhead composition XD can be attained using the XF and L/V shown in the diagram. This is not the case. The situation depicted in Figure 5 has no physical significance. For a saturated liquid feed having a composition of XF, the lowest value for the overhead composition is XD'. This is true because the vapor in equilibrium with the feed would have the composition XD' (= YD'). Since XD' is greater than XD, the specification of XD as the composition of the overhead product is impossible.

If a feed having a composition of XF were introduced into a column having zero reflux, the overhead composition would be XD'. For a finite amount of reflux the overhead composition would be greater than XD'. Consequently, all possible values for the overhead composition lie between XD', (obtained by drawing a horizontal line through the intersection of the q line with the equilibrium curve), and 1.0.

This discussion has been included to caution the programmer against specifying a situation similar to the one which exists in Figure 5. For each feed composition there exists a minimum overhead composition XD'. If an attempt is made to optimize a

column where the overhead composition is less than this minimum, the computer will respond by asking for lower and lower values of L/V. It will not identify the condition specifically as an error. It should be noted that the possibility of encountering this difficulty is much more pronounced in the acetone-water system than in other binary systems. This is due to the extremely high relative volatility of acetone and the peculiar hump in the system equilibrium curve.

Another convergence problem was encountered during the debugging of the subroutine for calculating the number of trays. The difficulty has since been resolved but a discussion of the problem and its solution may prove to be of some interest.

The initial version of the subroutine treated the number of trays as an integer variable, which is physically the case. This procedure introduced discontinuities into the cost versus L/V curve as shown in Figure 6. The numbers represent the integral number of trays required for the separation. Consider the situation where the cost/# is calculated at Points a and b. The L/V was not increased enough in going from a to b to reduce the integral number of trays required, ie, 18. Consequently, there was no reduction in the fixed capital, but rather an increase since the reboiler and condenser had to be larger at b to accommodate the higher reflux. The operating cost at b was also higher than at a. Since a greater quantity of steam and cooling water was required to attain the

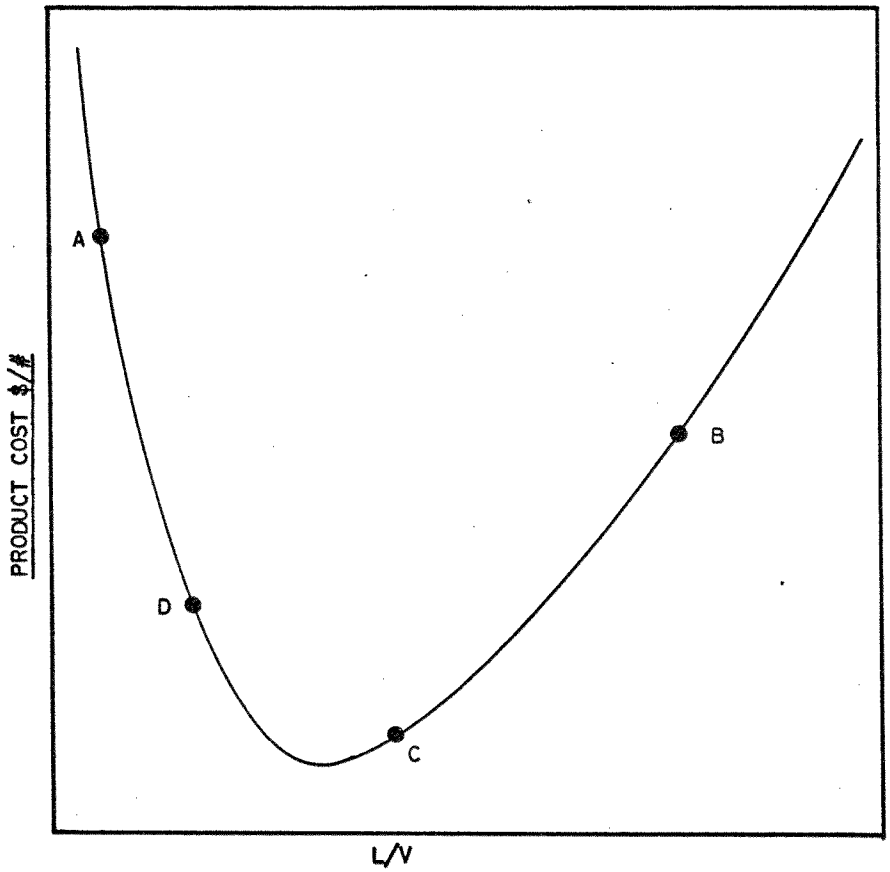


FIGURE 4: HALF-INTERVAL SEARCH TECHNIQUE

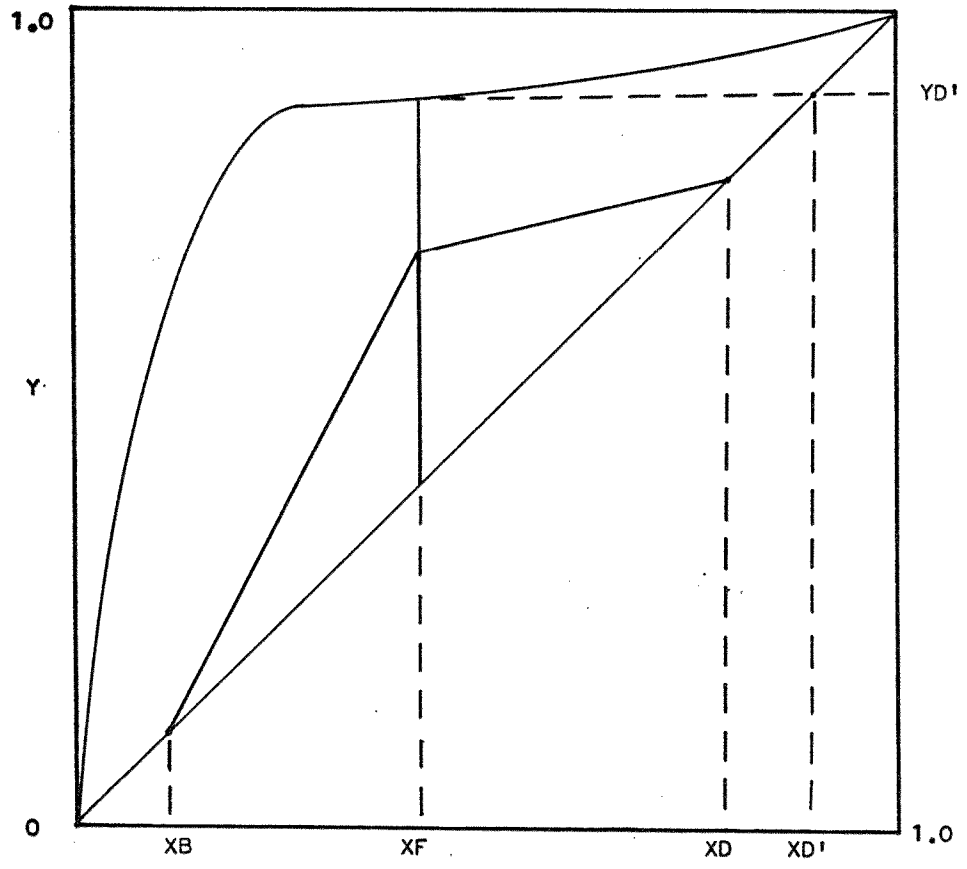


FIGURE 5: MINIMUM OVERHEAD CONCENTRATION

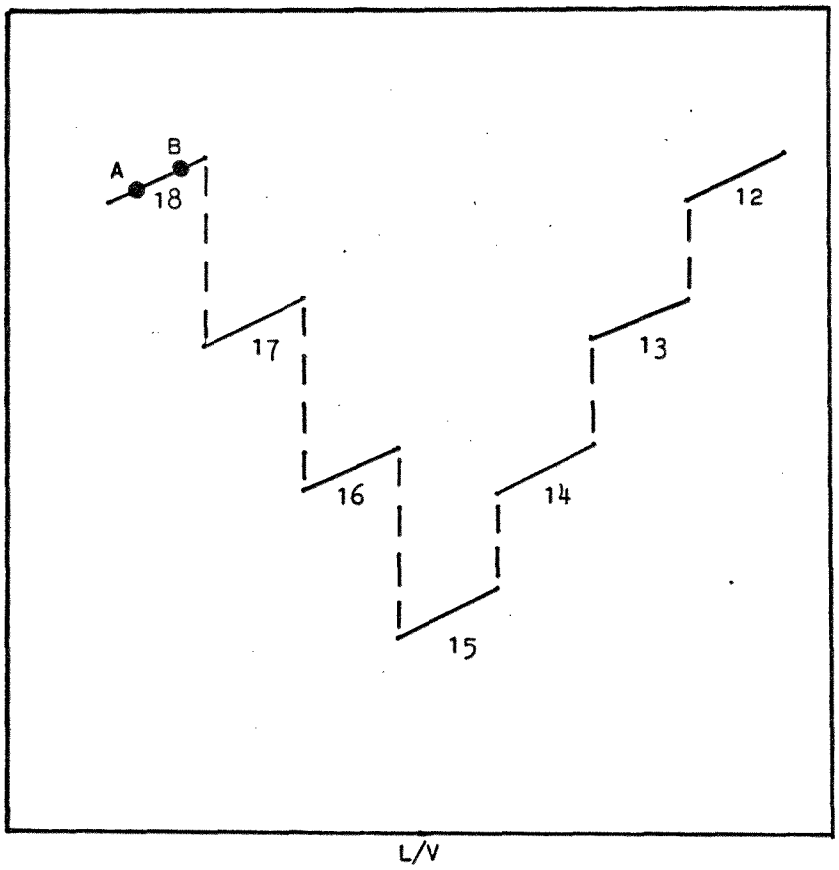


FIGURE 6: DISCONTINUOUS COST CURVE

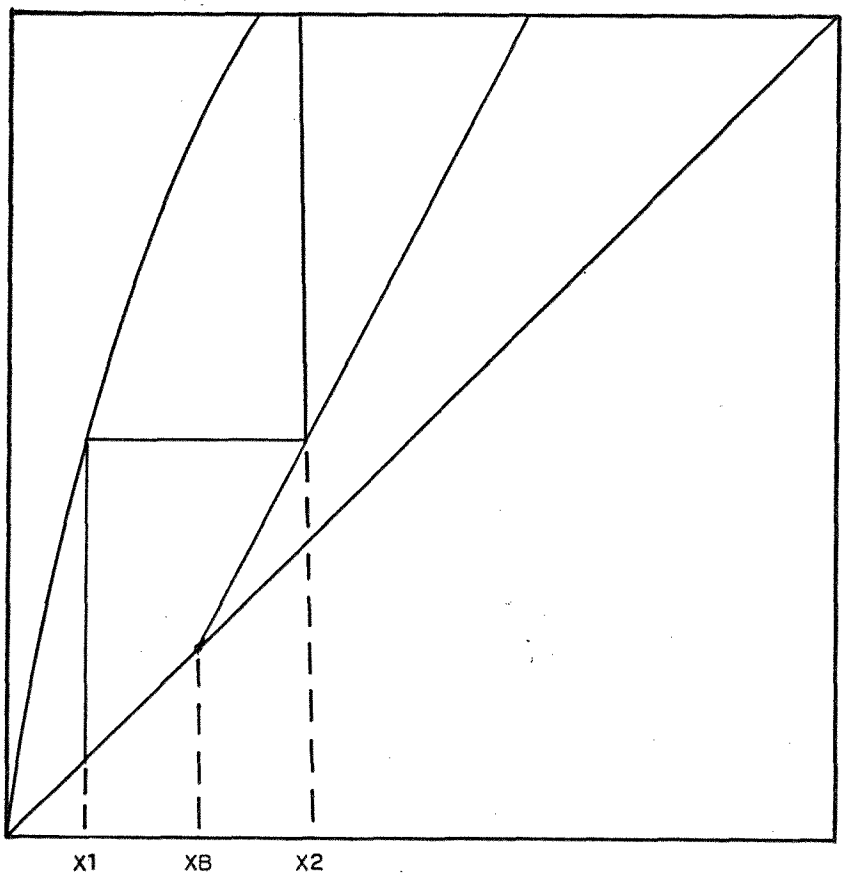


FIGURE 7: FRACTIONAL NUMBER OF STAGES

the higher reflux at b. The result was that the slope calculated in the vicinity of a and b was positive. The computer interpreted the positive slope to mean the optimum was located the left of a and b and decreased the L/V for the next trial. Inspection of Figure 6 indicates that the "macroscopic" slope in the vicinity of a and b was negative, and that the optimum lay to the right not the left. The computation, obviously, could never have converged.

The problem was rectified by redefining the number of trays as a floating point (rather than a fix point) variable. The fractional number of stages was defined in the standard manner by the equation:

$$\text{stages} = \text{integral number of trays} + \frac{X2 - XB}{X2 - X1}$$

where the values of X1, X2, and XB are as shown in Figure 7

If the assumption of unimodality is valid, then all points to the left of the optimum must have a negative slope and all points to the right a positive slope. Defining the equilibrium stages as above eliminates the discontinuities in the cost curve and assures convergence for a unimodal function. The assumption of unimodality is usually valid for a distillation optimization of the type presented in this thesis.

IV INPUT INSTRUCTIONS

A general discussion of input procedures is presented in the following sections. These topics include the choice of initial reflux ratios and several important programming options. Following the general discussion are given the specific, detailed input instructions.

A. General Considerations

1.) Initial reflux ratios As indicated previously, the convergence procedure used by the program requires that the optimum reflux ratio be known to lie within a specific interval. Certainly, the optimum L/V for any column must lie between the minimum reflux ratio and total reflux. Experience narrows the interval even further. Robinson[13] notes that in most cases the optimum reflux ratio lies very close to the minimum reflux ratio. The usual factor of 1.3 applied to the minimum external L/D is employed to yield a design which is less sensitive to slight inaccuracies in the equilibrium data. The actual optimum lies even closer to the minimum L/D than this.

The input data requires two initial values of L/V in each column for each XD1 considered. Say the minimum reflux was determined graphically, for the first column in the system, to be 0.40. A good set of initial L/V values for Column I would be 0.41 and 0.7. Note that the lesser L/V, (0.41), is chosen slightly greater than the minimum. The programmer should avoid picking a

reflux ratio too close to the minimum since this could result in a pinch if there was an inaccuracy in the determination of the minimum L/V. The larger reflux ratio, (0.7), should be chosen at a distance approximately halfway between the minimum reflux ratio and total reflux. If, however, the optimum L/V is known to lie within a narrower interval, then by all means the initial L/V's corresponding to the narrower interval should be used.

In case a pinch should be encountered, there exists an internal safeguard which prevents the computer from going through endless iterations. The computer will signify a pinch by the following message, then terminate execution:

A PINCH HAS BEEN ENCOUNTERED

THE STAGE TO STAGE CALCULATIONS APPEAR BELOW

The computer would then proceed to print the stage to stage calculations which led to the pinch.

When this error message is printed the programmer has either specified a reflux ratio which is below the minimum or has attempted some other procedure which has resulted in a pinch. Another condition which results in a pinch is the specification of too low a "q" value for the feed. It is best at this point to plot the operating line and the "q" line to find out exactly what is causing the pinch.

The programmer will not always bracket the optimum L/V in the first try. The computer will signify this by the message:

THE VALUES CHOSEN FOR THE INITIAL L/V'S IN COLUMN (AA) ARE TOO (BBBB).

THEY DO NOT BRACKET THE OPTIMUM L/V.

THE SLOPE AT L/V = (CCCC) IS:

(DDDD)

THE SLOPE AT L/V = (EEEE) IS:

(FFFF)

FOR THE NEXT RUN CHOOSE THE (GGGG) INITIAL L/V = (HHHH)

where AA is the column number (I or II)

BBBB (HIGH or LOW)

CCCC is the input value of the lower L/V plus a small increment

DDDD is the slope of the cost vs L/V curve at L/V = CCCC

EEEE is the input value of the higher L/V plus a small increment

FFFF is the slope of the cost vs L/V curve at L/V = EEEE

GGGG (LARGER or SMALLER)

HHHH The programmer should use this as the larger or smaller (depending upon GGGG) initial L/V for the next run

Execution would then be terminated.

A typical output for the case where the initial L/V's were chosen too high in Column II is given below:

THE VALUES CHOSEN FOR THE INITIAL L/V'S IN COLUMN II ARE TOO HIGH.

THEY DO NOT BRACKET THE OPTIMUM L/V.

THE SLOPE AT L/V = 7.0025000E-01 is:

7.9646545E-03

THE SLOPE AT L/V = 8.0025000E-01 IS:

1.8656216E-02

FOR THE NEXT RUN CHOOSE THE LARGER INITIAL L/V = 7.0025000E-01

The initial L/V's used in the input data which led to the above result were 0.7 and 0.8. Note that the L/V's stated in the message, (0.70025000 and 0.80025000), differ from the input values by 0.00025. The discrepancy is a result of a procedure for determining the slope of the cost vs L/V curve and need not concern the programmer.

The message states that the initial choices for L/V were too high and suggests a value of the higher L/V to be used in the next run. A reasonable set of L/V's for the next run would be 0.65 and 0.70025, assuming of course that the minimum L/V was less than 0.65. The program would be run with these new values of initial L/V's. If the new set of L/V's were still too high, the error message would appear once more, this time suggesting a larger initial L/V of 0.65. The programmer would choose a new set of L/V's and repeat the procedure until the optimum L/V was bracketed.

When the initial L/V's are chosen too low, the appropriate error message would be printed along with a suggestion for the smaller L/V in the next run.

When the initial L/V's are properly chosen to bracket the optimum L/V, the optimization will continue to the degree of accuracy specified by the "OUT" variable. (See the section of this thesis entitled "Escape Options".) The computer will print the optimum L/V for the current XD1, the cost per pound of product, the accuracy of the convergence, details of equipment design and costs, the tray to tray calculations for the optimum L/V and the material balances for the two column system. An example of the output is given in Appendix I.

In some cases the optimum L/V may lie so close to the minimum L/V that it becomes difficult to bracket it. One case was investigated where the optimum L/V was within 0.002 of the minimum L/V. The minimum L/V for this example was determined graphically to be approximately 0.33. The optimum L/V was finally computed to be 0.340125. An analysis of the approach used in this problem will now be presented. The table below indicates the input L/V's and the computer responses.

RUN	SMALLER L/V	LARGER L/V	COMPUTER RESPONSE
1	0.36000	0.60000	L/V's too high
2	0.33000	0.36000	Pinch was encountered
3	0.34025	0.36000	L/V's too high
4	0.33800	0.34025	Pinch was encountered
5	0.33950	0.34025	Optimization executed
	OPTIMUM L/V =	0.340125	

In the computation of the optimum five distinct computer runs were required. (It should be emphasized that this is an unusually severe case since the optimum L/V was located extremely close to the minimum. Normally, if the minimum L/V is known from graphical methods the optimum L/V can be bracketed on the first try.)

Run 1: The input values for L/V (0.36 and 0.60) were too high. They did not bracket the optimum. The computer suggested that 0.36 be used for the larger L/V in the next run. The choice of the smaller L/V is up to the discretion of the programmer. The input tape was modified to specify 0.33 and 0.36 as the L/V's for the next run.

Run 2: The computer encountered a pinch during the stage to stage calculations for L/V = 0.33. The appropriate message was printed and execution terminated. The choice of L/V = 0.33 was obviously below the minimum L/V so the smaller initial L/V was increased to 0.34025. The input tape was modified to specify 0.34025 and 0.36 for the next run.

Run 3: The values of L/V were too high. We conclude that the optimum is less than 0.34025 but more than 0.33. The larger L/V for the next run is set equal to 0.34025. The smaller L/V is set equal to 0.33800.

Run 4: A pinch was encountered. This means the value chosen for the smaller L/V (0.338) was too low. The optimum is now known to lie between 0.338 and 0.34025. The value of the smaller L/V is chosen as 0.3395 for the next trial.

Run 5: The optimum L/V has finally been bracketed by L/V = 0.3395 and L/V = 0.34025. The computer calculates the optimum L/V = 0.340125.

Note that graphical estimate of the minimum L/V was 0.33 but the minimum L/V implied by the above calculation was greater than 0.338 (since a pinch was encountered at 0.338). In a normal situation the minimum L/V need not be known to this degree of accuracy. The difficulty illustrated by the above analysis was caused by the close proximity of the optimum L/V to the minimum L/V.

When a situation such as the one described in this example is investigated, it is desirable to analyze the system one column at a time. The analysis is facilitated by the use of the variable "NUMBER". (See the section of this thesis entitled "Tower Options".)

2.) Escape options There are two escape options written into the program to allow for exiting when the optimum reflux has been attained.

The first of these is simply the specification of the slope of the cost vs reflux ratio curve at which the computations are to be terminated. Mathematically this value should be zero. Since a slope of zero would be obtained only under the most fortuitous situations a tolerance is allowed (to be specified by the programmer). This option is rather inconvenient to use since a prior knowledge of the unit product cost is required to set an intelligent value for the tolerance. Also if the optimum is very shallow, the computer might terminate execution before the optimum L/V has been determined to any degree of accuracy. If the cost per pound is about 5 cents, a reasonable value for this escape tolerance is 0.0001. A value of zero may be used for this tolerance to essentially negate the effect of this option.

A far more useful escape procedure is available. This is instrumented through the variable "OUT". If the initial set of L/V's were 0.42 and 0.7, the interval between the two L/V's would be approximately 0.300. If the variable "OUT" were set equal to 0.01, the iterations would continue until the value of the optimum reflux ratio was known to within 1 percent of the original interval. That is, the value of the optimum reflux ratio would be known to $\pm$0.003, which is 0.01 x 0.300. The ratio of the current interval to the original interval is calculated after each point on the cost curve has been computed. When the value of the ratio falls below the specified value for "OUT", execution is terminated.

3.) Tower options The program may be used to optimize a single column as well as a two column system. This is accomplished through the specification of the variable "NUMBER". The normal value is zero which should be used in the two column analysis. If a single column system is to be analyzed, a value of 1 is assigned to the variable "NUMBER". This causes control to "skip over" the Column II section of the program. When using this option, dummy variables must be supplied in the input for Column II, even though they will never be used. These are variables such as Column II reflux rate, stream compositions, stream rates, and so on. They must be included to satisfy the request for input. Any values could probably be used for these Column II variables, but it is safest to assign them numbers having a reasonable order of magnitude for the variable. Perhaps the easiest way to specify these is to use the same values which are used for the Column I variables. The Column I optimization will be carried out for as many values of the variable XD1 (the overhead composition from Column I) as are specified in the input.

It is also possible to have control "skip over" the Column I section and proceed directly to Column II. This instruction is implemented by setting the value of "NUMBER" equal to 2. In order to appreciate the utility of this last option, let us imagine the programmer at the console. He has graphically determined the minimum L/V required in Column I and the minimum L/V required in Column II. He enters a set of initial L/V's for each column and

begins the run. Say the initial L/V set for Column I did, indeed, bracket the optimum L/V for Column I. The optimization of Column I would continue until the desired interval were reached; then the computer would move on to Column II. Suppose that the L/V set used for Column II was too high to bracket the optimum. The computer would print the error message stating that the optimum had not been bracketed by the initial set of L/V's and stop. The programmer would then prepare a new input tape with a new set of L/V's for Column II. Also he would change the value of the variable "NUMBER" from its original value of zero to a new value of two. He must include the same Column I variables as used in the first run. In this second run the Column I section of the program would not be executed. Control would jump directly to the Column II portion of the program. As soon as execution begins, the following message will be printed:

TYPE IN COST PER LB FOR COL I OVERHEAD?

The programmer should enter the cost per pound obtained for the optimum L/V in the first computer run. (See "Example Run" section for an illustration.) The computer will then proceed to optimize Column II for as many values of XD1 as are specified in the input.

This may seem like a rather clumsy and complicated procedure, but it has been included to save precious computer run time.

B. Specific Input Instructions

Here is a list of the input variables with a brief description of how to specify them. They are listed in the order in which they appear in the input statements on lines 36100 through 37600 inclusive. (See Appendix II.)

XF1 — Is the mole fraction of the lighter component in the feed to Column I

XD2 — Is the mole fraction of the lighter component in the overhead from Column II

XB1 — Is the mole fraction of the lighter component in the bottoms product from Column I

XB2 — Is the mole fraction of the lighter component in the bottoms product from Column II

D2 — Is the flow rate in moles per hour of the overhead product from Column II

P — Is the flow rate in moles per hour of the intermediate product stream (See Figure 1)

NXD1 — Is the number of values for XD1 to be tried. If it is desired to investigate 10 different values of XD1, NXD1 should be set = 10. This is an integer variable.

DELTA — Is a convergence parameter which establishes the width of the "differential" slice used to determine the slope of the cost vs L/V curve.

RECOMMENDED VALUE: 0.0005

TOLSLP Is an escape tolerance. It is the slope tolerance discussed in the "Escape" section of this thesis.

RECOMMENDED VALUES:

1. If escape based upon slope is desired - 0.0001
2. If escape based upon slope is not desired - 0

LOOPKN Is a loop delimiter. It appears in the statement "DO 17 K = 1, KOOPKN". This is an integer variable.

RECOMMENDED VALUE: 20

NLOOPN Is a loop delimiter. It appears in the statement "DO 9 N = 1, NLOOPN". This is an integer variable.

RECOMMENDED VALUE: 20

WMB1 Is the average molecular weight of the bottoms product from Column I

WMT2 Is the average molecular weight of the overhead product from Column II

WMB2 Is the average molecular weight of the bottoms product from Column II

CV Is the constant for the Souders-Brown Equation. See reference 6 for recommended values. Note that the value of CV for a bubble cap column is not the same as that for a sieve tray column

SF Is the factor of safety to be applied to the maximum velocity used to calculate the column diameter

RECOMMENDED VALUE: 0.6 - 0.7

RHOLT1 Is the liquid density of the overhead product from Column I (#/ft^3). Note that if several XD1 values are investigated, an average value may be taken for the liquid density of the various concentrations. This is not a critical variable and the averaging procedure will cause only a small error in the determination of column diameter. The same comment applies to all physical properties of the Column I overhead.

RHOLB1 Is the liquid density of the Column I bottoms product (#/ft^3)

RHOLT2 Is the liquid density of the overhead product from Column II (#/ft^3)

RHOLB2 Is the liquid density of the bottoms product from Column II (#/ft^3)

DCA Is the fraction of column area to be allowed for the downcomer

RECOMMENDED VALUE: 0.10

FUDGE This is a factor to be applied, if desired, to approximate the cost of a sieve tray column. For further description see the section of this thesis entitled "Cost Equations". If the programmer supplies his own cost curve for sieve tray columns, this variable should be set equal to 1.0

RECOMMENDED VALUE: 0.6 - 0.7

If it is desired to approximate the cost of a sieve tray column by taking a percentage of the cost of a bubble cap column.

OAEFF — Is the overall tray efficiency. See references 5 and 6 for recommended values.

CINDEX — Is the inflation adjustment factor. The value used should be the ratio of the current cost index (eg, the Marshal and Stevens Index) to the cost index for June 1962. For the Marshal and Stevens Index, CINDEX = 290.7/236.2 = 1.24

FACMAT — Is the material of construction adjustment factor. The cost equations used in the program were based upon carbon steel. If other materials are to be used an adjustment can be made using "FACMAT". This variable is a simple multiplier.

CC1,CC2, CC3 — If the programmer supplies his own cost curve for sieve tray columns he places the three equation constants in this position. See the section of this thesis entitled "Cost Equations" for further description.

HEATT1 — Is the latent heat of the overhead product from Column I (Btu/#). See note under RHOLT1.

HEATB1 — Is the latent heat of the bottoms product from Column I (Btu/#)

HEATT2 Is the latent heat of the overhead product from Column II (Btu/#)

HEATB2 Is the latent heat of the bottoms product from Column II (Btu/#)

UTOP1 Is the U for the Column I condenser (Btu/hr/ft^2/^{o}F)

UBOT1 Is the U for the Column I reboiler (Btu/hr/ft^2/^{o}F)

UTOP2 Is the U for the Column II condenser (Btu/hr/ft^2/^{o}F)

UBOT2 Is the U for the Column II reboiler (Btu/hr/ft^2/^{o}F)

TSTEAM Is the steam temperature (^{o}F) supplied to the reboilers

CWIN Is the cooling water inlet temperature for the condensers (^{o}F)

CWOUT Is the cooling water outlet temperature for the condensers (^{o}F)

SBCOL1 Is the number of degrees of subcooling (^{o}F) desired in the Column I condenser

SBCOL2 Is the number of degrees of subcooling (^{o}F) desired in the Column II condenser

CORR1 Is the LMTD correction factor for the Column I condenser

CORR2 Is the LMTD correction factor for the Column II condenser

STMCST Is the cost of steam in $/1000 Btu

CP1 Is the heat capacity of the liquid reflux to Column I (Btu/#/^{o}F)

CP2 Is the heat capacity of the liquid reflux to Column II (Btu/#/^{o}F)

CWCST Is the cost of cooling water in $/1000 gal

WMF1 Is the average molecular weight of the feed to Column I

RMCST Is the value of the feed to Column I in $/# of feed

SPACE Is the tray spacing in ft

TMCST Is the tower maintenance cost in $/ft^3/yr

CMCST Is the condenser maintenance cost in $/ft^2/yr

RBMCST Is the reboiler maintenance cost in $/ft^2/yr

ELCOST Is the cost of electricity, $/KW hr

OLABCST Is the cost of labor, $/man-hour

KIND This variable determines which cost equation is used to determine tower cost

IF KIND = 0 the column cost will be calculated via the bubble cap column cost equation

IF KIND = 1 the variable "FUDGE" is multiplied by the bubble cap column cost in order to approximate the cost of a sieve tray column

IF KIND = 2 the programmer's equation for sieve tray columns will be used. See comments for the variables CC1, CC2, and CC3. See also the section in this thesis entitled "Cost Equations".

ILOOPN — A convergence parameter

RECOMMENDED VALUE = 300

JLOOPN — Represents the maximum number of temperature trials allowed.

RECOMMENDED VALUE = 40

KLOOPN — Represents the maximum number of trials allowed in concentration LOOP K

RECOMMENDED VALUE = 40

PT — Total pressure in mm Hg

TEMPT — Represents the initial temperature guess for the first X-Y point (^{o}C)

RECOMMENDED VALUE = BP OF THE MORE VOLATILE COMPONENT

A1,B1,C1, A2,B2,C2 — These are the Antoine constants for the lighter and heavier components respectively. If acetone is the lighter component, use A1 = B1 = C1 = 0. If water is the heavier component, use A2 = B2 = C2 = 0.

A12,A21 — These are the Margules constants. If the Wilson equation is to be used to calculate the entire X-Y curve, use A12 = A21 = 0.

AA12,AA21 — These are the Wilson constants. If the Margules equation is to be used to calculate the entire X-Y curve, use AA12 = AA21 = 0.

TOLERY — A convergence parameter

RECOMMENDED VALUE = 0.0005

TOL — A convergence parameter

RECOMMENDED VALUE = 0.2

TOLTEM — A convergence parameter

RECOMMENDED VALUE = 3.0

TOLSUM — A convergence parameter

RECOMMENDED VALUE = 0.0005

CHANGE — If this variable is set equal to 0, the program will use the Wilson equation for the entire X-Y diagram. If the variable is set equal to 1, the Margules equation will be used to calculate the entire X-Y diagram. If the variable is specified as any value between 0 and 1, say 0.4, the Wilson equation will be used for all points above X = 0.4 and the Margules equation will be used for all points below X = 0.4.

IACET — If acetone is one of the components, use IACET = 0. If acetone is not one of the components, use IACET = 1.0. This parameter allows the use of a special equation, already in the program, for the vapor pressure of acetone. If IACET is set = 1.0, the Antoine equation will be used to calculate the vapor pressure of the lighter component.

IWATER — If water is one of the components, use IWATER = 0. If water is not one of the components, use IWATER = 1.0. This parameter allows the use of a special equation (already in the program) for the vapor

pressure of water. If IWATER is set = 1.0, the Antoine equation will be used to calculate the vapor pressure of the heavier component.

TOL1 A convergence parameter

RECOMMENDED VALUE = 0.2

TOLTM1 A convergence parameter

RECOMMENDED VALUE = 3.0

Q1 Is the q value for the feed to Column I used in the q line equation for the McCabe-Thiele calculation

Q2 Is the q value for the feed to Column II used in the q line equation for the McCabe-Thiele calculation

DUMMY A dummy variable. Use 0.5

NUMBER This variable allows access to either column routine. The value is either 0, 1, or 2. See this thesis section entitled "Tower Options". This is an integer variable.

OUT This is an escape variable. A value of 0.01 for "OUT" will cause the iterations to continue until the optimum L/V is known to 1 percent of the original interval. See this thesis section entitled "Escape".

XD1(MOP) This array includes all the values of XD1 which are to be investigated. The number of data pieces in this position must be equal to NXD1. In a sense XD1 is the independent variable of the optimization. Once it has been specified, the system is fixed. The programmer

can then plot the cost/# vs XD1 to find the true optimum of the system. No rules can be given for choosing XD1's. The programmer must use his judgment and common sense. As many values of XD1 as desired may be specified.

GLOV1(IT) This array contains the initial L/V's for Column I. The data should be arranged in sets of two. That is, two values for L/V in Column I should appear for each XD1 investigated, the lower L/V being listed first, then the higher L/V. The two values in a set must be chosen to bracket the optimum L/V. The total number of data pieces in this location must be equal to 2 x "NXD1". See the section of this thesis entitled "Initial Reflux Ratios".

GLOV2(IT) This array contains the initial L/V's for Column II. The data should be arranged in sets of two. That is, two values for L/V in Column II should appear for each XD1 investigated, the lower L/V being listed first, then the higher L/V. The two values in a set must be chosen to bracket the optimum L/V. The total number of data pieces in this location must be equal to 2 x "NXD1". See the section of this thesis entitled "Initial Reflux Ratios".

WEIGHT(MG) This array contains the molecular weights of the overhead product from Column I. A molecular weight should appear for each value of XD1 to be investigated. The number of data pieces in this location must be equal to the value of NXD1.

Inspection of lines 36100 through 37600 in the program reveals a total of eight INPUT statements. In GE Mark II Fortran the data for each new INPUT statement must begin on a new record. The data pieces within a single INPUT statement may, however, appear on several records. To clarify this restriction, observe the input list in the sample run on page 1 of Appendix I. The variables "XF1" and "LOOPKN" which are the first and last variables in INPUT statement one correspond to the numbers 0.2366 and 20 on line one of the data list. Note that the data for INPUT statement one happens to be listed on a single record. There is no particular format required when typing in this group of variables. Each data piece could have been listed on a separate record just as well. The first variable in INPUT statement two, however, (NLOOPN = 20), must appear as the first data piece in a record. Below is a list of the variables which must appear as the first data piece in a record. The variables in between, aside from being in the proper sequence, may be listed in any convenient manner.

VARIABLE	VALUE IN EXAMPLE
XF1	0.2366
NLOOPN	20
ILOOPN	28
NUMBER	0
XD1(1)	0.87
GLOV1(1)	0.14
GLOV2(1)	0.42
WEIGHT(1)	54.54

The most convenient way to input the data is by tape. The tape must begin with a series of rub-outs, then the data (no intervening punches such as line feeds or carriage returns). Each record must end with the following sequence of punches: LINE FEED, (CONTROL X-OFF), CARRIAGE RETURN, RUBOUT. Unless these instructions are carried out exactly, the data will be scrambled and the program will not be executed.

On a request for input the computer will transmit a question mark along with a signal to activate the tape drive. On most teletypes the tape drive will be activated automatically (the TD call-in button on the Model 35 must be in the ON position). On other units the tape drive can be started manually each time the "?" appears. The tape drive will feed in one record at a time stopping after each line to wait for another "?" to be transmitted. If the tape drive is being activated by depressing the TD ON button manually the programmer must wait for the question mark each time.

Dimensions: The program is presently dimensioned for a maximum of 30 theoretical trays in each column. There is no other limit in the program for the number of trays. If the programmer wishes to increase the allowable number of trays he may change the dimensions of the variables indicated below. The allowable number of trays should replace XX in these statements.

LINE NUMBER	DIMENSIONED VARIABLE
10400	PP(5,XX), IP(4,XX)
19100	T(XX,50), Y1(XX)
19300	EE(XX)
19500	PP(5,XX), IP(4,XX)
35300	PP(5,XX), IP(4,XX)

If memory capacity becomes a problem the programmer has two choices.

1. Use of the NOLINE mode. The statement:

   100 NOLINE

   may be inserted. This command will prevent generation of line numbers and thereby release a considerable section of the core for computation.

2. The programmer can delete the following statements: 10400, 19500, 31600, 31700, 31800, 32300, 32400, 32700, 32800, 32900, 33200, 33300, 35300, 55800, 56100, 56200, 56300, 56600, 56900. The deletion of these lines will eliminate the printing of the stage to stage calculations for the optimum design. All other calculations and outputs will be

unaffected. The deletion should release a minimum of 2000 memory locations for computation.

VII EXAMPLE RUN

Appendix I contains a sample computer run of this program. The original intent was to study the acetone-water system up to concentrations of 99.99 percent acetone. At the higher reflux ratios columns of 100 stages or more would have been required. The cost for a complete optimization of a two-column system having 100 trays in each column would have been approximately $500. This is by no means an unreasonable figure for an industrial program of this complexity. However, budget considerations demanded a lower overhead concentration. The sample run uses 95 percent for the concentration of acetone in the overhead from Column II. Two values of XD1 are investigated, 0.87 and 0.875.

The example will be explained page by page starting with the input list appearing on page 1 of Appendix I.

The data are listed according to the INPUT statements on lines 36100 through 37600 of the program. (See Appendix II for a listing of the program and the section of this thesis entitled "Input Instructions" for a detailed description of the input variables.) Each data piece in the list shall now be identified and a brief discussion presented where necessary.

0.2366	XF1
0.95	XD2
0.001	XB1
0.001	XB2
17.24	D2

17.24	P	
2	NXD1	Since two values of XD1 are to be investigated (viz, 0.87 and 0.875), NXD1 is set equal to 2
0.0005	DELTA	
0.0001	TOLSLP	
20	LOOPKN	
20	NLOOPN	
18.0	WMB1	
58.0	WMT2	
18.0	WMB2	
0.1	CV	
0.6	SF	
54.9	RHOLT1	
62.4	RHOLB1	
54.9	RHOLT2	
62.4	RHOLB2	
0.1	DCA	
0.7	FUDGE	
0.7	OAEFF	
1.24	CINDEX	
1.0	FACMAT	
0,0,0	CC1,CC2,CC3	
220.0	HEATT1	
970.0	HEATB1	

220.0	HEATT2
970.0	HEATB2
150.0	UTOP1
300.0	UBOT1
150.0	UTOP2
300.0	UBOT2
298.0	TSTEAM
70.0	CWIN
90.0	CWOUT
10.0	SBCOL1
0	SBCOL2
1.0	CORR1
1.0	CORR2
1.0	STMCST
0.5	CP1
0.5	CP2
0.1	CWCST
18.1	WMF1
0.02	RMCST
1.0	SPACE
30.0	TMCST
3.0	CMCST
7.0	RBMCST
0.02	ELCOST
8.0	OLABCST

1	KIND	
28	ILOOPN	
40	JLOOPN	
40	KLOOPN	
760	PT	
63	TEMPT	
0,0,0,0,0,0	A1,B1,C1,A2,B2,C2	
0.94,0.7293	A12,A21	
0.597754,0.767919	AA12,AA21	
0.0005	TOLERY	
0.2	TOL	
3	TOLTEM	
0.0005	TOLSUM	
0.7	CHANGE	
0	IACET	
0	IWATER	
0.2	TOL1	
3	TOLTM1	
1	Q1	
1	Q2	
0.5	DUMMY	
0	NUMBER	Since it is desired to analyze a two-column system, this variable is set equal to 0
0.25	OUT	

0.87,0.875 XD1 array These are the values of XD1 to be investigated. The total number of data pieces (2) in this location must equal the value of NXD1.

0.14,0.144,0.14,0.16 GLOV1 array The first two figures (0.14 and 0.144) represent the initial L/V's in Column I corresponding to XD1 = 0.87. They were chosen to bracket the optimum L/V. The second two figures (0.14 and 0.16) represent the initial L/V's in Column I corresponding to XD1 = 0.875. They were chosen to bracket the optimum L/V. The total number of data pieces in this location (4 pieces in all) is equal to twice NXD1 (2 x 2).

0.41,0.60,0.70,0.80 GLOV2 array The first two figures (0.41 and 0.60) represent the initial L/V's in Column II corresponding to XD1 = 0.87. They were chosen to bracket the optimum L/V. The second two figures (0.70 and 0.80) represent the initial L/V's in Column II corresponding to XD1 = 0.875. Normally, they would have been chosen to bracket the optimum L/V. For illustrative purposes, however, they were chosen higher

than the optimum L/V. The total number of data pieces in this location (4 pieces in all) is twice the value of NXD1 (2 x 2).

54.54,54.75 WEIGHT array The first Figure (54.54) is the molecular weight of the overhead product from Column I corresponding to XD1 = 0.87. The second figure (54.75) is the molecular weight of the overhead product from Column I corresponding to XD1 = 0.875. The total number of data pieces in this location (2) must equal the value of NXD1.

This completes the input list. When two values of XD1 are investigated, and the initial L/V's have been chosen properly, the output will be printed in four sections as shown in Appendix I on pages 2, 3, 4, and 5. The output sections will be appropriately titled and appear in the following order:

1. Optimization of Column I for 1st XD1
2. Optimization of Column II for 1st XD1
3. Optimization of Column I for 2nd XD1
4. Optimization of Column II for 2nd XD1

There is no limit on the number of values of XD1 which can be specified. If 10 values of XD1 are specified, there will be 20 blocks of output, 10 for each column. This assumes, of course, that

the initial L/V's are chosen to bracket the optimum in each case. If the initial L/V's were chosen improperly, all computations up to that point will be printed out and execution irreversibly terminated after printing of an error message.

The output is self-explanatory except for the following points:

1. The cost/# of overhead product from Column I is the cost to produce the intermediate product stream P. It is also the cost per pound of the feed to Column II, F2.
2. All compositions in the printout refer to the most volatile component.
3. The block of print immediately below "TOTAL UTILITY COST" represents the stage to stage calculations for the optimum L/V.
4. The three columns under the heading "TRIAL" have been included to give the programmer a check on the number of iterations required for the calculations. Consider the 1st line under "TRIAL" on page 2 of Appendix I.

   1 11 8

   The calculation of the activity coefficients at a given temperature is a trial and error procedure since the vapor composition is specified for each tray. (See the section of this thesis entitled "Iteration Schemes; Equilibrium Calculations".) The figure in the right most column, (8),

is the number of trials associated with the determination of the activity coefficients for a given temperature. This value will vary between 1 and 25 depending upon the particular point. The value of this variable must be less than the variable KLOOPN. If it is equal to KLOOPN, (the number appearing in this position will never be greater than KLOOPN), then the loop has not converged and a higher value of KLOOPN must be chosen. A value of KLOOPN = 40 will probably be sufficient for most systems.

The number appearing in the middle column, (11), is the number of temperature trials required to get the sum of the y's to equal 1.0000. The value of this variable must be less than the variable JLOOPN. If it is equal to JLOOPN, (it will never be greater), then the temperature loop has not converged and a higher value of JLOOPN must be chosen. A value of JLOOPN = 40 will probably suffice for most systems.

The number appearing in the left most column is the theoretical tray number. The value of this variable must be less than ILOOPN. If not, the value of ILOOPN must be must be increased. A value of 300 may be used to cover most systems.

The approximate number of iterations required to converge tray 1 may be obtained by multiplying 11 x 8 = 88. The approximate number of iterations to converge tray 5 is 19 x 10 = 190.

A similar discussion applies to each tray in the printout.

The initials L/V's in Column II for XD1 = 0.875 (0.70 and 0.80) were purposely chosen too high to bracket the optimum L/V. The result was the printout on page 5 of Appendix I.

The computer printed the slope of the cost vs L/V curve at the two initial L/V's chosen. (Actually, the slope is calculated about an L/V which is greater than the L/V specified in the input by 0.00025, hence the output values of 0.70025 and 0.80025 rather than 0.70 and 0.80.) The computer suggested that the higher L/V for the next trial should be 0.70025.

It was known that the optimum L/V lay between 0.41 and 0.60 so this last message was ignored for the next run shown on pages 6 and 7 of Appendix I. Initial L/V's of 0.41 and 0.60 were used to obtain the output on page 6.

Before proceeding it will be instructive to review the input list on page 6 of Appendix I. In the 1st run Column I had been optimized for XD1 = 0.87 and XD1 = 0.875. Column II had been optimized for XD1 = 0.87. In order to avoid rerunning these cases, the following changes were made in the input list:

1. NXD1 (1st line, 7th variable) was changed from the original value of 2 to a new value of 1. This instructs the computer to analyze the system for one value of XD1 rather than 2.

2. NUMBER (8th line, 1st variable) was changed from 0 to 2. This causes control to skip over the Column I section of the program and proceed directly to Column II.
3. XD1 (9th line): The original array containing two values of XD1 (0.80 and 0.875) was replaced by a single value of XD1 = 0.875.
4. GLOV1 (10th line): The original array of 4 variables (0.14, 0.144, 0.14, 0.16) was replaced by an array of two variables (0.1, 0.1). Since these variables are not used in the calculation, (control skipped over Column I), they are dummy variables. Although two numbers must appear in this position of the input list, they may have any value.
5. GLOV2 (11th line): The original array of 4 variables (0.41, 0.60, 0.70, 0.80) was replaced by an array of two variables (0.41 and 0.60) representing the new initial L/V's for Column II.
6. WEIGHT (12th line): The original array of 2 variables is replaced by a single variable (54.72) which is the molecular weight of D1 for XD1 = 0.875.

After the input was fed into the computer, the following message appeared at the console:

TYPE IN COST PER LB ($/#) FOR COL I OVERHEAD?

The cost/# of overhead product from Column I (0.034049425) was obtained from the printout of the previous computer run for

Column I, XD1 = 0.875. (Appendix I page 4) This value was manually typed in as soon as the question mark appeared.

The optimization for Column II with XD1 = 0.875 was completed and the results are shown on page 7 of Appendix I.

In an actual run the programmer will specify more values of XD1, say 10. The resulting cost/# of overhead product from Column II would be manually plotted against XD1. The minimum of this curve is the optimum XD1 for the system. The corresponding L/V's could be interpolated or a new computer run made with the optimum XD1.

The output on page 8 of Appendix 1 illustrates what can be expected if a pinch is encountered. In this case the programmer has probably specified an L/V which is below the minimum.

APPENDIX I

EXAMPLE PRINTOUT

```
RVBS          20:59       04/15/70
?0.2366,0.95,0.001,0.001,17.24,17.24,2,0.0005,0.0001,20
?20,18.0,53.0,18.0,0.1,0.6,54.9,62.4,54.8,62.4,0.1,0.7,0.7,1.24
?1.0,0,0,0,220.0,970.0,220.0,970.0,150.0,300.0,150.0,300.0,298.0,70.0
?90.0,10.0,0,1.0,1.0,1.0,0.5,0.5,0.1,18.1,0.02,1.0,30.0,3.0,7.0,0.02
?3.0,1
?28,40,40,760,63,0,0,0,0,0,0,0.94,0.7293,0.597754,0.787919,0.0005
?0.2,3,0.0005,0.7,0,0,0.8,3,1,1,0.5
?0,0.25
?0.87,0.375
?0.14,0.144,0.14,0.16
?0.41,0.60,0.70,0.80
?54.54,54.75
```

COLUMN I OPTIMIZATION FOR XD1 = 0.87000000

THE OPTIMUM L/V IN COLUMN I IS 0.14337500
THIS CORRESPONDS TO XD1 = 8.7000000E-01
THE OPTIMUM L/V IS ACCURATE TO +OR- 8.1249970E-04
THE COST OF OVERHEAD PRODUCT FROM COL I ($/#)=
3.3962549E-02

TOWER DIAMETER (INCHES) = 88.689880
ACTUAL NUMBER OF TRAYS = 8.5884000E+00
TOWER COST ($) = 2.7824368E+03
REBOILER AREA (SQ. FT.) = 2.6123535E+01
REBOILER COST ($) = 1.1176350E+03
CONDENSER AREA (SQ. FT.) = 8.5674933E+01
CONDENSER COST ($) = 1.9884417E+03
FEED PUMP COST ($) = 2.9605638E+02
BOTTOMS PUMP COST ($) = 2.7680352E+02

TOTAL PURCHASED EQUIPMENT COST ($) = 5831.7704
TOTAL MAINTENANCE COST ($/#PRODUCT) = 1.0472517E-04
TOTAL UTILITY COST ($/#PRODUCT) = 0.5340498OE-03

TRIAL			X1	Y1	GAMMA1	GAMMA2	TEMP (C)	
1	11	3	0.566875	0.870000	1.19307	2.10988	53.6375	0
2	6	7	0.538750	0.840775	1.41803	1.85395	58.3750	1
3	8	16	0.204375	0.822341	3.47152	1.10781	60.4687	1
4	14	130.619924E-01		0.672470	6.36915	1.01000	72.7500	1
5	19	10.7390630E-02		0.202374	8.35509	1.00016	93.9844	1
6	12	10.7353140E-030		.2375090E-01	8.67344	1.00000	99.3516	1

A ZERO IN THE RIGHTMOST COLUMN INDICATES THE WILSON EQUATION WAS USED

A ONE IN THE RIGHTMOST COLUMN INDICATES THE MARGULES EQUATION WAS USED

MATERIAL BALANCES

XF1 = 2.3660000E-01
XD1 = 8.7000000E-01
XB2 = 9.5000000E-01
XB1 = 1.0000000E-03
XD2 = 1.0000000E-03
D2 = 1.7840000E+01 LBS/HR
F = 1.7840000E+01 LBS/HR
B2 = 1.5371117E+00 LBS/HR
F2 = 1.5271117E+01 LBS/HR
F1 = 1.3307192E+02 LBS/HR
B1 = 9.9965455E+01 LBS/HR
D1 = 8.6673600E+01 LBS/HR
V = 4.8128814E+01
L = 6.9612546E+00

COLUMN II OPTIMIZATION FOR XD1 = 0.87000000

THE OPTIMUM L/V IN COLUMN II IS 0.50525001
THIS CORRESPONDS TO XD1 = 8.70000000E-01
THE OPTIMUM L/V IS ACCURATE TO +/R- 4.73750010-02
THE COST OF OVERHEAD PRODUCT FROM COL II ($/#) =
5.04818140-02

TOWER DIAMETER (INCHES) = 26.411399
ACTUAL NUMBER OF TRAYS = 1.11983380+01
TOWER COST ($) = 3.35899830E+03
REBOILER AREA (SQ. FT.) = 2.35036570+01
REBOILER COST ($) = 1.00803620+05
CONDENSER AREA (SQ. FT.) = 5.59829150+01
CONDENSER COST ($) = 1.10516150+05
FEED PUMP COST ($) = 2.83307960+03
BOTTOMS PUMP COST ($) = 1.71190820+02

TOTAL PURCHASED EQUIPMENT COST ($) = 5873.1889
TOTAL MAINTENANCE COST ($/#PRODUCT) = 2.15821150-04
TOTAL UTILITY COST ($/#PRODUCT) = 0.37827760E-03

TRIAL			XI	YI	GAMMA1	GAMMA2	TEMP (C)	
1	16	1	0.926563	0.950000	1.00995	4.11493	56.4609	0
2	8	11	0.903125	0.938147	1.01705	3.81603	56.6464	0
3	12	13	0.875782	0.920293	1.02763	3.51106	56.8828	0
4	12	14	0.839844	0.918464	1.04524	3.16878	57.1875	0
5	7	13	0.710157	0.878012	1.14555	2.30915	58.5125	0
6	15	15	0.135938	0.742424	3.69480	1.05180	68.1094	0
7	21	10	0.58000810-02	0.142078	8.47382	1.00007	95.9062	1
8	10	10	0.17150830-03	0.53919420-02	8.70172	1.00000	99.8437	1

A ZERO IN THE RIGHTMOST COLUMN INDICATES THE WILSON EQUATION WAS USED

A ONE IN THE RIGHTMOST COLUMN INDICATES THE MARGULES EQUATION WAS USED

MATERIAL BALANCES

XF1 = 2.30000000E-01
XD1 = 8.70000000E-01
XB2 = 9.50000000E-01
XC1 = 1.00000000E-03
XB2 = 1.00000000E-03
D2 = 1.72400000E+01 #MOLES/HR
F = 1.78400000E+01 #MOLES/HR
B2 = 1.55711170E+00 #MOLES/HR
F2 = 1.83271120E+01 #MOLES/HR
F1 = 1.33031900E+02 #MOLES/HR
B1 = 9.69645560E+01 #MOLES/HR
D1 = 3.60673600E+01 #MOLES/HR
V = 3.48811540E+01
L = 1.78411540E+01

COLUMN I OPTIMIZATION FOR XD1 = 0.87500000

THE OPTIMUM L/V IN COLUMN I IS 0.15537500
THIS CORRESPONDS TO XD1 = 8.7500000E-01
THE OPTIMUM L/V IS ACCURATE TO +OR- 2.3125000E-03
THE COST OF OVERHEAD PRODUCT FROM COL I ($/#)=
5.4049489E-02

INNER DIAMETER (INCHES) = 28.812177
ACTUAL NUMBER OF TRAYS = 9.4610379E+00
TOWER COST ($) = 5.1073779E+03
REBOILER AREA (SQ. FT.) = 2.3735146E+01
REBOILER COST ($) = 1.1315036E+03
CONDENSER AREA (SQ. FT.) = 6.7206939E+01
CONDENSER COST ($) = 1.2345985E+03
FEED PUMP COST ($) = 2.9602637E+02
BOTTOMS PUMP COST ($) = 2.7708262E+02

TOTAL PURCHASED EQUIPMENT COST ($) = 6036.7833
TOTAL MAINTENANCE COST ($/#PRODUCT) = 1.1416270E-04
TOTAL UTILITY COST ($/#PRODUCT) = 0.5401568E-03

TRIAL			X1	Y1	GAMMA1	GAMMA2	TEMP (C)	
1	15	11	0.694531	0.875000	1.16166	2.33339	58.4531	0
2	9	13	0.825781	0.846869	1.24368	2.28510	58.5408	1
3	9	9	0.303906	0.856153	2.47411	1.24094	58.2031	1
4	10	15	0.188516	0.735981	4.70744	1.04258	63.9844	1
5	20	200	2.1728372E-01	0.420133	7.77734	1.00124	85.9087	1
6	13	10	2.2368837E-02	0.3914152E-01	8.80121	1.00001	98.0605	1
7	9	10	1.7111056E-03	0.5498252E-02	8.70174	1.00000	99.3437	1

A ZERO IN THE RIGHTMOST COLUMN INDICATES THE WILSON EQUATION WAS USED

A ONE IN THE RIGHTMOST COLUMN INDICATES THE MARGULES EQUATION WAS USED

MATERIAL BALANCES

XF1 = 2.3660000E-01
XD1 = 8.7500000E-01
XD2 = 9.3000000E-01
XB1 = 1.0000000E-03
XB2 = 1.0000000E-03
D2 = 1.7240000E+01 MOLES/HR
F = 1.7240000E+01 MOLES/HR
B2 = 1.4794061E+00 MOLES/HR
F2 = 1.8719405E+01 MOLES/HR
F1 = 1.3339779E+02 MOLES/HR
B1 = 9.7453095E+01 MOLES/HR
D1 = 3.5959497E+01 MOLES/HR
V = 4.0599730E+01
L = 6.6400330E+00

COLUMN II OPTIMIZATION FOR XD1 = 0.87500000

THE VALUES CHOSEN FOR THE INITIAL L/V'S IN COLUMN II ARE TOO HIGH.
THEY DO NOT BRACKET THE OPTIMUM L/V.
THE SLOPE AT L/V = 7.0025001E-01 IS :
7.9637232E-03
THE SLOPE AT L/V = 8.0025000E-01 IS :
1.8657147E-02
FOR THE NEXT RUN CHOOSE THE LARGER INITIAL L/V =
7.0025001E-01

PROGRAM STOP AT 49200

```
RV310          19:55        04/24/70
?0.2366,0.95,0.001,0.001,17.24,17.24,1,0.0005,0.0001,20
?20,13.0,58.0,13.0,0.1,0.6,54.9,62.4,54.9,62.4,0.1,0.7,0.7,1.24
?1.0,0,0,0,220.0,970.0,220.0,970.0,150.0,300.0,150.0,300.0,298.0,70.0
?90.0,10.0,0,1.0,1.0,1.0,0.5,0.5,0.1,13.1,0.02,1.0,30.0,3.0,7.0,0.02
?8.0,1
?23,40,40,750,63,0,0,0,0,0,0,0.94,0.7093,0.597754,0.767919,0.0005
?0.2,3,0.0005,0.7,0,0,0.2,3,1,1,0.5
?2,0.25
?0.875
?.1,.1
?0.41,0.60,←
?54.75

TYPE IN COST PER LB ($/#) FOR COL I OVERHEAD?0.034049435
```

COLUMN II OPTIMIZATION FOR XD1 = 0.87500000

THE OPTIMUM L/V IN COLUMN II IS 0.50525001
THIS CORRESPONDS TO XD1 = 3.75000000E-01
THE OPTIMUM L/V IS ACCURATE TO +/- 4.73750001E-02
THE COST OF OVERHEAD PRODUCT FROM COL II ($/#)=
5.04411835E-02

TOWER DIAMETER (INCHES) = 26.411399
ACTUAL NUMBER OF TRAYS = 1.09775342E+01
TOWER COST ($) = 3.69427803E+03
REBOILER AREA (SQ. FT.) = 2.35630011E+01
REBOILER COST ($) = 1.00839197E+03
CONDENSER AREA (SQ. FT.) = 5.59829165E+01
CONDENSER COST ($) = 1.10510157E+03
FEED PUMP COST ($) = 3.33857336E+02
BOTTOMS PUMP COST ($) = 1.19481657E+02

TOTAL PURCHASED EQUIPMENT COST ($) = 5807.3703
TOTAL MAINTENANCE COST ($/#PRODUCT) = 6.18257615E-04
TOTAL UTILITY COST ($/#PRODUCT) = 8.87827749E-03

TRIAL			XI	YI	GAMMA1	GAMMA2	TEMP (C)	
1	16	1	0.926563	0.950000	1.00995	4.11493	56.4609	0
2	3	11	0.903125	0.938147	1.01705	3.81603	56.6484	0
3	12	13	0.875782	0.926293	1.02763	3.51133	56.8885	0
4	12	14	0.839844	0.912464	1.04524	3.16876	57.1875	0
5	10	11	0.894532	0.875422	1.16166	2.23339	58.4551	0
6	12	170	.319342E-01	0.723946	5.79660	1.01740	69.0937	1
7	12	240	.295489E-03	0.353606E-01	3.57463	1.00002	97.5937	1
8	13	10	.952463E-04	0.303760E-02	3.70510	1.00000	99.9141	1

A ZERO IN THE RIGHTMOST COLUMN INDICATES THE WILSON EQUATION WAS USED

A ONE IN THE RIGHTMOST COLUMN INDICATES THE MARGULES EQUATION WAS USED

MATERIAL BALANCES

XF1 = 2.50000000E-01
XD1 = 8.75000000E-01
XD2 = 9.50000000E-01
XB1 = 1.00000000E-03
XB2 = 1.00000000E-03
D1 = 1.70400000E+01 LBS/HR
F1 = 1.70400000E+01 LBS/HR
D2 = 1.47940051E+00 LBS/HR
F2 = 1.57194057E+01 LBS/HR
F1 = 1.00000000E+01 LBS/HR
B1 = 5.74020957E+01 LBS/HR
B1 = 3.59594977E+01 LBS/HR
V = 3.13611547E+01
L = 1.70411547E+01

```
RVSID          20:03        04/24/70

?0.2568,0.95,0.001,0.001,17.24,17.24,1,0.0005,0.0001,20

?20,18.0,58.0,18.0,0.1,0.8,54.9,62.4,54.9,62.4,0.1,0.7,0.7,1.24

?1.0,0,0,0,220.0,970.0,220.0,970.0,150.0,300.0,150.0,300.0,298.0,70.0

?90.0,10.0,0,1.0,1.0,1.0,0.5,0.5,0.1,16.1,0.02,1.0,30.0,3.0,7.0,0.02

?8.0,1

?28,40,40,700,55,0,0,0,0,0,0,0.94,0.7293,0.597754,0.707919,0.0005

?0.8,3,0.0005,0.7,0,0,0.2,3,1,1,0.5

?2,0.05

?0.375

?.1,.1

?.33,0.60,←

?54.75

TYPE IN COST PER LB ($/#) FOR COL I OVERHEAD?0.064049425


          COLUMN II OPTIMIZATION FOR XD1 =       0.87500000
          ----------------------------------------------------

A PINCH HAS BEEN ENCOUNTERED
THE STAGE TO STAGE CALCULATIONS APPEAR BELOW

 TRIAL          X1          Y1          GAMMA1       GAMMA2       TEMP (C)
 1  16  1    0.926563    0.950000    1.00995      4.11493      56.4639   0
 2   9 13    0.913281    0.942266    1.01375      3.94096      56.5547   0
 3   5 12    0.902344    0.937833    1.01736      3.80676      56.6434   0
 4  11 11    0.895313    0.934274    1.01983      3.72449      56.6953   0
 5  11 12    0.890625    0.931953    1.02159      3.67130      56.7402   0
 6  11 12    0.886719    0.930406    1.02311      3.62795      56.7891   0
 7  12 14    0.883594    0.929117    1.02436      3.59389      56.8125   0
 8   1 12    0.882032    0.928086    1.02500      3.57706      56.8125   0
 9  10 13    0.881251    0.927571    1.02532      3.56839      56.8125   0
10   1  1    0.881251    0.927313    1.02532      3.56369      56.8125   0
0 IN RIGHTMOST COLUMN INDICATES WILSON EQ WAS USED
1 IN RIGHTMOST COLUMN INDICATES MARQULES EQ WAS USED
```

APPENDIX II

COMPUTER PROGRAM

RV010

```
10000       SUBROUTINE COST(TV,RHOLT,RHOLB,BOTV,HEATT,HEATB,UTOP,UBOT,
10100 &     BOTL,SBCOOL,CORR,CP,Z,D,WMT,WMB,WMF,B,FEED,RMCST,
10200 &     UNTCST)
10300       COMMON IC
10400       COMMON PP(5,200),IP(4,200)
10500       COMMON STAGES,BTEMP,TTEMP,CV,SF,DCA,FUDGE,OAEFF,CINDEX,
10600 &     FACMAT,CC1,CC2,CC3,TSTEAM,CWIN,CWOUT,STMCST,CWCST,
10700 &     OLABCST,SPACE,TMCST,CMCST,RBMCST,
10800 &     ELCOST,KIND
10900       COMMON DIAM,ATRAYS,COSTA,RBAREA,COSTB,CDAREA,
11000 &     COSTC,COSTFP,COSTBP,PURCST,OMAINT,UTIL
11100       RHOVT=WMT*492/(359*(TTEMP+460))
11200       UMAXT=CV*(((RHOLT-RHOVT)/RHOVT)**0.5)
11300       RHOVB=WMB*492/(359*(BTEMP+460))
11400       UMAXB=CV*(((RHOLB-RHOVB)/RHOVB)**0.5)
11500       IF(UMAXB-UMAXT) 1,1,2
11600 1     UMAX=UMAXB; RHOV=RHOVB; RHOL=RHOLB; WM=WMB
11700       GO TO 3
11800 2     UMAX=UMAXT; RHOV=RHOVT; RHOL=RHOLT; WM=WMT
11900 3     CONTINUE
12000       UACT=SF*UMAX; TVLB=TV*WM
12100       AREA=(1+DCA)*TVLB/(RHOV*UACT*3600)
12200       DIAM=((4*AREA/3.141592)**0.5)*12
12300       TPRICE=10**(1.89108-0.111341*0.43429*ALOG(DIAM)
12400 &     +0.398702*(0.43429*ALOG(DIAM))**2)
12500       IF(1-KIND) 6,4,7
12600 4     TPRICE=FUDGE*TPRICE
12700 5     GO TO 7
12800 6     TPRICE=10**(CC1+CC2*ALOG(DIAM)+CC3*(ALOG(DIAM))**2)
12900 7     CONTINUE
13000       ATRAYS=STAGES/OAEFF
13100       COSTA=TPRICE*ATRAYS*CINDEX*FACMAT
13200       BOTLLB=BOTL*WMB; BOTVLB=BOTV*WMB
13300       DELTB=TSTEAM- BTEMP
13400       TOUT=TTEMP-SBCOOL
13500       TERM1=TTEMP-CWOUT; TERM2=TOUT-CWIN
13600       IF(TERM2-TERM1) 9,10,8
13700 8     GTTD=TERM2; STTD=TERM1
13800       GO TO 11
13900 9     GTTD=TERM1; STTD=TERM2
14000       GO TO 11
14100 10    TMTD=TERM1
14200       GO TO 12
14300 11    CONTINUE
14400       TMTD=(GTTD-STTD)/(ALOG(GTTD/STTD))
14500 12    CONTINUE
14600       CMTD=CORR*TMTD
14700       DLB=D*WMT
14800       RBAREA=HEATB*BOTVLB/(UBOT*DELTB)
14900       PRICEB=131*(RBAREA)**0.578
```

RV010 CONTINUED

```
      COSTB=PRICEP*CINDEX*FACMAT
      QVAP=HEATD*BOILVLB
      CCOSTB=QVAP*STMCST/(1000000*DLB)
      TVLB=TV*WMT
      QTOP=TVLB*CP*SBCOOL+TVLB*HEATT
      CDAREA=QTOP/(UTOP*CMTD)
      CWRATE=QTOP/(CWPUT-CWIN)
      PRICEC=92.96*(CDAREA)**0.5615
      COSTC=PRICEC*CINDEX*FACMAT
      OCOSTC=CWRATE*CWCST/(1000*8.345*DLB)
      COSTFP=CINDEX*FACMAT*171.9*(Z*WMF/500)**0.209
      COSTBP=CINDEX*FACMAT*171.9*(B*WMB/500)**0.209
      PURCST=COSTA+COSTB+COSTC+COSTFP+COSTBP
      PHP=100*(Z*WMF+B*WMB)/(500*0.60*3960)
      OLABOR=0.25*OLABCST/DLB
      RAWMAT=RMCST*FEED*WMF/DLB
      IMAINT=AREA*SPACE*ATRAYS*1.1*TMCST/(8760*DLB)
      CMAINT=CDAREA*CMCST/(8760*DLB)
      RMAINT=RBAREA*RBMCST/(8760*DLB)
      PMAINF=(CINDEX*0.824*(Z*WMF/500)+72)/(8760*DLB)
      PMAINB=(CINDEX*0.824*(B*WMB/500)+72)/(8760*DLB)
      OMAINT=IMAINT+CMAINT+RMAINT+PMAINF+PMAINB
      COSTKW=PHP*0.746*ELCOST/DLB
      UTIL=OCOSTB+OCOSTC+COSTKW
      UNTCST=3.05*OLABOR+1.4*OMAINT
     &+0.595*PURCST/(8760*DLB)+1.22*UTIL+1.22*RAWMAT
      RETURN; END
      SUBROUTINE MATLBAL(XF1,XD1,XD2,XB1,XB2,D2,TLOV1,TLOV2,P,
     & B2,F2,F1,B1,D1,TV1,TV2,TL1,TL2)
      XF2=XD1
      B2=D2*(XD2-XF2)/(XF2-XB2); F2=B2+D2
      F1=(XB1*(B2+P+D2)-XB2*B2-XD1*P-XD2*D2)/(XB1-XF1)
      B1=(XF1*F1-XB2*B2-XD1*P-XD2*D2)/XB1; D1=F1-B1
      TV1=D1/(1-TLOV1); TV2=D2/(1-TLOV2)
      TL1=TLOV1*TV1; TL2=TLOV2*TV2
      RETURN; END
      SUBROUTINE TRAYS(ILOOPN,JLOOPN,KLOOPN,PT,TEMPT,TEMPXD,
     &                 A1,B1,C1,A2,B2,C2,A12,A21,AA12,AA21,
     & TOLERY,TOL,TOLTEM,TOLSUM,CHANGE,
     &                 IACET,IWATER,TOL1,TOLTM1,E,XB,XF,IOPL,
     & TOPV,D,Q,F,B,I,BOTV,BOTL)
      DIMENSION T(30,50),Y1(30),GAMMA1(50),GAMMA2(50),X1(50),
     &          Y1TRY(30), YDELTA(30), DELSUM(30)
      DIMENSION EE(300)
      COMMON IC
      COMMON PP(5,200),IP(4,200)
      COMMON STAGES,BTEMP,TTEMP
      CONTINUE
      CONTINUE
      CONTINUE
```

RV010 CONTINUED

```
20000       CONTINUE
20100       T(1,1)=TEMPT; X1(1)=TEMPXD; Y1(1)=TEMPXD
20200       IC=0
20300       XI=(XF+(Q-1)*D*Y1(1)/TOPV)/(Q-(Q-1)*TOPL/TOPV)
20400       DO 47 I=1,ILOOPN
20500       DO 45 J=1,JLOOPN
20600       IF (IACET) 3,1,3
20700 1     P10 = 10**(22.57411-2312.5/(T(I,J)+273.2)
20800 &           -5.0325*0.434294*ALOG(T(I,J)+273.2))
20900       IF(1-I) 5,2,5
21000 2     CONTINUE
21100       GO TO 5
21200 3     P10 = 10**(A1-B1/(T(I,J)+C1))
21300       IF(1-I) 5,4,5
21400 4     CONTINUE
21500 5     IF(IWATER) 9,6,9
21600 6     PC=218.167; TA=T(I,J)+273.16; Z=(647.27-TA)
21700       AW=3.2437814;BW=5.86826E-3;CW=1.1702379E-8
21800       DW=2.1378462E-3
21900       P20ATM = 10**(-Z/TA*((AW+BW*Z+CW*Z**3)/(1+DW*Z))
22000 &                    +0.434294*ALOG(PC))
22100       P20 = 760.0*P20ATM
22200       IF(1-I) 8,7,8
22300 7     CONTINUE
22400 8     GO TO 11
22500 9     P20 = 10**(A2-B2/(T(I,J)+C2))
22600       IF(1-I) 11,10,11
22700 10    CONTINUE
22800 11    DO 26 K=1,KLOOPN
22900       IF(CHANGE-E) 12,12,13
23000 12    IW=0
23100       X2 = 1-X1(K)
23200       GAMMA1(K)=EXP(-ALOG(1-AA21*X2)+X2*(X2*AA12/(1-AA12*X1(K))
23300 &                    -X1(K)*AA21/(1-AA21*X2)))
23400       GAMMA2(K)=EXP(-ALOG(1-AA12*X1(K))-X1(K)*(X2*AA12/(1-AA12*X1(K
23500 &                   )-X1(K)*AA21/(1-AA21*X2)))
23600       GO TO 14
23700 13    IW=1
23800       X2 = 1-X1(K)
23900       GAMMA1(K)=10**((2*A21-A12)*X2**2
24000 &                    +2*(A12-A21)*X2**3)
24100       GAMMA2(K)=10**((2*A12-A21)*X1(K)**2
24200 &                    +2*(A21-A12)*X1(K)**3)
24300 14    Y1TRY(K) = GAMMA1(K)*X1(K)*P10/PT
24400       YDELTA(K) = Y1TRY(K)-Y1(I)
24500       IF(ABS(YDELTA(K))-TOLERY) 28,28,15
24600 15    IF(1-K) 17,16,17
24700 16    X1(K+1) = X1(K)-TOL
24800       GO TO 26
24900 17    IF(YDELTA(K-1)) 22,27,18
```

RV010 CONTINUED

```
25000 18   IF(YDELTA(K)) 21,27,19
25100 19   IF(YDELTA(K-1)-YDELTA(K)) 20,27,16
25200 20   T0L = -2.0*T0L
25300      G0 T0 16
25400 21   T0L = -0.5*T0L
25500      G0 T0 16
25600 22   IF(YDELTA(K)) 23,27,25
25700 23   IF(YDELTA(K-1)-YDELTA(K)) 16,27,24
25800 24   T0L = -2.0*T0L
25900      G0 T0 16
26000 25   T0L = -0.5*T0L
26100      G0 T0 16
26200 26   CONTINUE
26300      G0 T0 28
26400 27   PRINT,"ZER0 VALUE IN STATEMENT 17,18,19,22 OR 23"
26500      GO T0 48
26600 28   CONTINUE
26700 29   C0NTINUE
26800      C0NTINUE
26900      CONTINUE
27000 30   CONTINUE
27100      C0NTINUE
27200      C0NTINUE
27300      C0NTINUE
27400 31   CONTINUE
27500      C0NTINUE
27600 32   C0NTINUE
27700      CONTINUE
27800 33   C0NTINUE
27900      T0L=T0L1
28000      X1(1) = X1(K)
28100      X2 = 1-X1(K)
28200      Y2TRY = GAMMA2(K)*X2*P20/PT
28300      SUMY = Y1TRY(K)+Y2TRY
28400      DELSUM(J) = 1-SUMY
28500      C0NTINUE
28600 330  C0NTINUE
28700      IF(ABS(DELSUM(J))-T0LSUM) 46,46,34
28800 34   IF(1-J) 36,35,36
28900 35   T(I,J+1) = T(I,J)+T0LTEM
29000      G0 T0 45
29100 36   IF(DELSUM(J-1)) 41,27,37
29200 37   IF(DELSUM(J)) 40,27,38
29300 38   IF(DELSUM(J-1)-DELSUM(J)) 39,27,35
29400 39   T0LTEM = -2.0*T0LTEM
29500      G0 T0 35
29600 40   T0LTEM = -0.5*T0LTEM
29700      G0 T0 35
29800 41   IF(DELSUM(J)) 42,27,44
29900 42   IF(DELSUM(J-1)-DELSUM(J)) 35,27,43
```

```
RV010        CONTINUED


30000 43    TOLTEM = -2.0*TOLTEM
30100       GO TO 35
30200 44    TOLTEM = -0.5*TOLTEM
30300       GO TO 35
30400 45    CONTINUE
30500 46    T(I+1,1) = T(I,J)
30600       TOLTEM=TOLTM1
30700       BTEMP=T(I,J)*1.8 + 32
30800       IF(1-I) 459,458,459
30900 458
31000       TTEMP=T(1,J)*1.8 + 32
31100 999   FORMAT(2X,"TRIAL",10X,"X1",10X,"Y1",
31200 &             8X,"GAMMA1",6X,"GAMMA2",5X,"TEMP (C)"//)
31300 459
31400 460   FORMAT(/3I3,5G12.6,I3)
31500       IC=IC+1
31600       IP(1,IC)=I; IP(2,IC)=J; IP(3,IC)=K
31700       PP(1,IC)=X1(K); PP(2,IC)=Y1(I); PP(3,IC)=GAMMA1(X)
31800       PP(4,IC)=GAMMA2(K); PP(5,IC)=T(I,J); IP(4,IC)=IW
31900       E=X1(K)
32000       EE(I+1)=E;EE(1)=0
32100       IF(EE(I)-EE(I+1))  4605,4601,4605
32200 4601  PRINT,"A PINCH HAS BEEN ENCOUNTERED"
32300       PRINT,"THE STAGE TO STAGE CALCULATIONS APPEAR BELOW"
32400       PRINT 4602
32500 4602  FORMAT(//2X,"TRIAL",10X,"X1",10X,"Y1",
32600 &     8X,"GAMMA1",6X,"GAMMA2",5X,"TEMP (C)"/)
32700       DO 4604 IZ=1,IC
32800       PRINT 4603, IP(1,IZ),IP(2,IZ),IP(3,IZ),PP(1,IZ),
32900 &     PP(2,IZ),PP(3,IZ),PP(4,IZ),PP(5,IZ),IP(4,IZ)
33000 4603  FORMAT(3I3,5G12.6,I3)
33100 4604  CONTINUE
33200       PRINT,"0 IN RIGHTMOST COLUMN INDICATES WILSON EQ WAS USED"
33300       PRINT,"1 IN RIGHTMOST COLUMN INDICATES MARGULES EQ WAS USED"
33400       STOP
33500 4605  CONTINUE
33600       STAGES=(I-1)+(EE(I)-XB)/(EE(I)-EE(I+1))
33700       IF(E-XB) 48,48,461
33800 461   IF(E-XI) 463,463,462
33900 462   TOPLOV=TOPL/TOPV
34000       Y1(I+1)=TOPLOV*E + D*Y1(1)/TOPV
34100       GO TO 47
34200 463   BOTL=TOPL+Q*F
34300       BOTV=TOPV-(1-Q)*F
34400       BOTLOV=BOTL/BOTV
34500       Y1(I+1)=BOTLOV*E - B*XB/BOTV
34600 47    CONTINUE
34700 48    CONTINUE
34800       RETURN; END
34900       DIMENSION COST1(50),COST2(50),XD1(50),TLOV1(50),TLOV2(50)
```

```
RV010       CONTINUED

35000       DIMENSION REFLUX(50),GLOV1(50),GLOV2(50)
35100       DIMENSION WEIGHT(50)
35200       COMMON IC
35300       COMMON PP(5,200),IP(4,200)
35400       COMMON STAGES,BTEMP,TTEMP,CV,SF,DCA,FUDGE,OAEFF,CINDEX,
35500 &     FACMAT,CC1,CC2,CC3,TSTEAM,CWIN,CWOUT,STMCST,CWCST,
35600 &     OLABCST,SPACE,TMCST,CMCST,RBMCST,
35700 &     ELCOST,KIND
35800       COMMON DIAM,ATRAYS,COSTA,RDAREA,COSTB,CDAREA,
35900 &     COSTC,COSTFP,COSTBP,PURCST,OMAINT,UTIL
36000
36100       INPUT,XF1,XD2,XB1,XB2,D2,P,
36200 &     NXD1,DELTA,TOLSLP,LOOPKN
36300       INPUT,NLOOPN,WNB1,WNT2,WMB2,CV,SF,RHOLT1,
36400 &     RHOLB1,RHOLT2,RHOLB2,DCA,FUDGE,OAEFF,CINDEX,FACMAT,
36500 &     CC1,CC2,CC3,HEATT1,HEATB1,HEATT2,HEATB2,UTOP1,
36600 &     UBOT1,UTOP2,UBOT2,TSTEAM,CWIN,CWOUT,SBCOL1,
36700 &     SBCOL2,CORR1,CORR2,STMCST,CP1,CP2,CWCST,WMF1,
36800 &     RMCST,SPACE,TMCST,CMCST,RBMCST,ELCOST,OLABCST,KIND
36900       INPUT,ILOOPN,JLOOPN,KLOOPN,PT,TEMPT,A1,B1,C1,A2,B2,C2,
37000 &           A12,A21,AA12,AA21,TOLERY,TOL,TOLTEM,TOLSUM,CHANGE,
37100 &           IACET,IWATER,TOL1,TOLTM1,Q1,Q2,DUMMY
37200       INPUT,NUMBER,OUT
37300       INPUT,(XD1(MOP), MOP=1,NXD1)
37400       KAT=4*NXD1; KL=0; KN=0
37500       INPUT,(GLOV1(IT),IT=1,KAT,2); INPUT,(GLOV2(IT),IT=1,KAT,2)
37600       INPUT,(WEIGHT(MG), MG=1,NXD1)
37700       DO 18  M=1,NXD1
37800       WMT1=WEIGHT(M)
37900       IF(2-NUMBER) 7777,7010,7777
38000 7777  PRINT 700, XD1(M)
38100 700   FORMAT(///10X,"COLUMN I OPTIMIZATION FOR XD1 = ",G16.8)
38200       PRINT 701
38300 701   FORMAT(10X,"----------------------------------------
38400       &-----",//)
38500 7010  KKK=0
38600       XF2=XD1(M)
38700       CONTINUE
38800       IF(2-NUMBER) 829,828,829
38900 828   PRINT,"TYPE IN COST PER LB ($/#) FOR COL I OVERHEAD"
39000       INPUT,UNTCST1; GO TO 99
39100 829   CONTINUE
39200       DO 1   L=1,4
39300       TEMPXD=XD1(M)
39400       KL=KL+1
39500       KLHALF=KL/2; KLTEST=2*KLHALF
39600       IF(KL-KLTEST) 831,830,831
39700 830   GLOV1(KL)=GLOV1(KL-1)+DELTA
39800 831   CONTINUE
39900       TLOV1(L)=GLOV1(KL)
```

RV010 CONTINUED

```
40000       TEMLV1=TL0V1(L)
40100       CALL MATLBAL(XF1,TEMPXD,XD2,XB1,XB2,D2,TEMLV1,DUMMY,P,
40200 &                  B2,F2,F1,B1,D1,TV1,TV2,TL1,TL2)
40300       CALL TRAYS(IL00PN,JL00PN,KL00PN,PT,TEMPT,TEMPXD,
40400 &                A1,B1,C1,A2,B2,C2,A12,A21,AA12,AA21,
40500 &     T0LERY,T0L,T0LTEM,T0LSUM,CHANGE,
40600 &                IACET,IWATER,T0L1,T0LTM1,TEMPXD,XB1,XF1,TL1,
40700 &     TV1,D1,Q1,F1,B1,ITRAY1,B0TV1,B0TL1)
40800       CALL C0ST(TV1,RH0LT1,RH0LB1,B0TV1,HEATT1,HEATB1,UT0P1,UB0T1,
40900 &     B0TL1,SBC0L1,C0RR1,CP1,F1,D1,WMT1,WMB1,WMF1,B1,
41000 &     F1,RMCST,UNTCST1)
41100       C0ST1(L)=UNTCST1
41200       CONTINUE
41300 1     CONTINUE
41400       FA=(C0ST1(2)-C0ST1(1))/(TL0V1(2)-TL0V1(1))
41500       FB=(C0ST1(4)-C0ST1(3))/(TL0V1(4)-TL0V1(3))
41600 222   CONTINUE
41700 2     A=(TL0V1(1)+TL0V1(2))/2
41800       B=(TL0V1(3)+TL0V1(4))/2
41900       SPAN1=ABS(B-A)
42000       IF(FA*FB) 3,3,19
42100 3     DO 9  N=1,NL00PN
42200       X=(A+B)/2
42300       REFLUX(N)=X
42400       IF(1-N) 33,333,33
42500 33    S=(REFLUX(N)-REFLUX(N-1))/SPAN1
42600       IF(ABS(S)-0UT) 99,99,333
42700 333   D0 5 I=1,2
42800       TEMPXD=XD1(M)
42900       TEMLV1=X
43000       CALL MATLBAL(XF1,TEMPXD,XD2,XB1,XB2,D2,TEMLV1,DUMMY,P,
43100 &                  B2,F2,F1,B1,D1,TV1,TV2,TL1,TL2)
43200       CALL TRAYS(IL00PN,JL00PN,KL00PN,PT,TEMPT,TEMPXD,
43300 &     A1,B1,C1,A2,B2,C2,A12,A21,AA12,AA21,T0LERY,
43400 &     T0L,T0LTEM,T0LSUM,CHANGE,
43500 &     IACET,IWATER,T0L1,T0LTM1,TEMPXD,XB1,XF1,TL1,
43600 &     TV1,D1,Q1,F1,B1,ITRAY1,B0TV1,B0TL1)
43700       CALL C0ST(TV1,RH0LT1,RH0LB1,B0TV1,HEATT1,HEATB1,UT0P1,
43800 &     UB0T1,B0TL1,SBC0L1,C0RR1,CP1,F1,D1,WMT1,WMB1,
43900 &     WMF1,B1,F1,RMCST,UNTCST1)
44000       C0ST1(I)=UNTCST1
44100       IF(2-I) 5,5,4
44200 4     X=X+DELTA
44300 5     CONTINUE
44400       FX=(C0ST1(I)-C0ST1(I-1))/DELTA
44500       IF(ABS(FX)-T0LSLP) 99,99,6
44600 6     IF(FX*FA) 7,22,8
44700 7     B=X-DELTA/2; FB=FX
44800       GO TO 9
44900 8     A=X-DELTA/2; FA=FX
```

RV010 CONTINUED

```
45000 9     CONTINUE
45100       PRINT,"(DO 9 N=1,NLOOPN) LOOP NOT CONVERGED"
45200       GO TO 24
45300 99    CONTINUE
45400       ACC1=ABS(S*SPAN1)
45500       IF(2-NUMBER) 7100,7110,7100
45600 7100  PRINT 711,REFLUX(N-1)
45700 711   FORMAT(// " THE OPTIMUM L/V IN COLUMN I IS ",G16.8)
45800       PRINT,"THIS CORRESPONDS TO XD1 = ",XD1(M)
45900       PRINT,"THE OPTIMUM L/V IS ACCURATE TO +OR- ",ACC1
46000       PRINT,"THE COST OF OVERHEAD PRODUCT FROM COL I ($/#)="
46100       PRINT,COST1(I); GO TO 714
46200 7110  CONTINUE
46300       IF(1-NUMBER) 999,18,999
46400 999   CONTINUE
46500       PRINT 702, XD1(M)
46600 702   FORMAT(///10X,"COLUMN II OPTIMIZATION FOR XD1 = ",G16.8)
46700       PRINT 703
46800 703   FORMAT(10X,"----------------------------------------------
46900       &-----",//)
47000       KKK=1
47100       OVHDCST=UNTCST1
47200       DO 10  N=1,4
47300       TEMPXD=XD1(N); TEMPXD2=XD2
47400       KN=KN+1
47500       KNHALF=KN/2; KNTEST=2*KNHALF
47600       IF(KN-KNTEST) 841,840,841
47700 840   GLOV2(KN)=GLOV2(KN-1)+DELTA
47800 841   CONTINUE
47900       TLOV2(N)=GLOV2(KN)
48000       TEMLV2=TLOV2(N)
48100       CALL MATLBAL(XF1,TEMPXD,XB2,XB1,XD2,D2,DUMMY,TEMLV2,P,
48200 &                  B2,F2,F1,B1,D1,TV1,TV2,TL1,TL2)
48300       CALL TRAYS(ILOOPN,JLOOPN,KLOOPN,PT,TEMPT,TEMPXD2,
48400 &              A1,B1,C1,A2,D2,C2,A12,A21,AA12,AA21,
48500 &     TOLERY,TOL,TOLTEM,TOLSUM,CHANGE,
48600 &     IACCT,IWATER,TOL1,TOLTM1,TEMPXD2,XB2,XF2,TL2,TV2,
48700 &     D2,Q2,F2,B2,ITRAY2,BOTV2,BOTL2)
48800       CALL COST(TV2,RHOLT2,RHOLB2,BOTV2,HEATT2,HEATB2,UTOP2,
48900 &     LBOT2,BOTL2,SBOIL2,CORR2,CP2,D1,D2,WMT2,WMB2,
49000 &     WMT1,B2,F2,OVHDCST,UNTCST2)
49100       COST2(N)=UNTCST2
49200       CONTINUE
49300 10    CONTINUE
49400       FA=(COST2(2)-COST2(1))/(TLOV2(2)-TLOV2(1))
49500       FB=(COST2(4)-COST2(3))/(TLOV2(4)-TLOV2(3))
49600 101   CONTINUE
49700 11    A=(TLOV2(1)+TLOV2(2))/2
49800       B=(TLOV2(3)+TLOV2(4))/2
49900       SPAN2=ABS(B-A)
```

RV010 CONTINUED

```
50000       IF(FA*FB) 600,600,20
50100 600   CONTINUE
50200       DO 17 K=1,LOOPKN
50300       X=(A+B)/2
50400       REFLUX(K)=X
50500       IF(1-K) 110,111,110
50600 110   S=(REFLUX(K)-REFLUX(K-1))/SPAN2
50700       IF(ABS(S)-OUT) 712,712,111
50800 111   DO 13 I=1,2
50900       TEMPXD=XD1(M); TEMPXD2=XD2
51000       TEMLV2=X
51100       CALL MATLBAL(XF1,TEMPXD,XD2,XB1,XB2,D2,DUMMY,TEMLV2,P,
51200 &     B2,F2,F1,B1,D1,TV1,TV2,TL1,TL2)
51300       CALL TRAYS(ILOOPN,JLOOPN,KLOOPN,PT,TEMPT,TEMPXD2,
51400 &     A1,B1,C1,A2,B2,C2,A12,A21,AA12,AA21,
51500 &     TOLERY,TOL,TOLTEM,TOLSUM,CHANGE,
51600 &     IACET,IWATER,TOL1,TOLIM1,TEMPXD2,XB2,XF2,TL2,TV2,
51700 &     D2,Q2,F2,B2,ITRAY2,BOTV2,BOTL2)
51800       CALL COST(TV2,RHOLT2,RHOLB2,BOTV2,HEATT2,HEATB2,UTOP2,
51900 &     UBOT2,BOTL2,SBCOL2,CORR2,CP2,D1,D2,WMT2,WMB2,
52000 &     WMT1,B2,F2,OVHDCST,UNTCST2)
52100       COST2(I)=UNTCST2
52200       IF(2-I) 13,13,12
52300 12    X=X+DELTA
52400 13    CONTINUE
52500       FX=(COST2(I)-COST2(I-1))/DELTA
52600       IF(ABS(FX)-TOLSLP) 170,170,14
52700 14    IF(FX*FA) 15,22,16
52800 15    B=X-DELTA/2; FB=FX
52900       GO TO 17
53000 16    A=X-DELTA/2; FA=FX
53100 17    CONTINUE
53200       PRINT,"(DO 17 K=1,LOOPKN) LOOP NOT CONVERGED"
53300       GO TO 24
53400 170   CONTINUE
53500 712   ACC2=ABS(S*SPAN2)
53600       PRINT 713,REFLUX(K-1)
53700 713   FORMAT(// " THE OPTIMUM L/V IN COLUMN II IS ",G15.8)
53800       PRINT,"THIS CORRESPONDS TO XD1 = ",XD1(M)
53900       PRINT,"THE OPTIMUM L/V IS ACCURATE TO +OR- ",ACC2
54000       PRINT,"THE COST OF OVERHEAD PRODUCT FROM COL II ($/#)="
54100       PRINT,COST2(I)
54200 714   CONTINUE
54300       PRINT 715, DIAM
54400 715   FORMAT(/ " TOWER DIAMETER (INCHES) =",G16.8)
54500       PRINT,"ACTUAL NUMBER OF TRAYS = ",ATRAYS
54600       PRINT,"TOWER COST ($) = ",COSTA
54700       PRINT,"REBOILER AREA (SQ. FT.) = ",RBAREA
54800       PRINT,"REBOILER COST ($) = ",COSTB
54900       PRINT,"CONDENSER AREA (SQ. FT.) = ",CDAREA
```

RV010 CONTINUED

```
55000       PRINT,"CONDENSER COST ($) = ",COSTC
55100       PRINT,"FEED PUMP COST ($) = ",COSTFP
55200       PRINT,"BOTTOMS PUMP COST ($) = ",COSTBP
55300       PRINT 716,PURCST
55400 716   FORMAT(/ " TOTAL PURCHASED EQUIPMENT COST ($) = ",G16.8)
55500       PRINT,"TOTAL MAINTENANCE COST ($/#PRODUCT) = ",OMAINT
55600       PRINT 717,UTIL
55700 717   FORMAT( " TOTAL UTILITY COST ($/#PRODUCT) =",G16.8///)
55800       PRINT 718
55900 718   FORMAT (8X,"TRIAL",10X,"X1",10X,"Y1",
56000 &     8X,"GAMMA1",6X,"GAMMA2",5X,"TEMP (C)"//)
56100       DO 720 IZ=1,IC
56200       PRINT 719,IP(1,IZ),IP(2,IZ),IP(3,IZ),PP(1,IZ),
56300 &     PP(2,IZ),PP(3,IZ),PP(4,IZ),PP(5,IZ),IP(4,IZ)
56400 719   FORMAT(3I3,5G12.6,I3)
56500 720   CONTINUE
56600       PRINT 721
56700 721   FORMAT(/" A ZERO IN THE RIGHTMOST COLUMN INDICATES
56800       & THE WILSON EQUATION WAS USED")
56900       PRINT 722
57000 722   FORMAT(/" A ONE IN THE RIGHTMOST COLUMN INDICATES
57100       & THE MARGULES EQUATION VAS USED"//)
57200       PRINT 723
57300 723   FORMAT(//3X," MATERIAL BALANCES")
57400       PRINT 724
57500 724   FORMAT(3X,"-----------------"//)
57600       PRINT,"XF1 = ",XF1
57700       PRINT,"XD1 = ",XD1(M)
57800       PRINT,"XD2 = ",XD2
57900       PRINT,"XB1 = ",XB1
58000       PRINT,"XB2 = ",XB2
58100       PRINT," D2 = ",D2," MOLES/HR"
58200       PRINT,"  P = ", P," MOLES/HR"
58300       PRINT," B2 = ",B2," MOLES/HR"
58400       PRINT," F2 = ",F2," MOLES/HR"
58500       PRINT," F1 = ",F1," MOLES/HR"
58600       PRINT," B1 = ",B1," MOLES/HR"
58700       PRINT," D1 = ",D1," MOLES/HR"
58800       IF(1-KKK) 726,727,726
58900 726   TLIQ=TL1; TVAP=TV1
59000       GO TO 728
59100 727   TLIQ=TL2; TVAP=TV2
59200 728   PRINT,"  V = ",TVAP
59300       PRINT,"  L = ",TLIQ
59400       PRINT 725
59500 725   FORMAT(///)
59600       IF(1-KKK) 7110,18,7110
59700 18    CONTINUE
59800       GO TO 24
59900 19    IF(FA) 706,704,704
```

RV010 CONTINUED

```
60000 704   PRINT 705
60100 705   FORMAT(// " THE VALUES CHOSEN FOR THE INITIAL L/V'S IN
60200               & COLUMN I ARE TOO HIGH.")
60300       PRINT,"THEY DO NOT BRACKET THE OPTIMUM L/V."
60400       PRINT,"THE SLOPE AT L/V =",A,"    IS :"
60500       PRINT,FA
60600       PRINT,"THE SLOPE AT L/V =",B,"    IS :"
60700       PRINT,FB
60800       PRINT,"FOR THE NEXT RUN CHOOSE THE LARGER INITIAL L/V ="
60900       PRINT,A
61000       PRINT,"THE COSTS OF COL I OVERHEAD PRODUCT FOR THE LESSER"
61100       PRINT,"AND GREATER L/V($/#) ARE, RESPECTIVELY"
61200       PRINT,COST1(1),COST1(3)
61300       GO TO 24
61400 706   PRINT 799
61500 799   FORMAT(// " THE VALUES CHOSEN FOR THE INITIAL L/V'S IN
61600               & COLUMN I ARE TOO LOW.")
61700       PRINT,"THEY DO NOT BRACKET THE OPTIMUM L/V."
61800       PRINT,"THE SLOPE AT L/V =",A,"    IS :"
61900       PRINT,FA
62000       PRINT,"THE SLOPE AT L/V =",B,"    IS :"
62100       PRINT,FB
62200       PRINT,"FOR THE NEXT RUN CHOOSE THE SMALLER INITIAL L/V ="
62300       PRINT,B
62400       PRINT,"THE COSTS OF COL I OVERHEAD PRODUCT FOR THE LESSER"
62500       PRINT,"AND GREATER L/V($/#) ARE, RESPECTIVELY"
62600       PRINT,COST1(1),COST1(3)
62700       GO TO 24
62800 20    IF(FA) 709,707,707
62900 707   PRINT 708
63000 708   FORMAT(// " THE VALUES CHOSEN FOR THE INITIAL L/V'S IN
63100               & COLUMN II ARE TOO HIGH.")
63200       PRINT,"THEY DO NOT BRACKET THE OPTIMUM L/V."
63300       PRINT,"THE SLOPE AT L/V =",A,"    IS :"
63400       PRINT,FA
63500       PRINT,"THE SLOPE AT L/V =",B,"    IS :"
63600       PRINT,FB
63700       PRINT,"FOR THE NEXT RUN CHOOSE THE LARGER INITIAL L/V ="
63800       PRINT,A
63900       PRINT,"THE COSTS OF COL II OVERHEAD PRODUCT FOR THE LESSER"
64000       PRINT,"AND GREATER L/V ARE, RESPECTIVELY"
64100       PRINT,COST2(1),COST2(3)
64200       GO TO 24
64300 709   PRINT 710
64400 710   FORMAT(// " THE VALUES CHOSEN FOR THE INITIAL L/V'S IN
64500               & COLUMN II ARE TOO LOW.")
64600       PRINT,"THEY DO NOT BRACKET THE OPTIMUM L/V."
64700       PRINT,"THE SLOPE AT L/V =",A,"    IS :"
64800       PRINT,FA
64900       PRINT,"THE SLOPE AT L/V =",B,"    IS :"
```

```
RV010       CONTINUED


65000       PRINT,FB
65100       PRINT,"FOR THE NEXT RUN CHOOSE THE SMALLER INITIAL L/V ="
65200       PRINT,B
65300       PRINT,"THE COSTS OF COL II OVERHEAD PRODUCT FOR THE LESSER"
65400       PRINT,"AND GREATER L/V ARE, RESPECTIVELY"
65500       PRINT,COST2(1),COST2(3)
65600       GO TO 24
65700 21    CONTINUE
65800       GO TO 24
65900 22    PRINT,"ZERO VALUE IN STATEMENT 6 OR 14. FA OR FB =0"
66000       GO TO 24
66100 24    STOP
66200       END



LENGTH

22852 CHARACTERS
READY
```

APPENDIX III

PROGRAM FLOW DIAGRAM

A. Dictionary of Important Flow Chart Variables in Order of Appearance

The definitions given below are for those variables referred to in the flow chart. This is not intended to be a complete list. Additional variables have been discussed in the section of this thesis entitled "Specific Input Instructions". Variables which appear in the program but are absent from the above are highly specialized and need not concern the programmer.

1.) Main program

LOOPKN	Loop delimiter[c]
TOLSLP	When the slope of the cost vs L/V curve is less than "TOLSLP" control shifts to a new case.[a,c]
OUT	When the ratio of the current interval to the original interval is less than "OUT" control shifts to a new case.[a,c]
NLOOPN	Loop delimiter[c]
DELTA	A cost is calculated for an input L/V. The L/V is then incremented by "DELTA" and a new cost is computed. These two costs are used together with the magnitude of "DELTA" to determine the slope of the cost vs L/V curve.[c]
NUMBER	is the "TOWER OPTION" variable.[b,c]
NXD1	is the number of values of XD1 to be investigated.[c]
KL	Index for L/V in Column I.
KN	Index for L/V in Column II

KKK	This variable is used to identify which column is currently being analyzed.
FA	is the slope of the L/V vs cost curve computed in the vicinity of the lesser input L/V, for the current case.
FB	is the slope of the L/V vs cost curve computed in the vicinity of the greater input L/V, for the current case.
X	is the value of L/V currently being investigated.
REFLUX(N)	is an array which stores the values of "X".
S	is the interval between the current L/V and the previous L/V.
ACC1	is the accuracy of the optimum L/V for Column I.
ACC2	is the accuracy of the optimum L/V for Column II.
COST1	This array contains the cost/# of overhead from Column I for all cases investigated.
COST2	This array contains the cost/# of overhead from Column II for all cases investigated.

2.) Subroutine trays

ILOOPN	Loop delimiter[c]
JLOOPN	Loop delimiter[c]
KLOOPN	Loop delimiter[c]
E	is the converged liquid composition on the current tray.

CHANGE	is the variable used for selecting either the Wilson or the Margules Equation.[C]
T(1,1)	is the initial trial temperature for the top tray.[C]
Y(1)	is equivalent to "XD1", the composition of the overhead product from Column I.[C]
X(1)	is the initial guess for the liquid composition on the top tray.[C]
TOLERY	is the tolerance allowed for the agreement of "Y(1)" and "Y1TRY".
TOL	is the variable used to increment the liquid composition.
TOLSUM	is the tolerance for Y's = 1.0.
TOLTEM	is the variable used to increment temperature.
XI	is the intersection of the "q-line" with the operating line. This variable determines the optimum feed location. Operating lines are switched when the liquid composition on a tray falls below "XI".
IACET	determines whether the acetone vapor pressure equation will be used.[C]
IWATER	determines whether the water vapor pressure equation will be used.[C]
Y1TRY	is the trial value for vapor composition. Iterations will continue until "Y1TRY" is equal

to the current value of Y1 ± TOLERY. This represents the vapor composition of the more volatile component.

YDELTA — (Y1TRY-Y1)

XB — Bottoms composition

3.) Subroutine cost

FUDGE,KIND — are the variables used to determine which cost equation should be used for the column.[c]

UMAXT — The vapor velocity computed at the top of the column.

UMAXB — The vapor velocity computed at the bottom of the column.

UMAX — The lesser of UMAXT and UMAXB.

TPRICE — Unadjusted cost per tray.

[a]See section entitled "Escape Options".

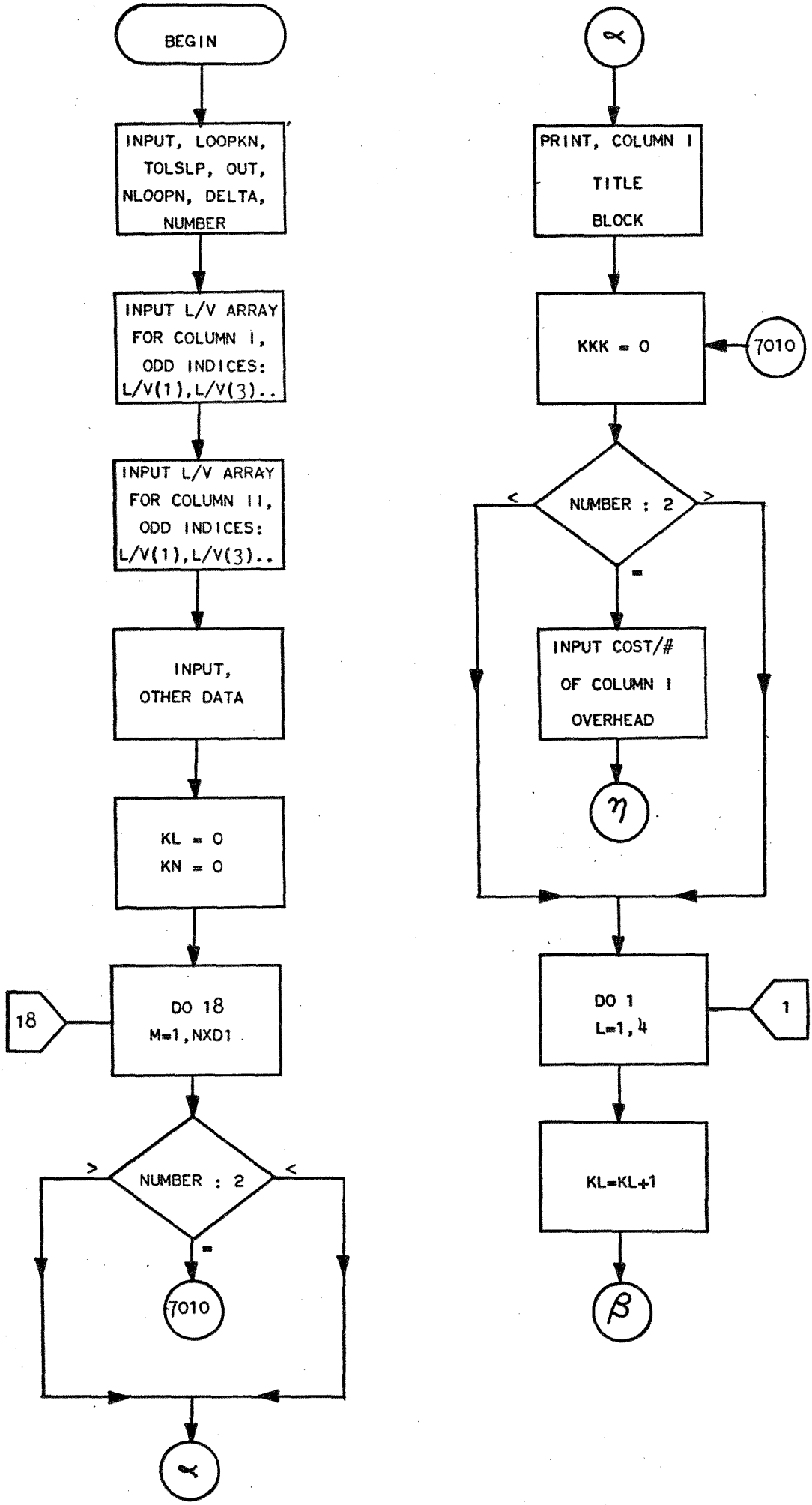
[b]See section entitled "Tower Options".

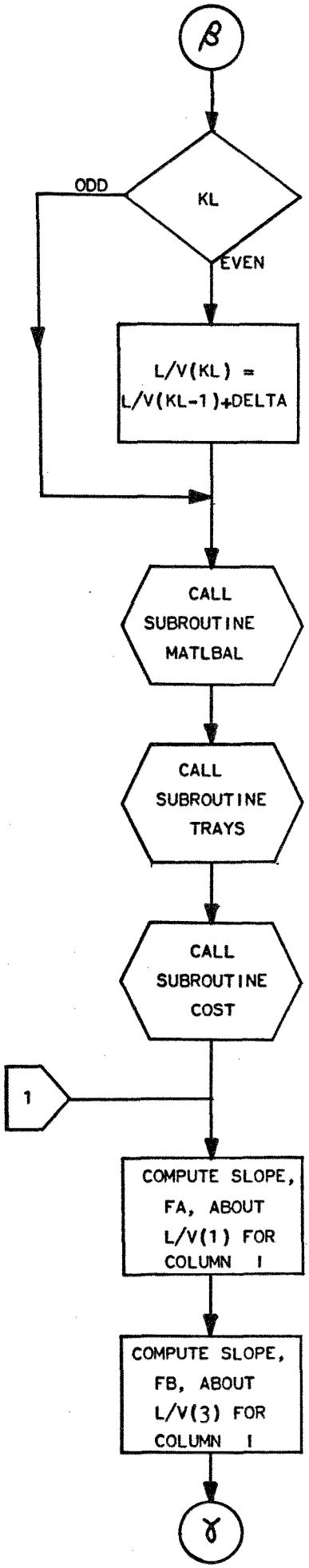
[c]See section entitled "Specific Input Instructions".

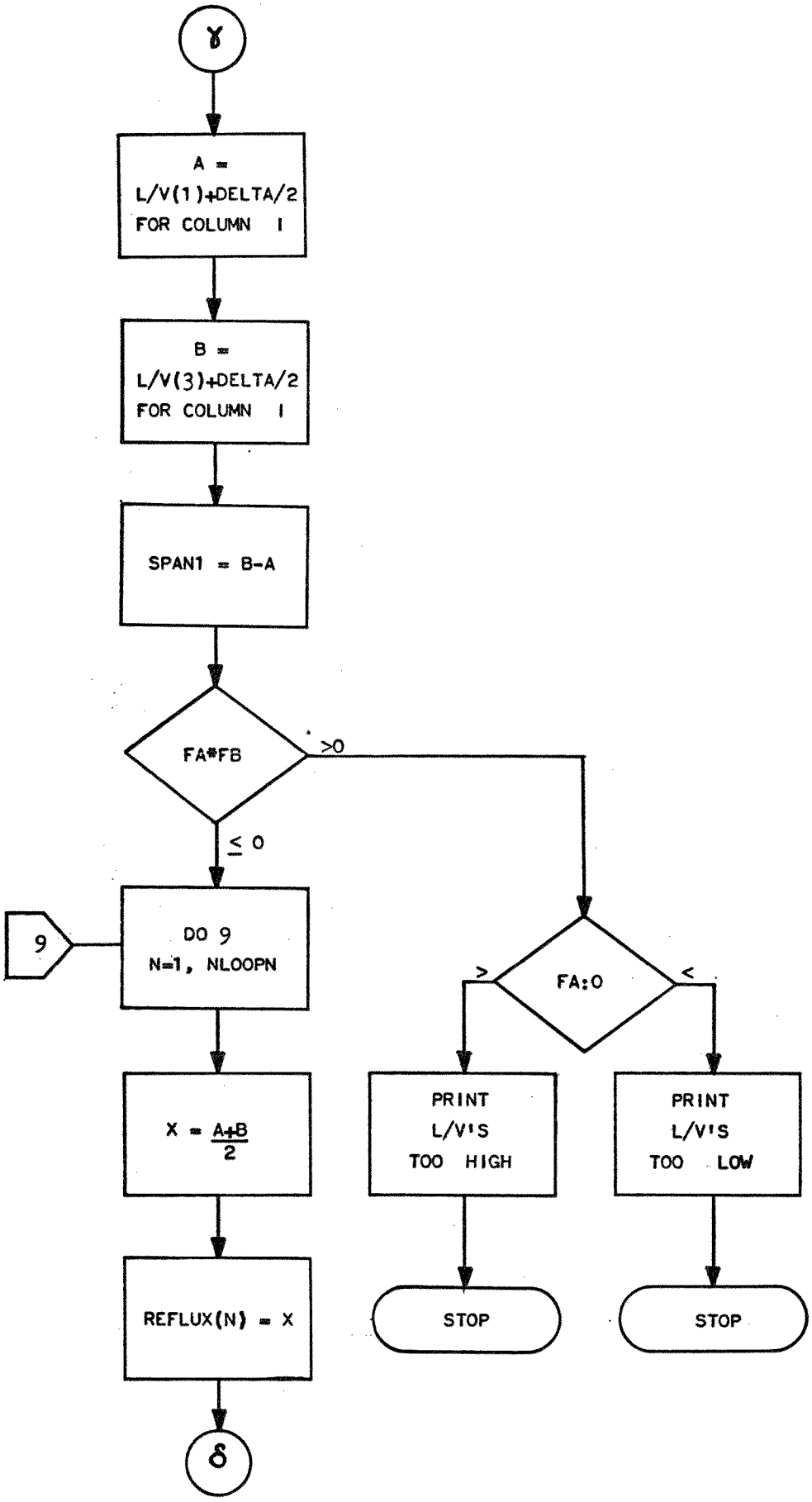
B. Program Flow Charts

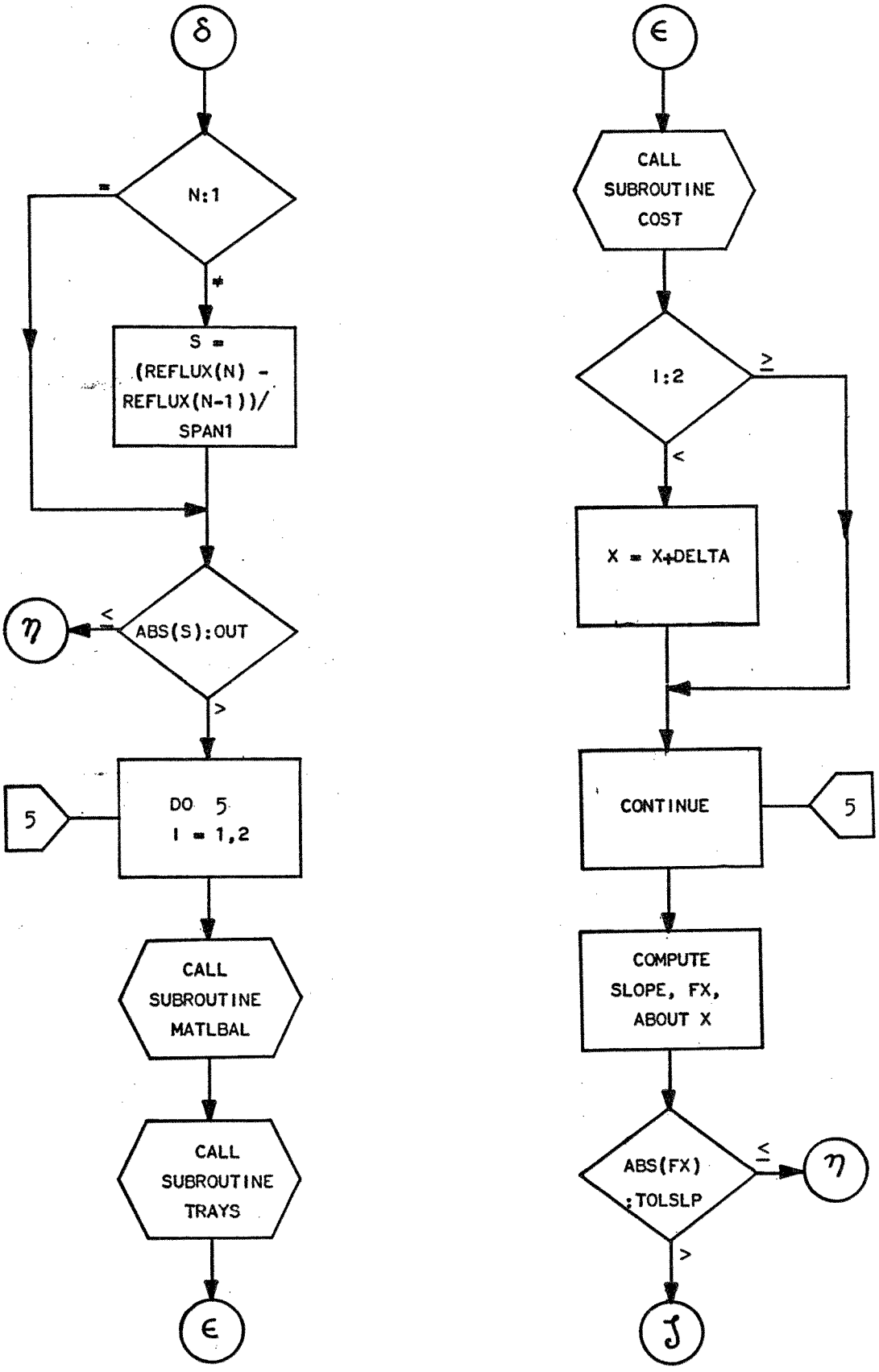
FLOW CHART FOR

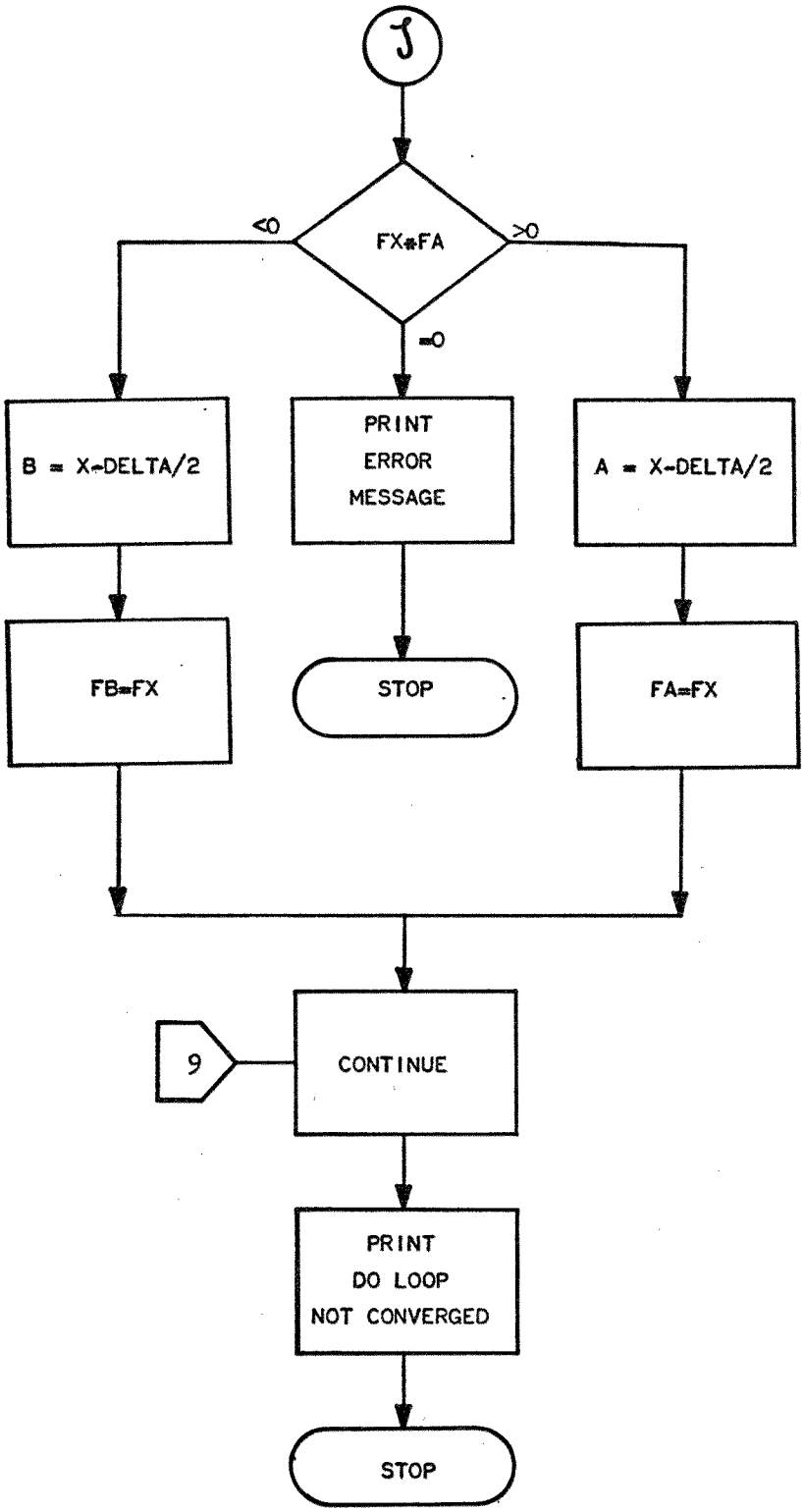
MAIN PROGRAM

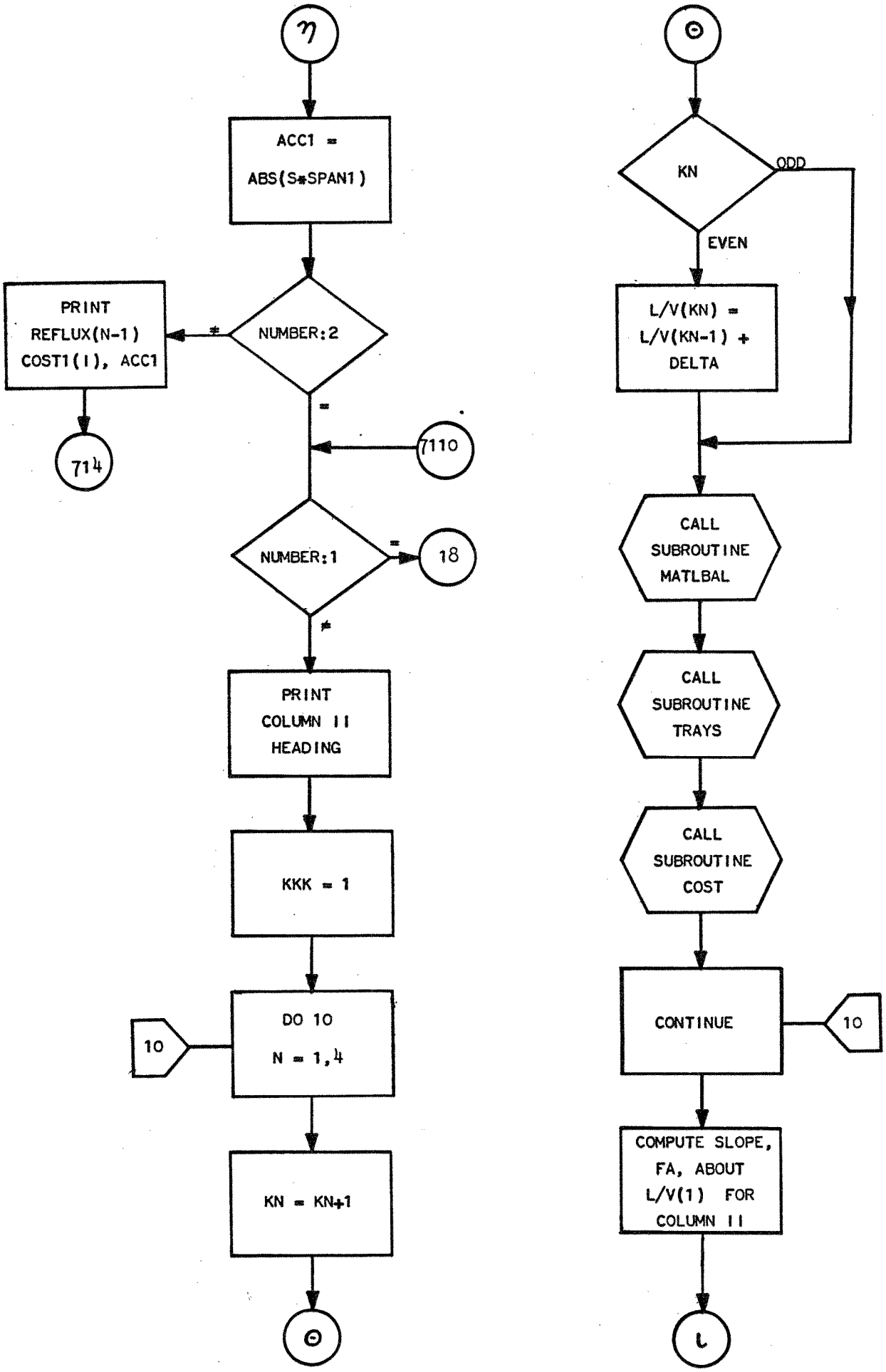

BEGIN
INPUT, LOOPKN, TOLSLP, OUT, NLOOPN, DELTA, NUMBER
INPUT L/V ARRAY FOR COLUMN I, ODD INDICES: L/V(1), L/V(3)..
INPUT L/V ARRAY FOR COLUMN II, ODD INDICES: L/V(1), L/V(3)..
INPUT, OTHER DATA
KL = 0
KN = 0
18
DO 18 M=1, NXD1
NUMBER : 2
>
=
<
7010
α
PRINT, COLUMN I TITLE BLOCK
KKK = 0
7010
NUMBER : 2
<
=
>
INPUT COST/# OF COLUMN I OVERHEAD
η
DO 1 L=1, 4
1
KL=KL+1
β

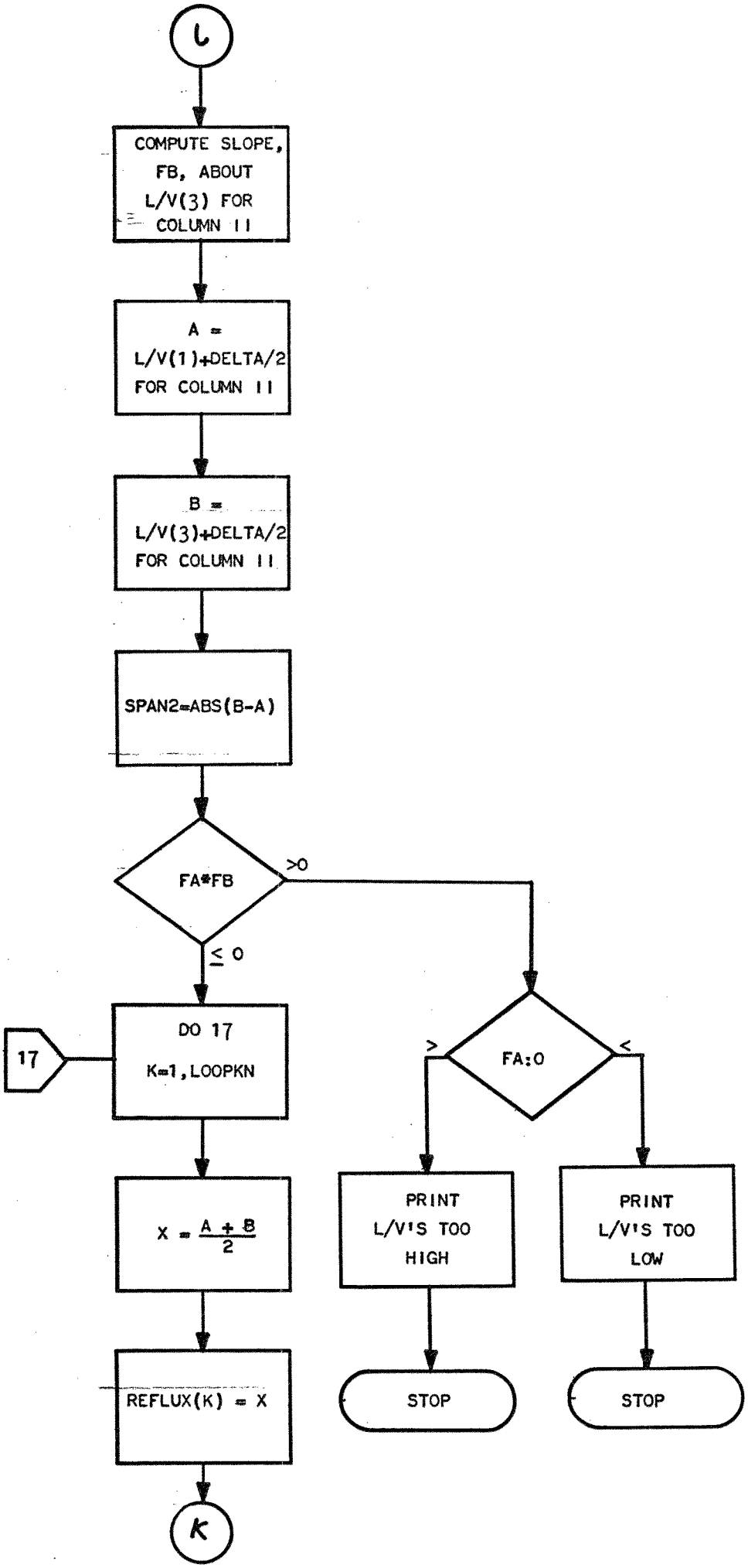

β
KL
ODD
EVEN
L/V(KL) =
L/V(KL-1)+DELTA
CALL
SUBROUTINE
MATLBAL
CALL
SUBROUTINE
TRAYS
CALL
SUBROUTINE
COST
1
COMPUTE SLOPE,
FA, ABOUT
L/V(1) FOR
COLUMN I
COMPUTE SLOPE,
FB, ABOUT
L/V(3) FOR
COLUMN I
γ

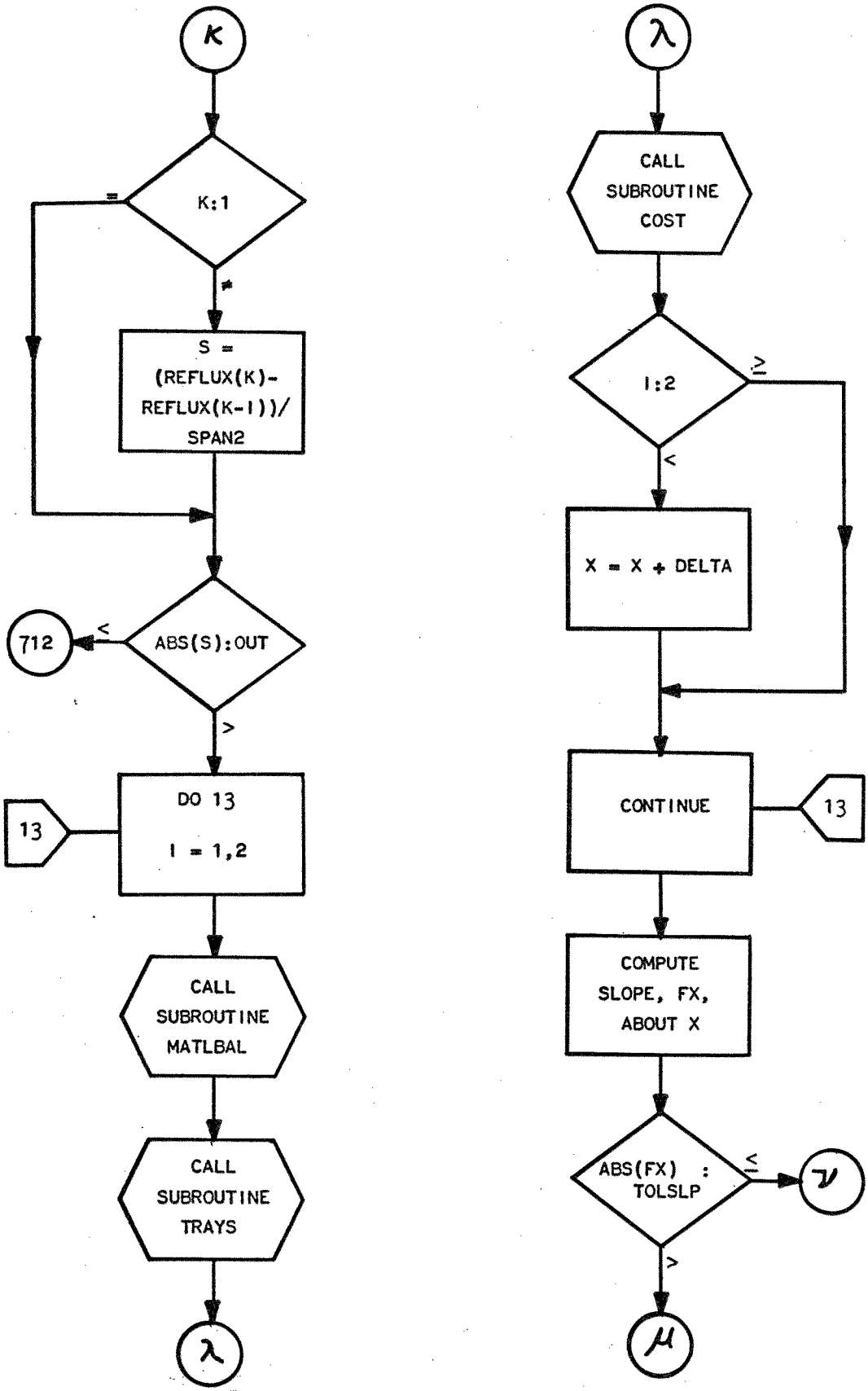

γ
A = L/V(1)+DELTA/2 FOR COLUMN I
B = L/V(3)+DELTA/2 FOR COLUMN I
SPAN1 = B-A
FA*FB
>0
≤ 0
9
DO 9 N=1, NLOOPN
FA:0
>
<
X = A+B/2
PRINT L/V'S TOO HIGH
PRINT L/V'S TOO LOW
REFLUX(N) = X
STOP
STOP
δ

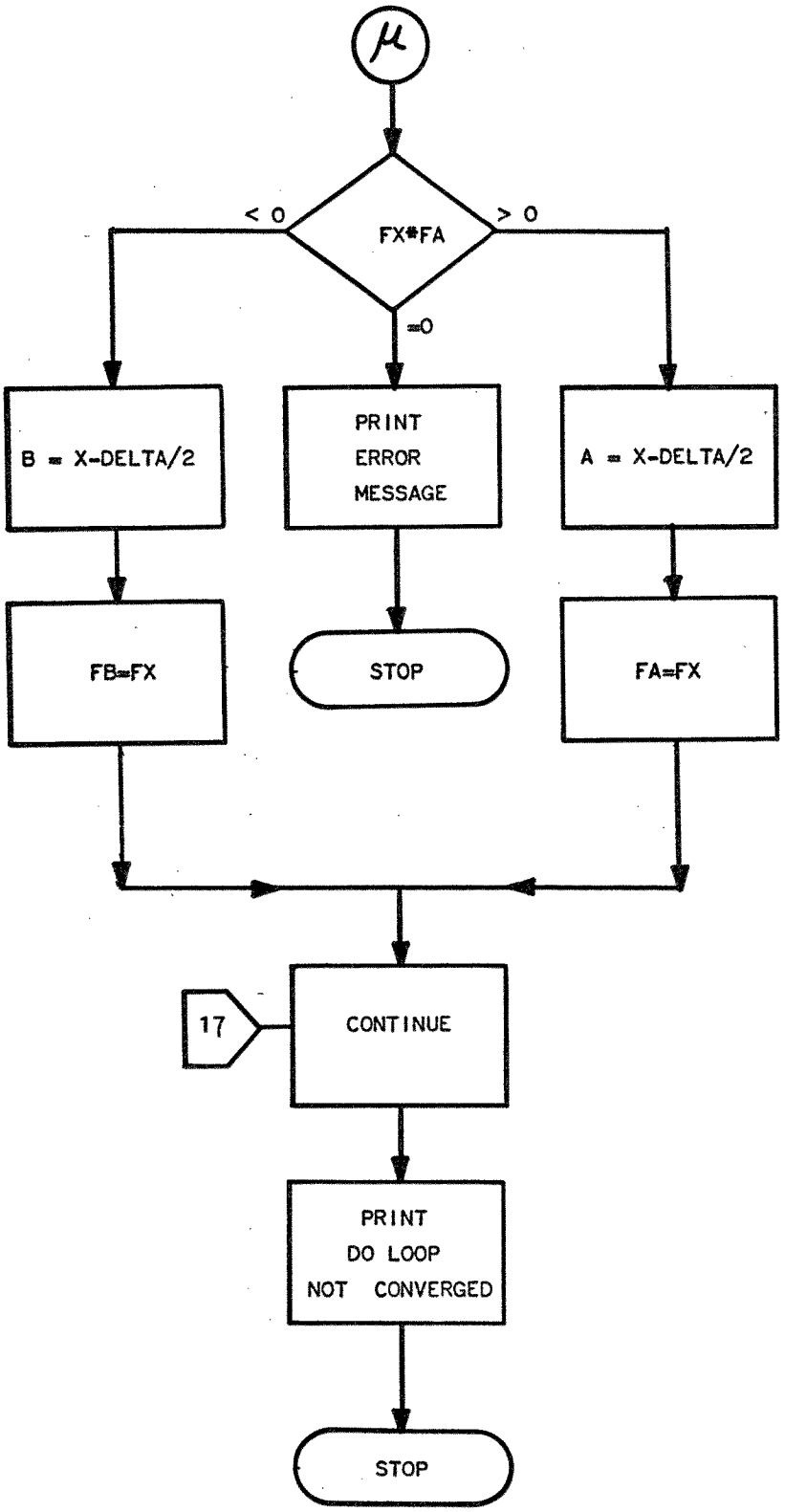

δ
N:1
=
*
S =
(REFLUX(N) -
REFLUX(N-1))/
SPAN1
η
≤
ABS(S):OUT
>
5
DO 5
I = 1,2
CALL
SUBROUTINE
MATLBAL
CALL
SUBROUTINE
TRAYS
ε
ε
CALL
SUBROUTINE
COST
I:2
≥
<
X = X+DELTA
CONTINUE
5
COMPUTE
SLOPE, FX,
ABOUT X
ABS(FX)
:TOLSLP
≤
η
>
J

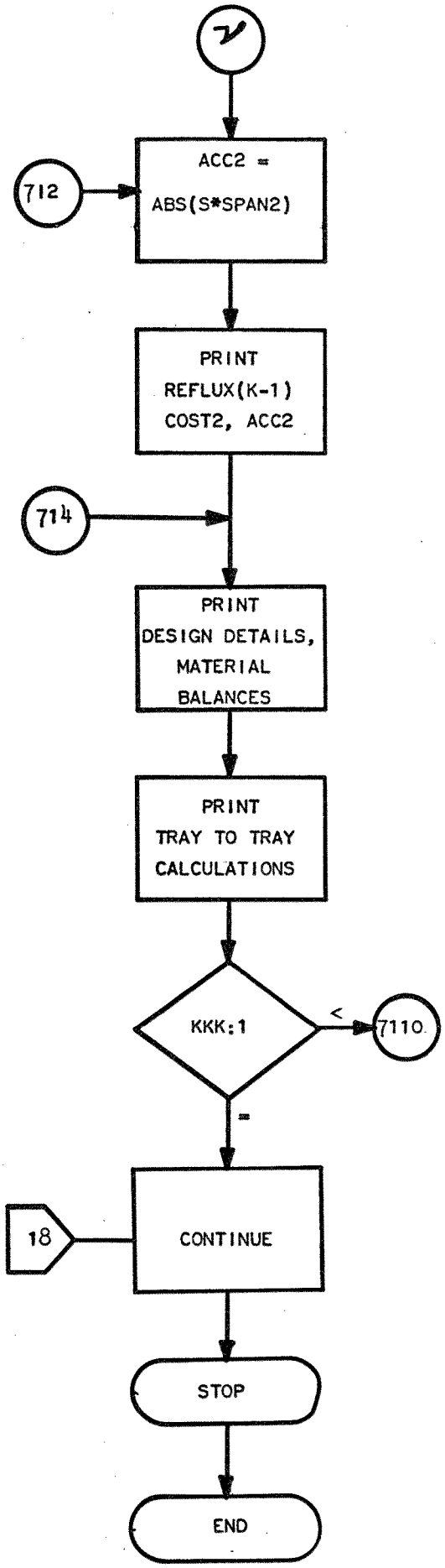

J
FX*FA
<0
=0
>0
B = X-DELTA/2
PRINT
ERROR
MESSAGE
A = X-DELTA/2
FB=FX
STOP
FA=FX
9
CONTINUE
PRINT
DO LOOP
NOT CONVERGED
STOP


η
ACC1 =
ABS(S*SPAN1)
NUMBER:2
*
PRINT
REFLUX(N-1)
COST1(I), ACC1
714
=
7110
NUMBER:1
=
18
*
PRINT
COLUMN II
HEADING
KKK = 1
10
DO 10
N = 1,4
KN = KN+1
Θ
Θ
KN
ODD
EVEN
L/V(KN) =
L/V(KN-1) +
DELTA
CALL
SUBROUTINE
MATLBAL
CALL
SUBROUTINE
TRAYS
CALL
SUBROUTINE
COST
CONTINUE
10
COMPUTE SLOPE,
FA, ABOUT
L/V(1) FOR
COLUMN II
ι


L
COMPUTE SLOPE, FB, ABOUT L/V(3) FOR COLUMN 11
A = L/V(1)+DELTA/2 FOR COLUMN 11
B = L/V(3)+DELTA/2 FOR COLUMN 11
SPAN2=ABS(B-A)
FA*FB
>0
≤ 0
17
DO 17 K=1,LOOPKN
FA:0
>
<
X = A + B / 2
REFLUX(K) = X
PRINT L/V'S TOO HIGH
PRINT L/V'S TOO LOW
STOP
STOP
K

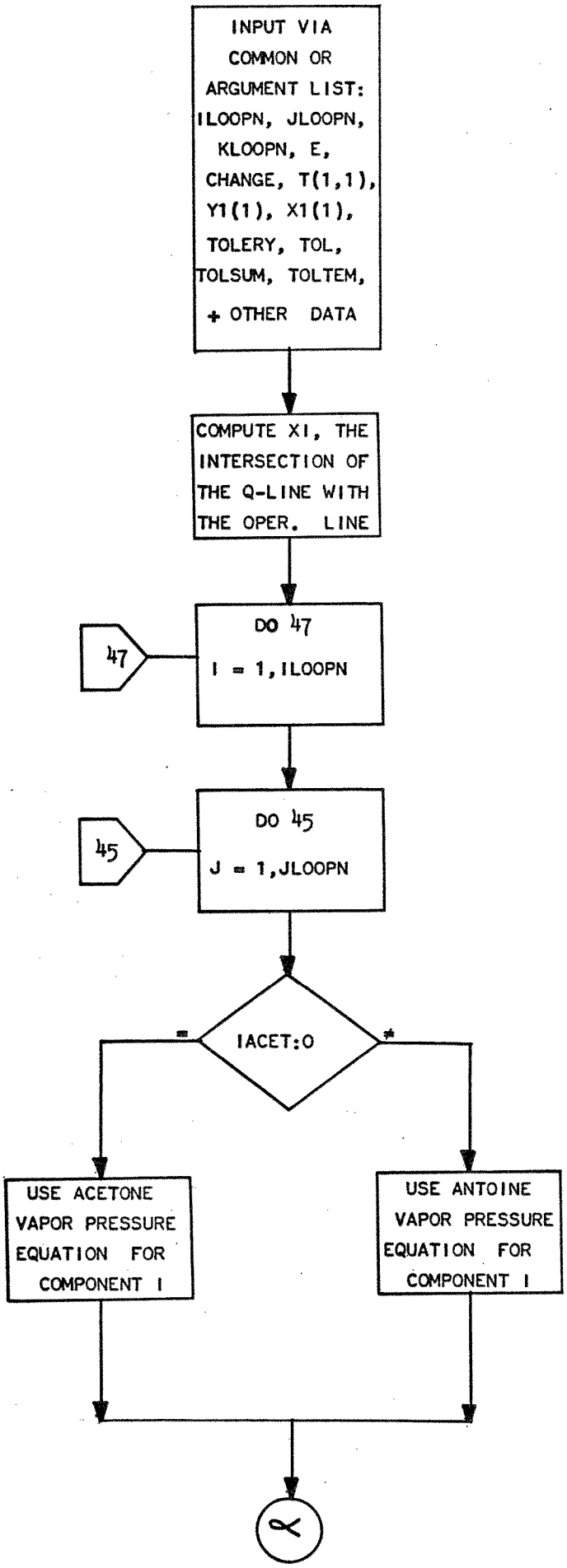

K
K:1
=
≠
S = (REFLUX(K)- REFLUX(K-1))/ SPAN2
712
<
ABS(S):OUT
>
13
DO 13 I = 1,2
CALL SUBROUTINE MATLBAL
CALL SUBROUTINE TRAYS
λ
λ
CALL SUBROUTINE COST
I:2
≥
<
X = X + DELTA
CONTINUE
13
COMPUTE SLOPE, FX, ABOUT X
ABS(FX) : TOLSLP
≤
ν
>
μ

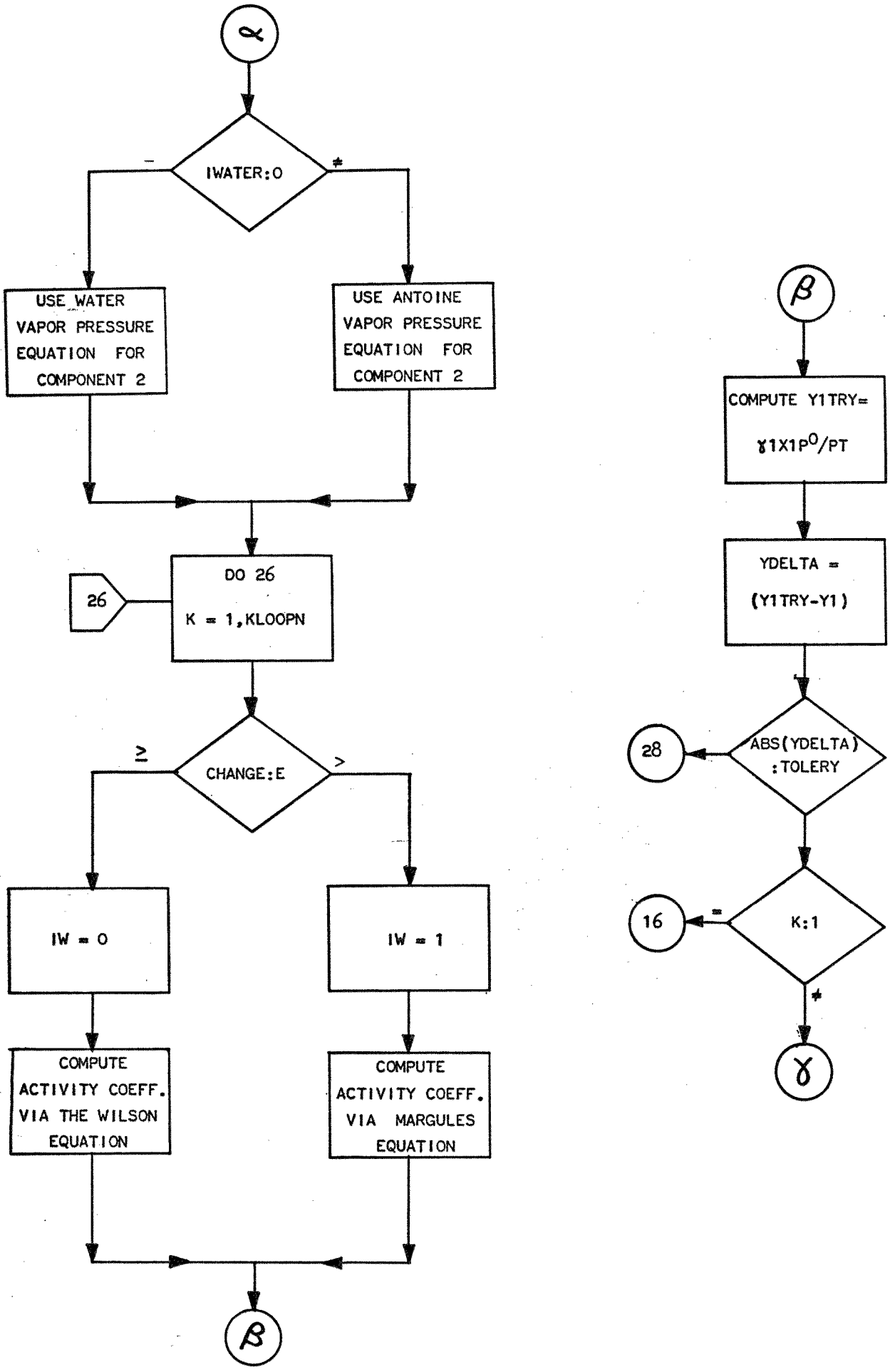

μ
FX*FA
< 0
=0
> 0
B = X-DELTA/2
PRINT
ERROR
MESSAGE
A = X-DELTA/2
FB=FX
STOP
FA=FX
17
CONTINUE
PRINT
DO LOOP
NOT CONVERGED
STOP

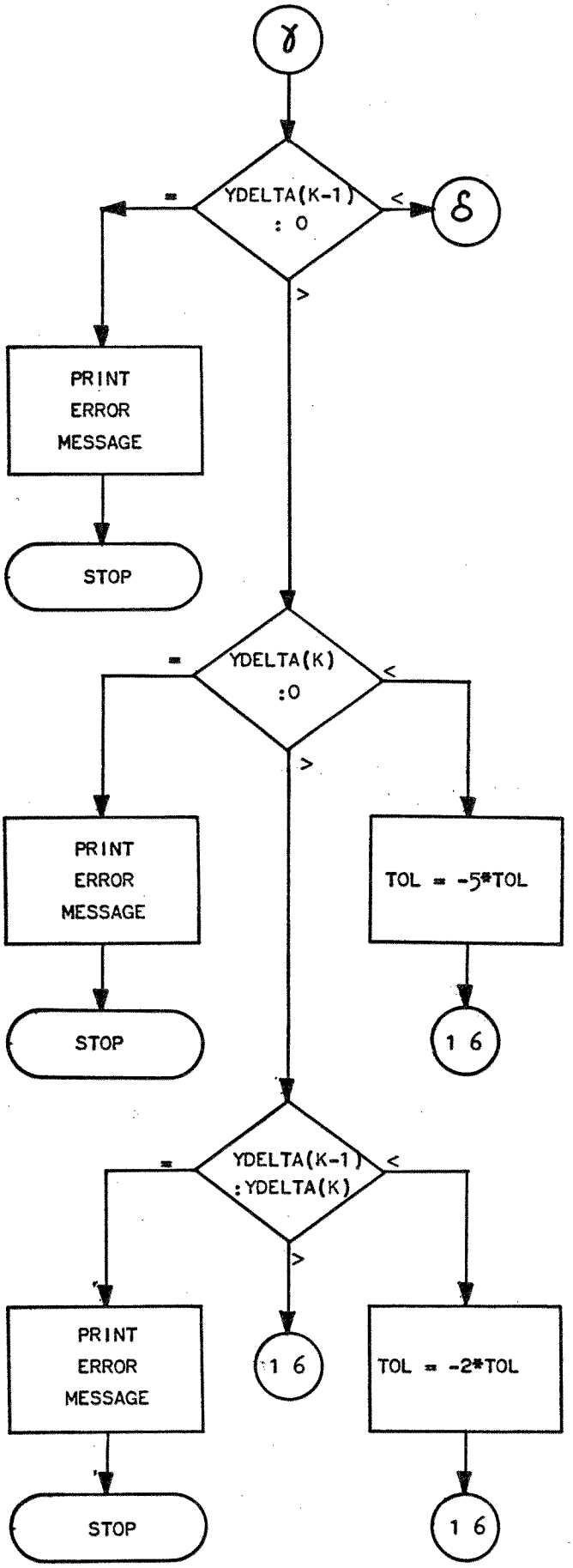

7
712
ACC2 =
ABS(S*SPAN2)
PRINT
REFLUX(K-1)
COST2, ACC2
714
PRINT
DESIGN DETAILS,
MATERIAL
BALANCES
PRINT
TRAY TO TRAY
CALCULATIONS
KKK:1
<
7110
=
18
CONTINUE
STOP
END

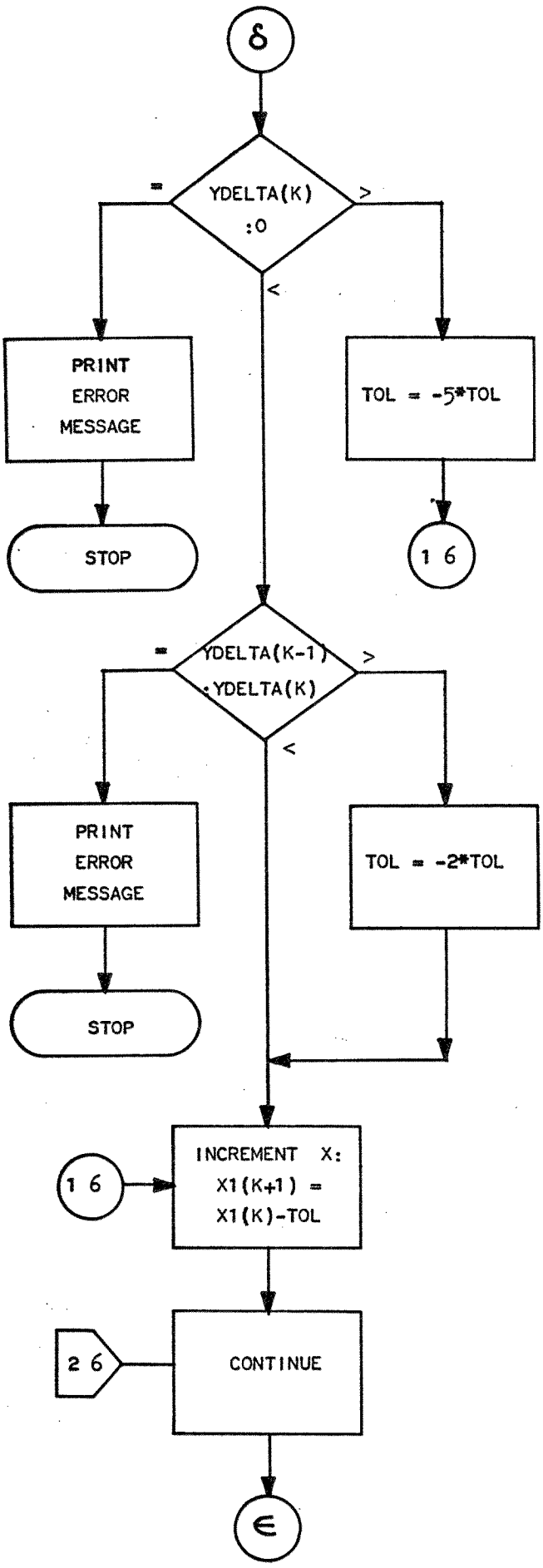
FLOW CHART FOR

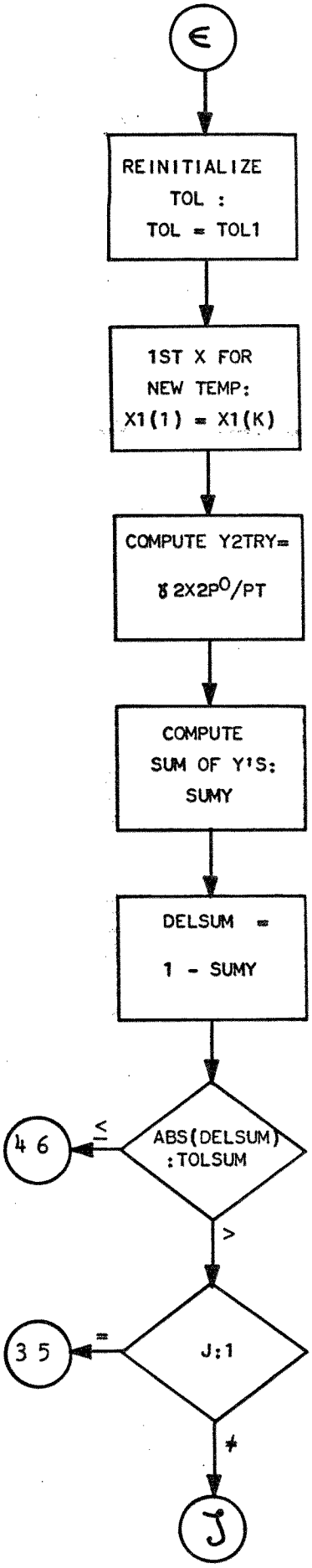
SUBROUTINE TRAYS

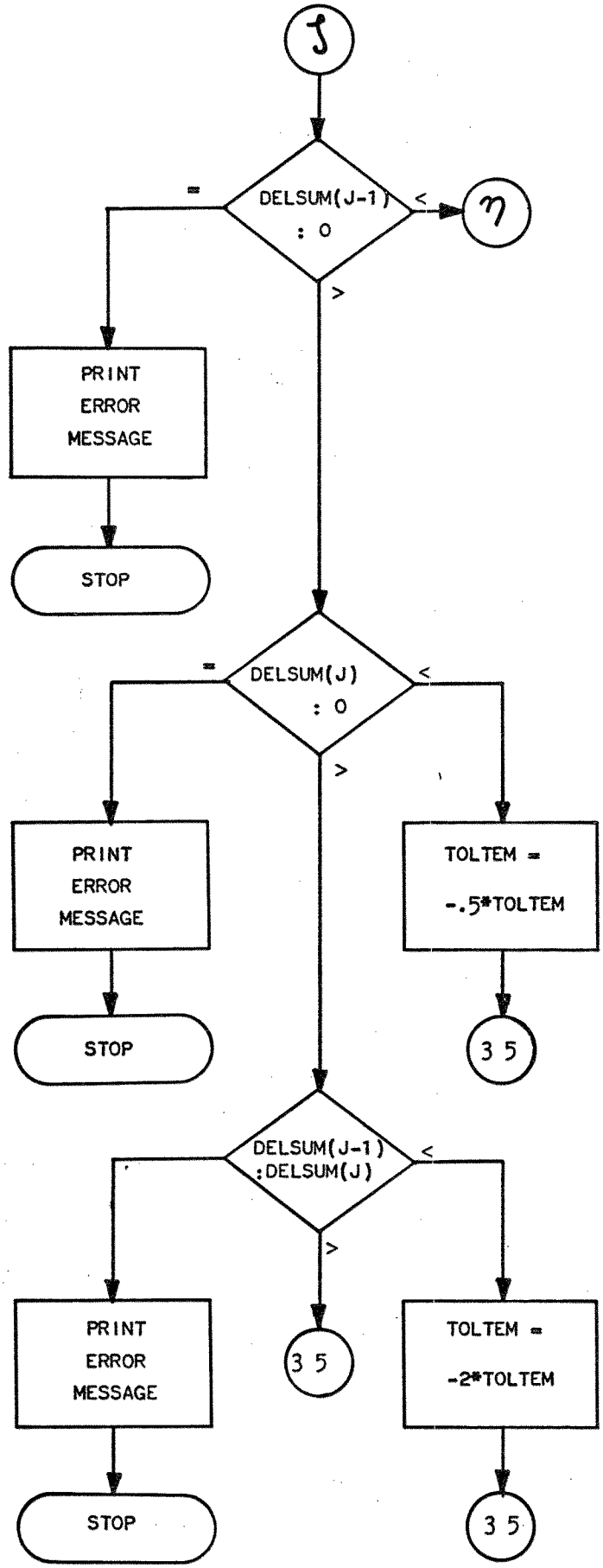

INPUT VIA COMMON OR ARGUMENT LIST: ILOOPN, JLOOPN, KLOOPN, E, CHANGE, T(1,1), Y1(1), X1(1), TOLERY, TOL, TOLSUM, TOLTEM, + OTHER DATA
COMPUTE XI, THE INTERSECTION OF THE Q-LINE WITH THE OPER. LINE
47
DO 47 I = 1,ILOOPN
45
DO 45 J = 1,JLOOPN
IACET:0
=
≠
USE ACETONE VAPOR PRESSURE EQUATION FOR COMPONENT I
USE ANTOINE VAPOR PRESSURE EQUATION FOR COMPONENT I
α

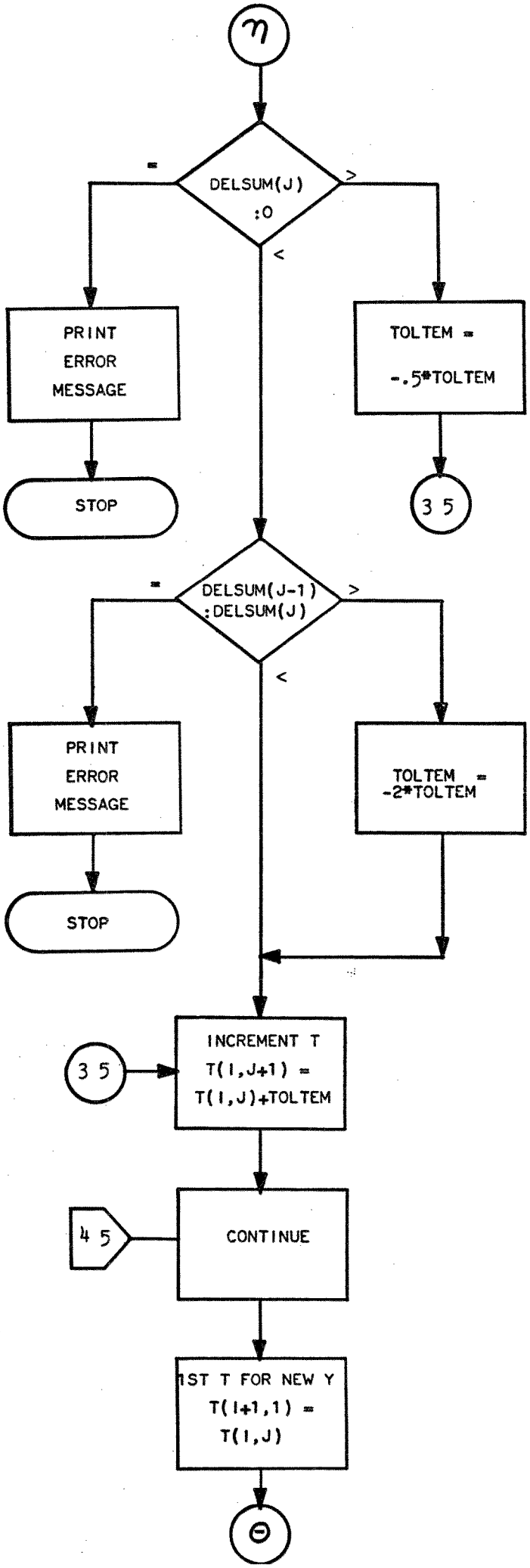

α
IWATER:0
=
≠
USE WATER VAPOR PRESSURE EQUATION FOR COMPONENT 2
USE ANTOINE VAPOR PRESSURE EQUATION FOR COMPONENT 2
26
DO 26
K = 1,KLOOPN
CHANGE:E
≥
>
IW = 0
IW = 1
COMPUTE ACTIVITY COEFF. VIA THE WILSON EQUATION
COMPUTE ACTIVITY COEFF. VIA MARGULES EQUATION
β
β
COMPUTE Y1TRY= γ1X1P^O/PT
YDELTA = (Y1TRY-Y1)
ABS(YDELTA) :TOLERY
28
16
=
K:1
≠
γ

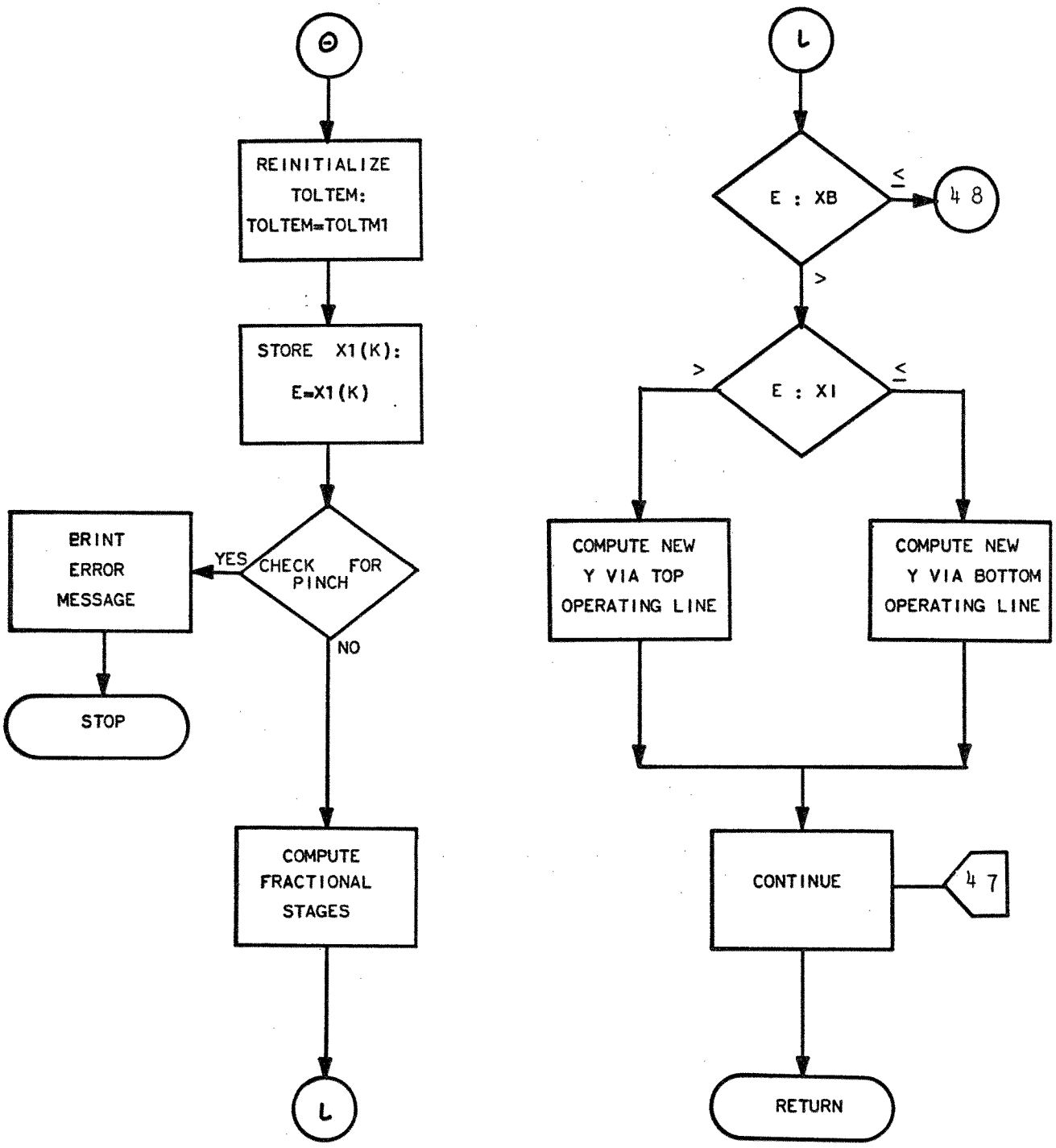

γ
YDELTA(K-1)
: 0
=
<
δ
>
PRINT
ERROR
MESSAGE
STOP
YDELTA(K)
:0
=
<
>
PRINT
ERROR
MESSAGE
STOP
TOL = -5*TOL
16
YDELTA(K-1)
:YDELTA(K)
=
<
>
PRINT
ERROR
MESSAGE
STOP
16
TOL = -2*TOL
16


δ
YDELTA(K)
:0
=
>
<
PRINT
ERROR
MESSAGE
STOP
TOL = -5*TOL
16
YDELTA(K-1)
:YDELTA(K)
=
>
<
PRINT
ERROR
MESSAGE
STOP
TOL = -2*TOL
16
INCREMENT X:
X1(K+1) =
X1(K)-TOL
26
CONTINUE
∈


∈
REINITIALIZE
TOL :
TOL = TOL1
1ST X FOR
NEW TEMP:
X1(1) = X1(K)
COMPUTE Y2TRY=
δ2X2P^O/PT
COMPUTE
SUM OF Y'S:
SUMY
DELSUM =
1 - SUMY
ABS(DELSUM)
:TOLSUM
≤
46
>
J:1
=
35
≠
J

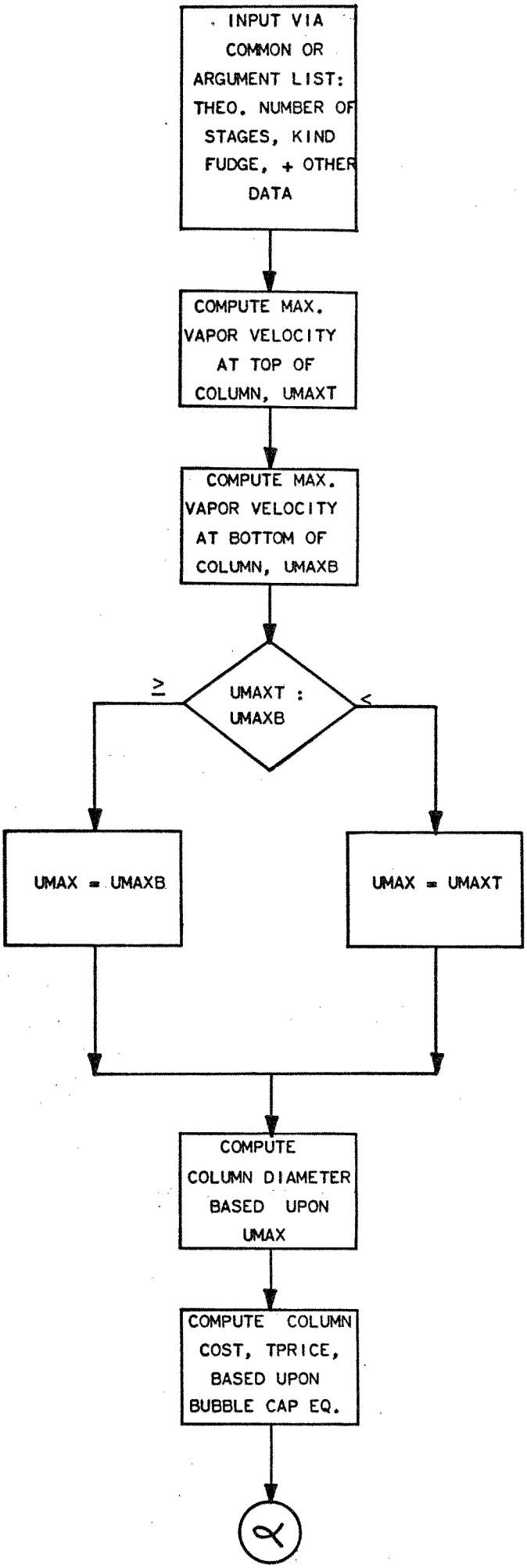

J
DELSUM(J-1)
: 0
=
<
η
>
PRINT
ERROR
MESSAGE
STOP
DELSUM(J)
: 0
=
<
>
PRINT
ERROR
MESSAGE
STOP
TOLTEM =
-.5*TOLTEM
35
DELSUM(J-1)
:DELSUM(J)
<
>
PRINT
ERROR
MESSAGE
STOP
35
TOLTEM =
-2*TOLTEM
35

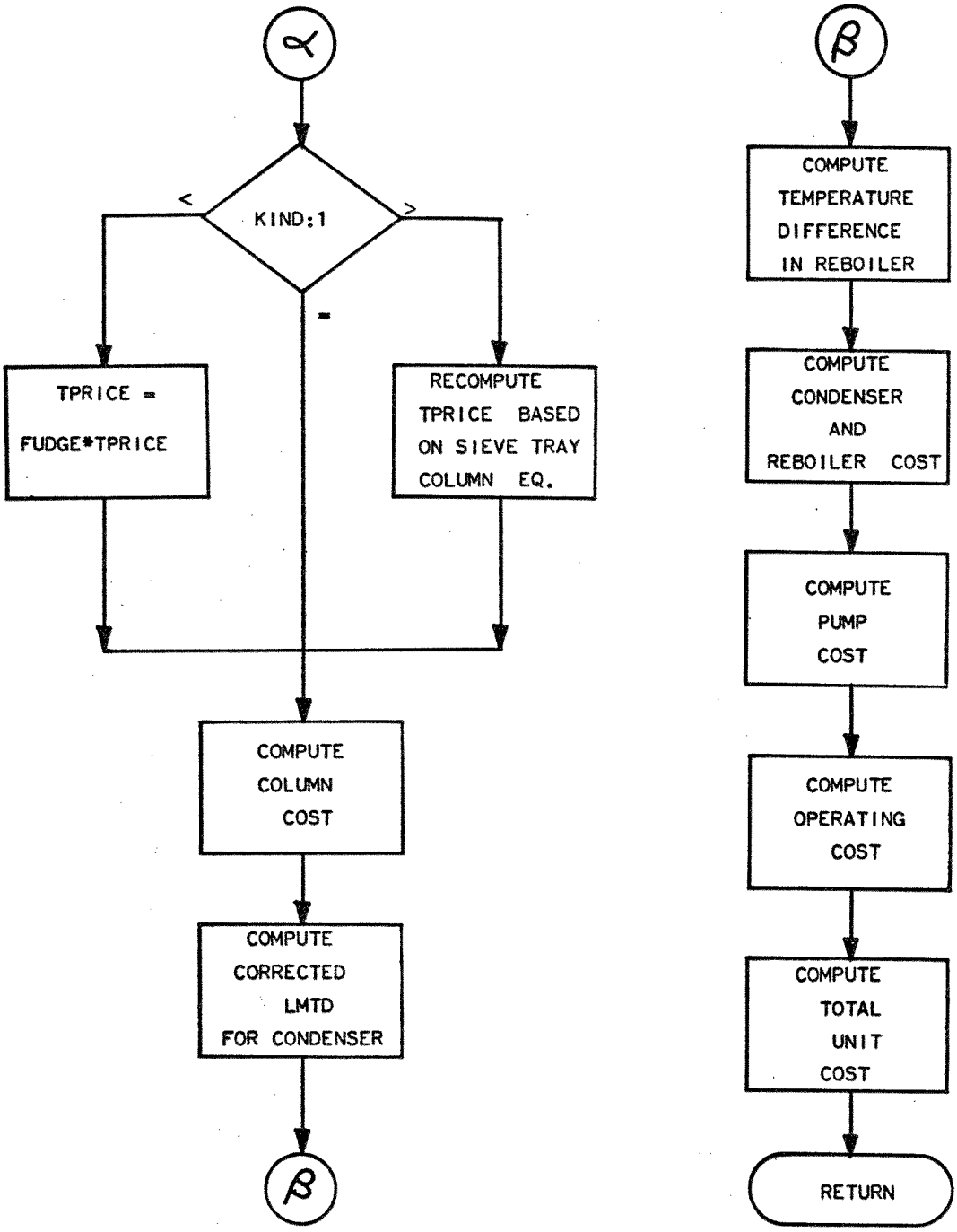

η
DELSUM(J)
:0
=
>
<
PRINT
ERROR
MESSAGE
STOP
TOLTEM =
-.5*TOLTEM
35
DELSUM(J-1)
:DELSUM(J)
=
>
<
PRINT
ERROR
MESSAGE
STOP
TOLTEM =
-2*TOLTEM
35
INCREMENT T
T(I,J+1) =
T(I,J)+TOLTEM
45
CONTINUE
1ST T FOR NEW Y
T(I+1,1) =
T(I,J)
Θ


Θ
REINITIALIZE TOLTEM: TOLTEM=TOLTM1
STORE X1(K): E=X1(K)
CHECK FOR PINCH
YES
PRINT ERROR MESSAGE
STOP
NO
COMPUTE FRACTIONAL STAGES
L
L
E : XB
≤
48
>
E : XI
>
≤
COMPUTE NEW Y VIA TOP OPERATING LINE
COMPUTE NEW Y VIA BOTTOM OPERATING LINE
CONTINUE
47
RETURN

FLOW CHART FOR

SUBROUTINE COST


INPUT VIA COMMON OR ARGUMENT LIST: THEO. NUMBER OF STAGES, KIND FUDGE, + OTHER DATA
COMPUTE MAX. VAPOR VELOCITY AT TOP OF COLUMN, UMAXT
COMPUTE MAX. VAPOR VELOCITY AT BOTTOM OF COLUMN, UMAXB
UMAXT : UMAXB
≥
<
UMAX = UMAXB
UMAX = UMAXT
COMPUTE COLUMN DIAMETER BASED UPON UMAX
COMPUTE COLUMN COST, TPRICE, BASED UPON BUBBLE CAP EQ.
α


α
KIND:1
<
=
>
TPRICE = FUDGE*TPRICE
RECOMPUTE TPRICE BASED ON SIEVE TRAY COLUMN EQ.
COMPUTE COLUMN COST
COMPUTE CORRECTED LMTD FOR CONDENSER
β
β
COMPUTE TEMPERATURE DIFFERENCE IN REBOILER
COMPUTE CONDENSER AND REBOILER COST
COMPUTE PUMP COST
COMPUTE OPERATING COST
COMPUTE TOTAL UNIT COST
RETURN

SUBROUTINE MATLBAL

Since control is straightforward, no Flow Chart is presented. See line 17700 in Appendix I.

NOMENCLATURE[d]

A_{12}, A_{21}	Constants for the Wilson equation or the Margules equation
B_{12}	Constant for the Redlich-Kister Equation
B1	Flow rate of bottoms product from Column I (moles/hr)
B2	Flow rate of bottoms product from Column II (moles/hr)
C	Constant for the Redlich-Kister Equation, Cost of overhead product ($/# product)
D	Constant for the Redlich-Kister Equation
D1	Flow rate of overhead product from Column I (moles/hr)
D2	Flow rate of overhead product from Column II (moles/hr)
F	Fixed capital cost ($)
F1	Flow rate of feed to Column I (moles/hr)
F2	Flow rate of feed to Column II (moles/hr)
K	Equilibrium constant
Kv	Constant for Souders-Brown equation
L	Labor cost ($/hr)
L'	Labor cost ($/# product)
L1	Internal liquid rate in Column I (moles/hr)
L2	Internal liquid rate in Column II (moles/hr)
L/V	Internal reflux ratio
L/D	External reflux ratio
Log	Logarithm to base 10
Ln	Logarithm to base e
M'	Equipment maintenance cost ($/# product)

m	Number of an intermediate tray in the stripping section
n	Number of an intermediate tray in the enriching section
N	Number of top tray
O	Operating cost ($/# product)
P	Flow rate of the intermediate product (moles/hr)
	Purchased equipment cost
P^O	Vapor pressure (mmHg)
PT	Total pressure (mmHg)
q	Thermal quality of the feed stream
R'	Raw materials cost ($/# product)
r	Annual production rate (#/product/yr)
T	Absolute temperature (^oK or ^oR)
t	Temperature (^oC or ^oF)
U'	Utilities cost ($/# product)
U	Vapor velocity (ft/sec)
V1	Vapor rate in Column I (moles/hr)
V2	Vapor rate in Column II (moles/hr)
X1	Mole fraction of Component 1 in the liquid
X2	Mole fraction of Component 2 in the liquid
XB1	Mole fraction of more volatile component in Column I bottoms product
XB2	Mole fraction of more volatile component in Column II bottoms product

XD1	Mole fraction of more volatile component in Column I overhead product
XD2	Mole fraction of more volatile component in Column II overhead product
XF1	Mole fraction of more volatile component in feed to Column I
XF2	Mole fraction of more volatile component in feed to Column II
XP	Mole fraction of more volatile component in intermediate product stream
$X_{n,1}$	Mole fraction of component 1 in the liquid on tray n
$X_{n,2}$	Mole fraction of component 2 in the liquid on tray n
Y	Mole fraction in the vapor
$Y_{n,1}$	Mole fraction of component 1 in the vapor on tray n
$Y_{n,2}$	Mole fraction of component 2 in the vapor on tray n

GREEK LETTERS

γ	Activity coefficients in the liquid
ρ	Density (#/Ft^3)
ϕ	Error function = $Y_{specified} - Y_{calc}$

[d]Also see Appendix 3A for program variables

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[13] Robinson & Gilliland, Elements of Fractional Distillation, 4th Ed., McGraw-Hill, 1950, page 130

[6b] Smith, B., Design of Equilibrium Stage Processes, McGraw-Hill, 1963, page 482 and page 545