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Computer program for binary distillation using the method of Pochon-Savarit with enthalpy data calculated by Lagrange interpolation

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COMPUTER PROGRAM FOR
BINARY DISTILLATION
USING THE METHOD OF POCHON-SAVARIT
WITH ENTHALPY DATA CALCULATED BY LAGRANGE
INTERPOLATION
BY
JOSEPH J. ROGUS

A THESIS
PRESENTED IN PARTIAL FULFILLMENT OF
THE REQUIREMENTS FOR THE DEGREE
OF
MASTER OF SCIENCE IN CHEMICAL ENGINEERING
AT
NEW JERSEY INSTITUTE OF TECHNOLOGY

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Newark, New Jersey
1975

APPROVAL OF THESIS
BINARY DISTILLATION USING THE METHOD
OF POCHON-SAVARIT WITH ENTHALPY DATA
CALCULATED BY LAGRANGE INTERPOLATION

BY

JOSEPH J. ROGUS

FOR

DEPARTMENT OF CHEMICAL ENGINEERING
NEW JERSEY INSTITUTE OF TECHNOLOGY

BY

FACULTY COMMITTEE

APPROVED:

NEWARK, NEW JERSEY

AUGUST, 1975

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August, 1975

Joseph J. Rogus

ABSTRACT

This thesis presents a Fortran Computer Program to solve binary distillation problems. The solution is obtained by the method of Pochon-Savarit which is based upon graphical use of an enthalpy-concentration diagram. The enthalpy data in this program is calculated using Lagrange interpolation. This is accomplished by utilizing the Lagrange interpolation to get values for the enthalpy of the vapor until we find that value which lies on the same line as the enthalpy of the liquid from the preceding tray and its corresponding dew point.

The required input data consist of liquid-vapor equilibrium data, heat of solution data with the reference temperature, the feed rate and temperature, the weight fraction of the lighter component in the feed, distillate, and bottoms, and the reflux ratio. In addition, for each component, the molecular weight, heat of vaporization, critical temperature, boiling point and specific heat of the liquid and vapor must be specified. The specific heats must be in terms of a third order polynomial with respect to temperature. The program output includes the mole fraction, quantity, and enthalpy of the feed, distillate, and bottoms, the condenser and reboiler heat loads, the feed tray location, the number of ideal trays, and the mole fraction and enthalpy of the vapor and the liquid at each tray. This program enables as many sets of data to be run within one execution of the program as desired by the user.

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I. INTRODUCTION

The solution to binary distillation problems requires obtaining the number of trays or plates necessary to achieve the desired distillate and bottoms concentrations for a specific feed. The number of trays is a function of the feed condition and the specified reflux ratio. The final number of trays is usually determined by utilizing that reflux value which will minimize the total system cost.

There are several methods available for solving binary distillation problems. Some of the common methods involve solution to the problem by either graphical procedures or by the use of analytical equations. The methods of Pochon-Savarit and McCabe-Theile employ the use of graphical techniques where as others such as Underwood and Colburn compute the solution analytically.

Each method has advantages and disadvantages associated with it.

The Pochon-Savarit method is the subject of this thesis. Some of the major advantages of this method over several other methods will be discussed briefly before the detailed procedure is developed.

The McCabe-Theile method requires that the system have equal molal overflow. This condition is not necessarily available for all applications. The Pochon-Savarit does not require this condition and therefore is more applicable to actual industrial calculations.

The graphical solutions allow less complex equations to be used. Non-ideal vapor-liquid equilibrium relationships required for analytical solutions often become very complex and cumbersome. The data required for the

Pochon-Savarit method are more readily available (Appendix I) and does not require the use of intermediates such as fugacity, K factor or relative volatility. This method, because of its relative simplicity, as compared to some of the more complex methods, readily lends itself to use on some of the smaller computers available in industry today.

Following the discussion of the theory, two (2) distinct systems will be solved utilizing the computer program.

II. DISTILLATION THEORY

The equations developed in the text of this thesis will use the same nomenclature used in the computer program to facilitate reference.

A. MATERIAL BALANCE CALCULATIONS

1. OVER-ALL BALANCES

Figure 1 represents a continuous distillation plant. The feed enters the column at a rate of FEED moles per hour and a concentration of ZFA. This results in the production of DIST moles per hour of overhead product with a concentration of XDA and BOT moles per hour of bottom product with a concentration of XBA. From this data, we can write two (2) over-all material balances for the system.

Total Material Balance:

$$\text{FEED} = \text{DIST} + \text{BOT} \quad (1)$$

Component A Balance:

$$(\text{FEED}) (\text{ZFA}) = (\text{DIST}) (\text{XDA}) + (\text{BOT}) (\text{XBA}) \quad (2)$$

Providing the values for FEED, ZFA, XDA and XBA are available, which is the case for our system, one can eliminate DIST from these equations. The result provides a solution for calculation of BOT.

$$\text{BOT} = (\text{FEED}) (\text{XDA} - \text{ZFA}) / (\text{XDA} - \text{XBA}) \quad (3)$$

The value of DIST can now be obtained from Equation 1.

For most industrial applications, we are not so fortunate as to have the feed given in moles per hour and the mole fractions of the feed, distillate and bottoms specified.

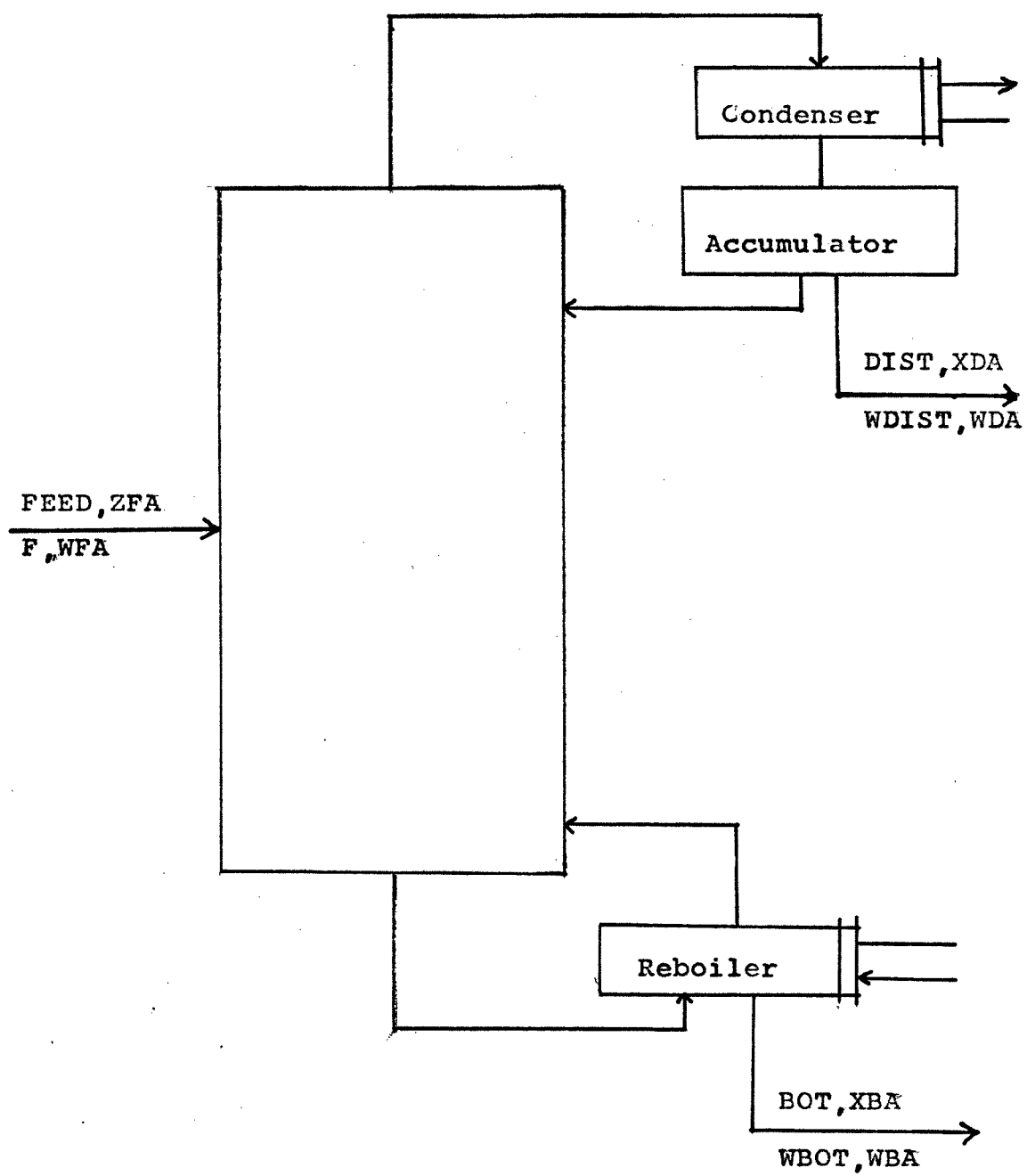


Figure 1
Overall Material Balance
of a Fractionator

A system is usually specified as follows:

The column is fed at a rate of F pounds per hour with a weight percent of WFA . This results in the production of an overhead product with weight percent of WDA and of a bottom product with a weight percent of WBA .

We must now determine the quantity of the products produced by this system.

We first determine the number of moles of components A and B , with molecular weights of MWA and MWB respectively, in the feed.

$$MOLA = (F)(WFA/MWA) \quad (4)$$

$$MOLB = (F)(WFB/MWB) \quad (5)$$

From these, we determine:

$$FEED = MOLA + MOLB \quad (6)$$

$$ZFA = MOLA/FEED \quad (7)$$

The mole fraction of the distillate and the bottom products are determined by use of Equation (8) and Equation (9) respectively.

$$XDA = (WDA/MWA)/(WDA/MWA + (1-WDA)/MWB) \quad (8)$$

$$XBA = (WBA/MWA)/(WBA/MWA + (1-WBA)/MWB) \quad (9)$$

With this data, we can now compute BOT and $DIST$ using Equation (3) and Equation (1).

We must now compute the average molecular weight of the distillate.

$$MWDAV = 1/(WDA/MWA + (1-WDA)/MWB) \quad (10)$$

This enables us to compute quantity of distillate, $WDIST$, in pounds per hour.

$$WDIST = (DIST)(MWDAV) \quad (11)$$

The quantity of bottom product produced, WBOT, in pounds per hour is determined by the total material balance in Equation (12)

$$WBOT = F - WDIST \quad (12)$$

2. NET FLOWS OF EACH SECTION

Now that we have discussed the total system, we consider the flows in each section of the column.

Consider the upper or enriching section of the column as shown in Figure 2. DIST represents the difference between the flow rates of the streams entering and leaving the top of the column. A balance around the condenser yields

$$DIST = G1 - L0 \quad (13)$$

Since DIST represents the difference between the flow rates of vapor and liquid anywhere in the enriching section, a total material balance for this section gives

$$DIST = G_{n+1} - L_n \quad (14)$$

A material balance for component A in the system yields the following

$$(DIST)(XDA) = (G1)(YA1) - (L0)(XAO) \quad (15)$$

$$(DIST)(XDA) = (G_{n+1})(Y_{An+1}) - (L_n)(X_{An}) \quad (16)$$

Similarly, for the bottom or stripping section of the column, Figure 3, the following equations apply

$$BOT = Lb - Gb = Lm - G_{m+1} \quad (17)$$

$$(BOT)(XBA) = (Lb)(XAb) - (Gb)(YAb) = (Lm)(XAm) - (G_{m+1})(Y_{Am+1}) \quad (18)$$

The subscripts n and m are used to represent a plate in the enrich-

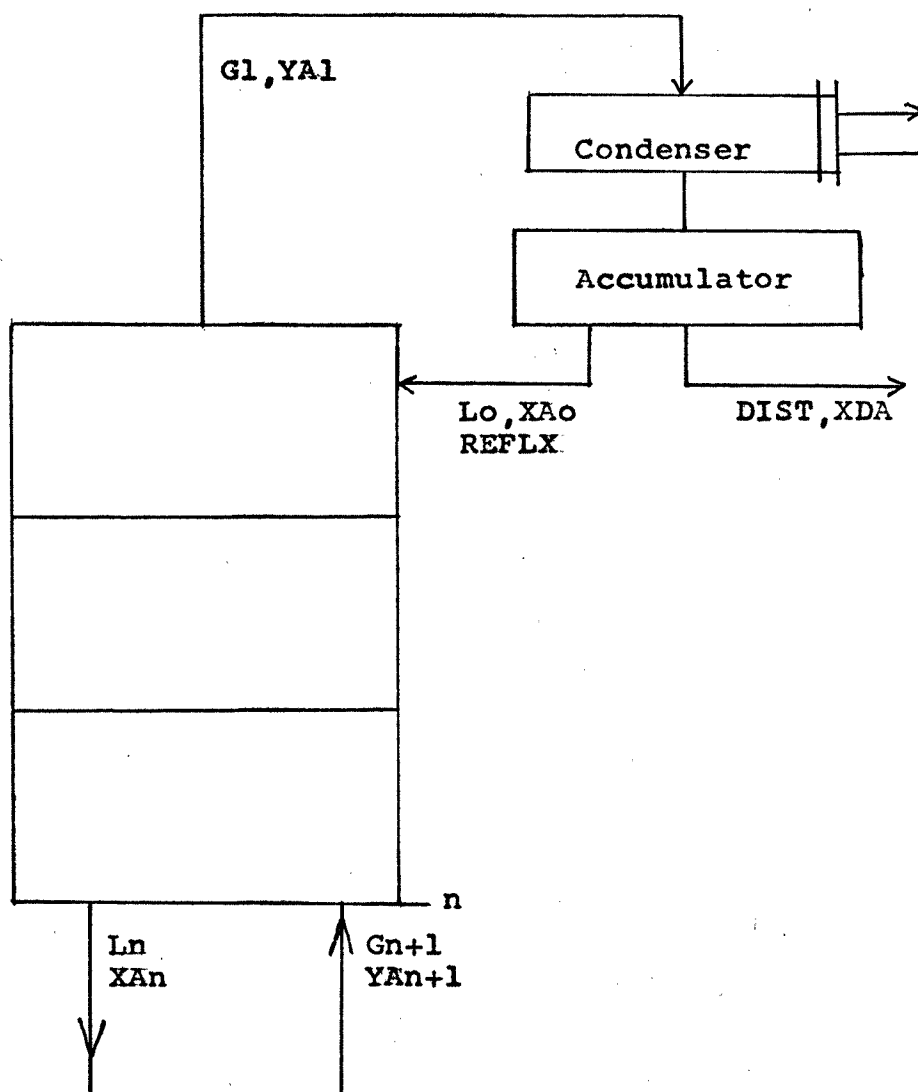


Figure 2
Material Balances for
Enriching Section

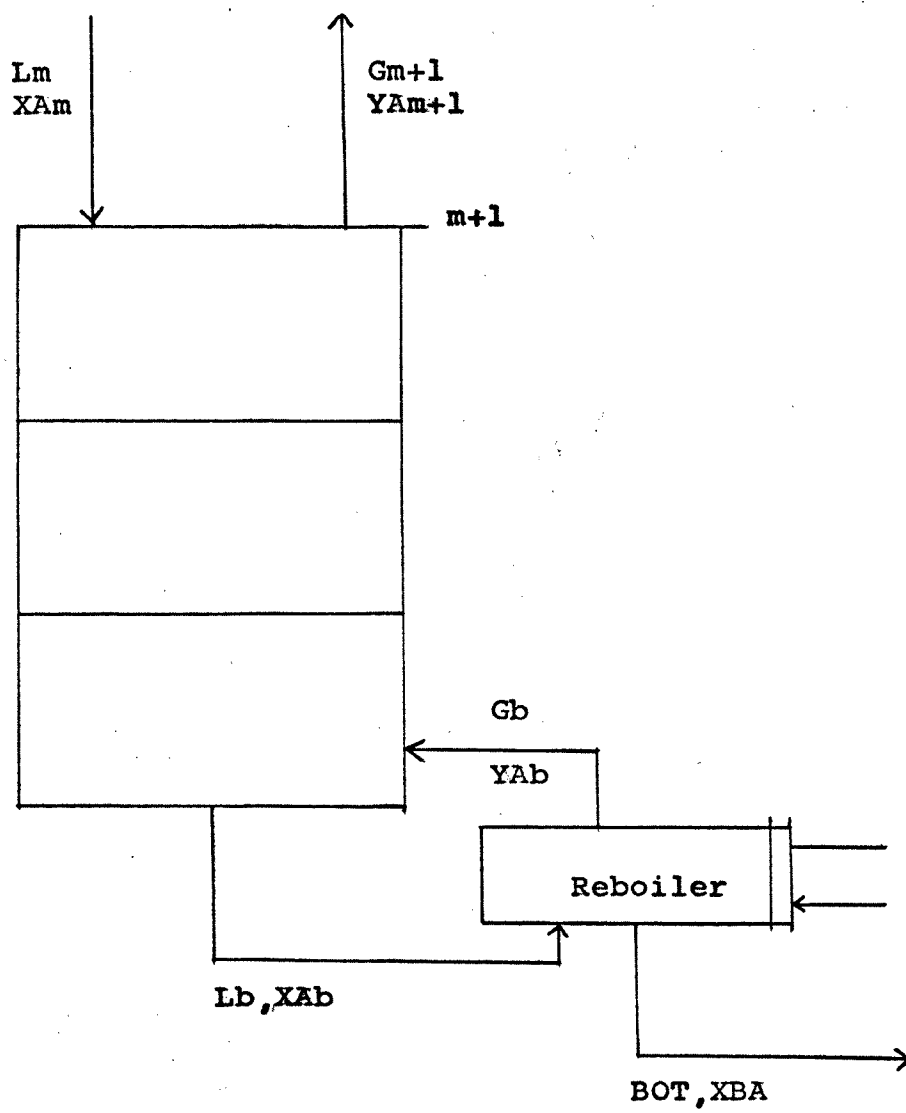


Figure 3
Material Balance for
Stripping Section

ing and stripping section respectively.

The feed plate is not included in either section. Since the feed plate separates the stripping and enriching sections and since the feed can have any condition from liquid below its bubble point to super-heated vapor, it requires special calculations.

B. ENTHALPY CALCULATIONS

OVER-ALL ENTHALPY BALANCE

Suppose we consider the overall enthalpy balances for a distillation plant with negligible heat losses. This system is represented in Figure 4.

We now define the reflux ratio as

$$\text{REFLX} = L_o/\text{DIST} \quad (19)$$

Consider the condenser, Section A(Figure 4). The total material balance is the same as Equation (13), but now we rewrite it as follows

$$G_1 = \text{DIST} + L_o \quad (13a)$$

Solving for L_o in Equation (19) and substituting that value in Equation (13a)

$$G_1 = \text{DIST}(\text{REFLX} + 1) \quad (20)$$

The enthalpy balance for Section A is

$$G_1(H_{G1}) = Q_{\text{COND}} + L_o(H_{L_o}) + \text{DIST}(H_{\text{DIST}}) \quad (21)$$

or

$$Q_{\text{COND}} = \text{DIST}(\text{REFLX} + 1)H_{G1} - \text{REFLX}(H_{L_o}) - H_{\text{DIST}} \quad (22)$$

Where Q_{COND} represents the condenser heat load.

To obtain the reboiler heat load, we consider Section B of Figure 4 and employ a complete enthalpy balance for this section to obtain

$$Q_{\text{BOIL}} = \text{DIST}(H_{\text{DIST}}) + B_o(H_{B_o}) + Q_{\text{COND}} - \text{FEED}(H_{\text{FEED}}) \quad (23)$$

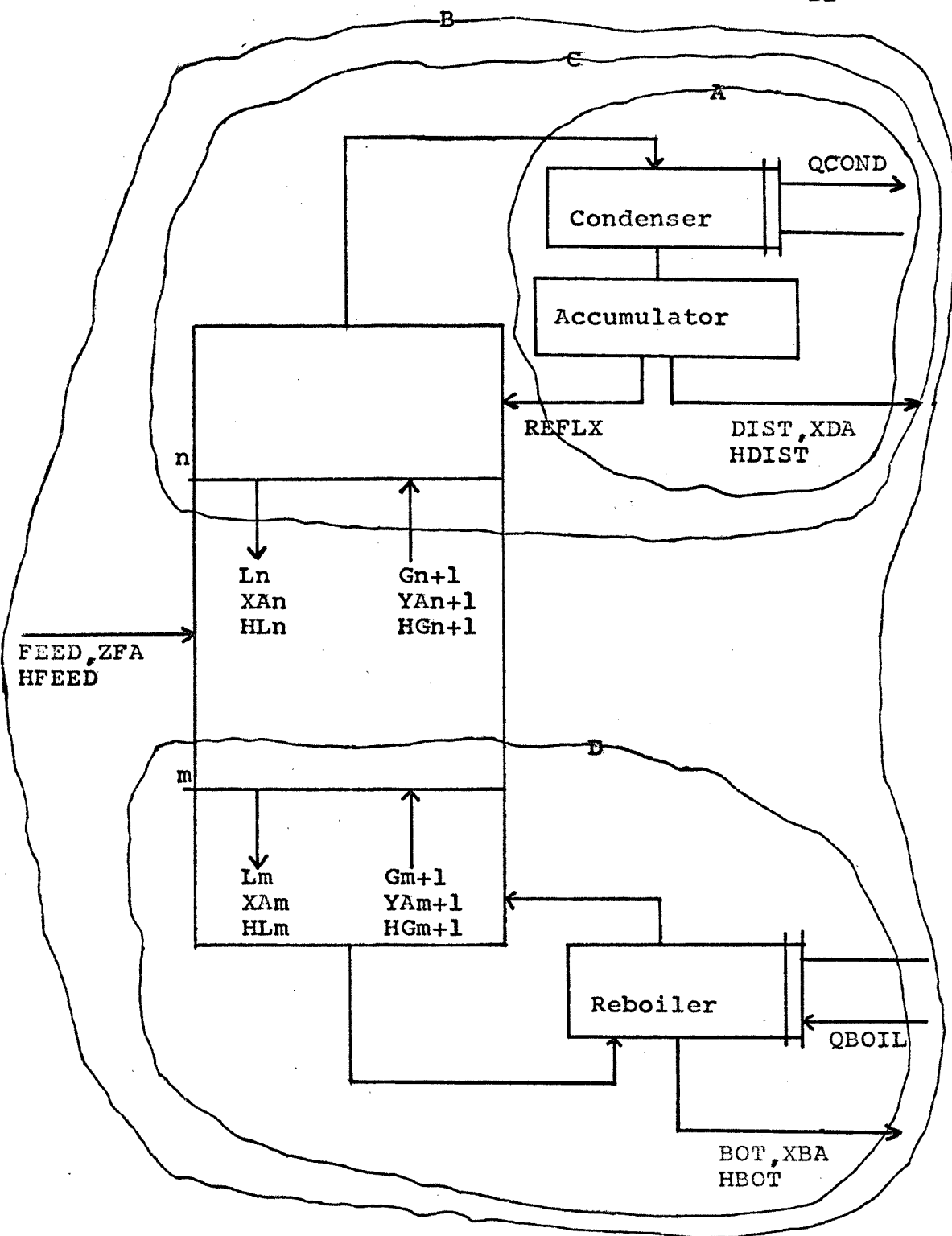


Figure 4
Enthalpy balance of
a distillation plant

III. METHOD OF POCHON-SAVARIT

As we mentioned previously, this thesis will only consider the case of negligible heat losses for the distillation plant.

A. THE ENRICHING SECTION

We will consider the enriching section through Tray n, Section C, Figure 4. As before, Tray n is any tray in this section. The material balances are developed in the same manner as those in Section IIA.

Total material balance from Equation (14)

$$G_{n+1} = L_n + \text{DIST} \quad (24)$$

For Component A

$$\text{Equation (16)} \quad \text{DIST}(X_{DA}) = G_{n+1}(Y_{n+1}) - L_n X_N$$

The enthalpy balance for this section is

$$(G_{n+1})H_{Gn+1} = (L_n)H_{Ln} + Q_{\text{COND}} + \text{DIST}(H_{\text{DIST}}) \quad (25)$$

If we let H_{DELD} represent the heat removed in the condenser and permanently removed with the distillate per mole of distillate, we get

$$H_{\text{DELD}} = \frac{Q_{\text{COND}} + \text{DIST}(H_{\text{DIST}})}{\text{DIST}} = Q_{\text{COND}}/\text{DIST} + H_{\text{DIST}} \quad (26)$$

and

$$(G_{n+1})H_{Gn+1} - (L_n)H_{Ln} = \text{DIST}(H_{\text{DELD}}) \quad (27)$$

Similar to the case of the material balance Equation (13) the left hand side of Equation (27) represents the difference in flow. This time, the difference is in heat flow. The right hand side of this equation as before is constant for a specific set of conditions. This difference remains constant in this section of the column, is independent of

the tray number, and is equal to the quantity of heat permanently removed at the top of the column with the distillate and at the condenser.

The elimination of DIST between Equations (24) and (16) and between Equations (24) and (27) yields

$$\frac{L_n}{G_{n+1}} = \frac{X_{DA} - Y_{An+1}}{X_{DA} - X_{An}} = \frac{H_{DELD} - H_{Gn+1}}{H_{DELD} - H_{Ln}} \quad (28)$$

Equation (28) represents a straight line on the Hxy diagram through points (H_{Gn+1}, Y_{An+1}) at G_{n+1} , (H_{Ln}, X_{An}) at L_n , and (H_{DELD}, X_{DA}) at Δ DIST.

Figure 5 represents a Hxy diagram for a total condenser. This is the only type of condenser considered in these calculations.

For a total condenser, the distillate, DIST, and the reflux L_o have identical coordinates. The saturated vapor from the top Tray G_1 , when totally condensed, has the same composition as DIST and L_o . The Liquid L_1 leaving Tray 1 is in equilibrium with the vapor G_1 and can be located by drawing a tie line from G_1 to the saturated liquid curve.

Since Equation (28) is applicable to all trays in the enriching section, G_2 can be located on the saturated vapor curve by the line drawn from Δ DIST to L_1 . Again, the Liquid L_2 is located using a tie line from G_2 to the saturated liquid curve. The number of ideal trays, represented by the number of tie lines, may now be determined for this section by alternate tie lines and construction lines through Δ DIST.

For any Tray n , the L_n/G_{n+1} value is given by the ratio of line lengths $H_{DELD}-G_{n+1}/H_{DELD}-L_n$. Utilizing Equations (24) and (28), we obtain

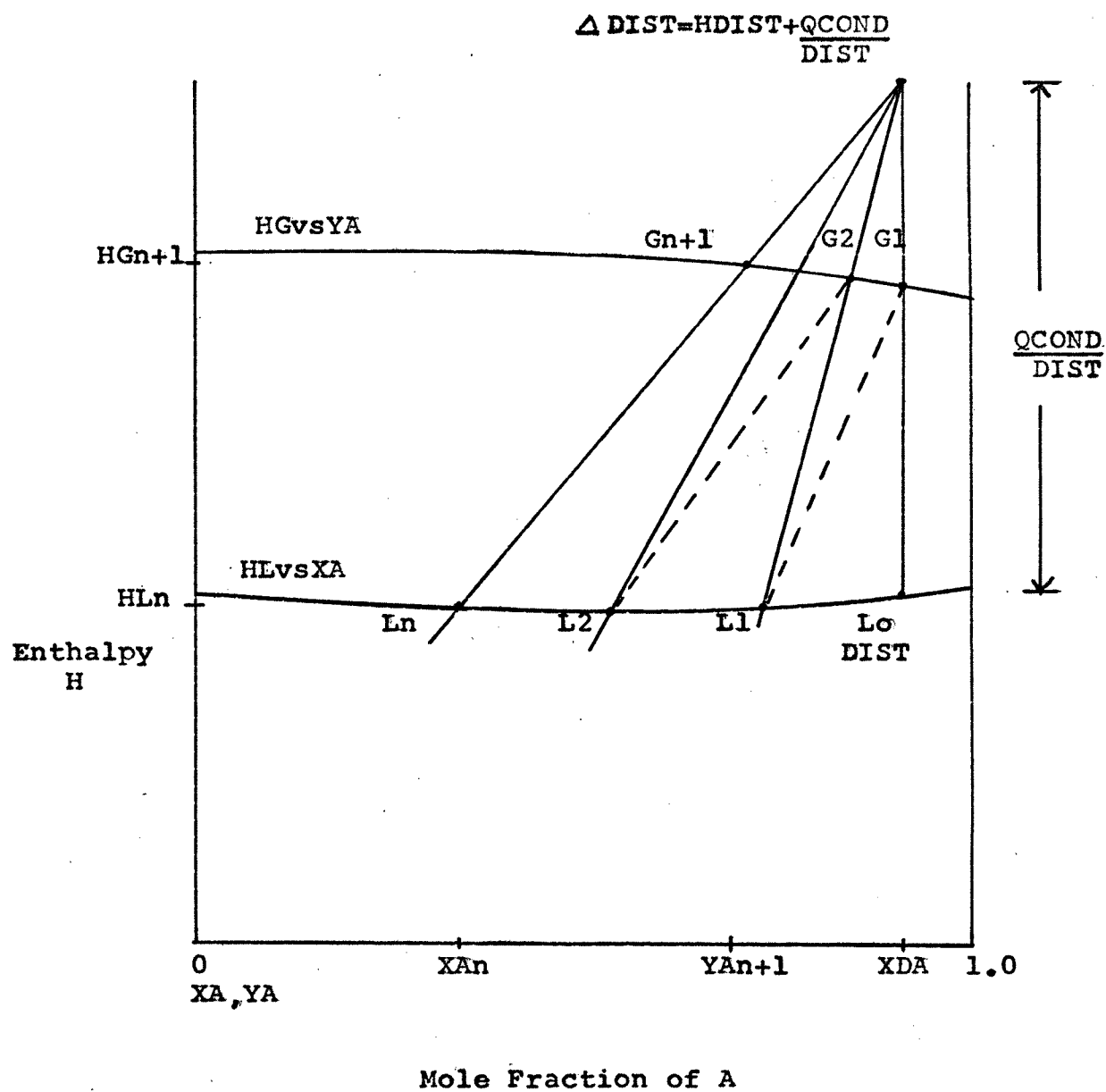


Figure 5
 HXY diagram for
 Enriching Section
 Total Condenser Reflux
 at Bubble Point

$$L_n/DIST = \frac{HDELD-HG_{n+1}}{HG_{n+1}-HL_n} = \frac{XDA-YA_{n+1}}{YA_{n+1}-XA_n} \quad (29)$$

If we apply Equation (29) to the top tray, we obtain the external reflux ratio, a value which is normally the one specified.

$$REFLX = L_o/DIST = \frac{HDELD-HG_1}{HG_1-HL_o} = \frac{\text{Line } HDELD \text{ } G_1}{\text{Line } G_1 L_o} = \frac{\text{Line } HDELD \text{ } G_1}{\text{Line } G_1 \text{ } DIST} \quad (30)$$

Thus, with the reflux ratio specified, Equation (30) may be used to locate Δ DIST on the Hxy diagram. The condenser heat load may now be calculated from the value of HDELD.

B. STRIPPING SECTION

In the stripping section, we will consider Section D of Figure 4. As we did in the enriching section, we will select a tray, m , and make our balances around it.

The total material balance is

$$\text{Equation (17) } BOT = L_m - G_{m+1}$$

and for Component A

$$\text{Equation (18) } BOT(X_B A) = (L_m)X_{A m} - G_{m+1}(Y_{A m+1})$$

The right hand side of Equation (18) represents the difference in the rate of flow of Component A. For a given distillation, the left hand side of the equation is constant. This difference is therefore independent of the tray selected in the stripping section. Similar to the case in the enriching section, this difference represents the rate of A removed permanently out of the bottom. We may now write the enthalpy balance for this section.

$$(L_m)H_{Lm} + Q_{BOIL} = (G_{m+1})H_{Gm+1} + BOT(H_{BOT}) \quad (31)$$

We now define $H_{DEL B}$ as the net flow of heat out of the stripping section per mole of bottom product

$$H_{DEL B} = \frac{BOT(H_{BOT}) - Q_{BOIL}}{BOT} = \frac{H_{BOT} - Q_{BOIL}}{BOT} \quad (32)$$

and

$$(L_m)H_{Lm} - (G_{m+1})H_{Gm+1} = (BOT)H_{DEL B} \quad (33)$$

This difference in heat as was the difference in mass in Equation (18) is constant for a given distillation and independent of the tray loca-

tion in the stripping section of the column.

If we now eliminate BOT, similarly to what we did for the enriching section, between Equations (17) and (18) and between Equations (17) and (33), we find

$$L_m/G_{m+1} = \frac{Y_{Am+1} - X_{BA}}{X_{Am} - X_{BA}} = \frac{H_{Gm+1} - H_{DEL B}}{H_{Lm} - H_{DEL B}} \quad (34)$$

As did Equation (28), Equation (34) represents a straight line on a Hxy diagram. This straight line is drawn through (H_{Gm+1}, Y_{Am+1}) at G_{m+1} , (H_{Lm}, X_{Am}) at L_m , and $(H_{DEL B}, X_{BA})$ at Δ_{BOT} . Analogous to the enriching section Equation (34) applies to all of the trays in the stripping section. If we consider the Hxy plot in Figure 6, the line from G_{Np+1} the vapor leaving the reboiler and entering the bottom tray N_p of the tower, to Δ_{BOT} intersects the enthalpy curve for the saturated liquid at L_{Np} , corresponding to the liquid leaving the bottom tray.

Similar to the enriching section, the number of trays can be determined on the Hxy diagram by alternating construction lines from $HG(i)$ to Δ_{BOT} and tie lines between $HG(i)$ and $HL(i)$. Each tie line again representing an ideal stage for this section.

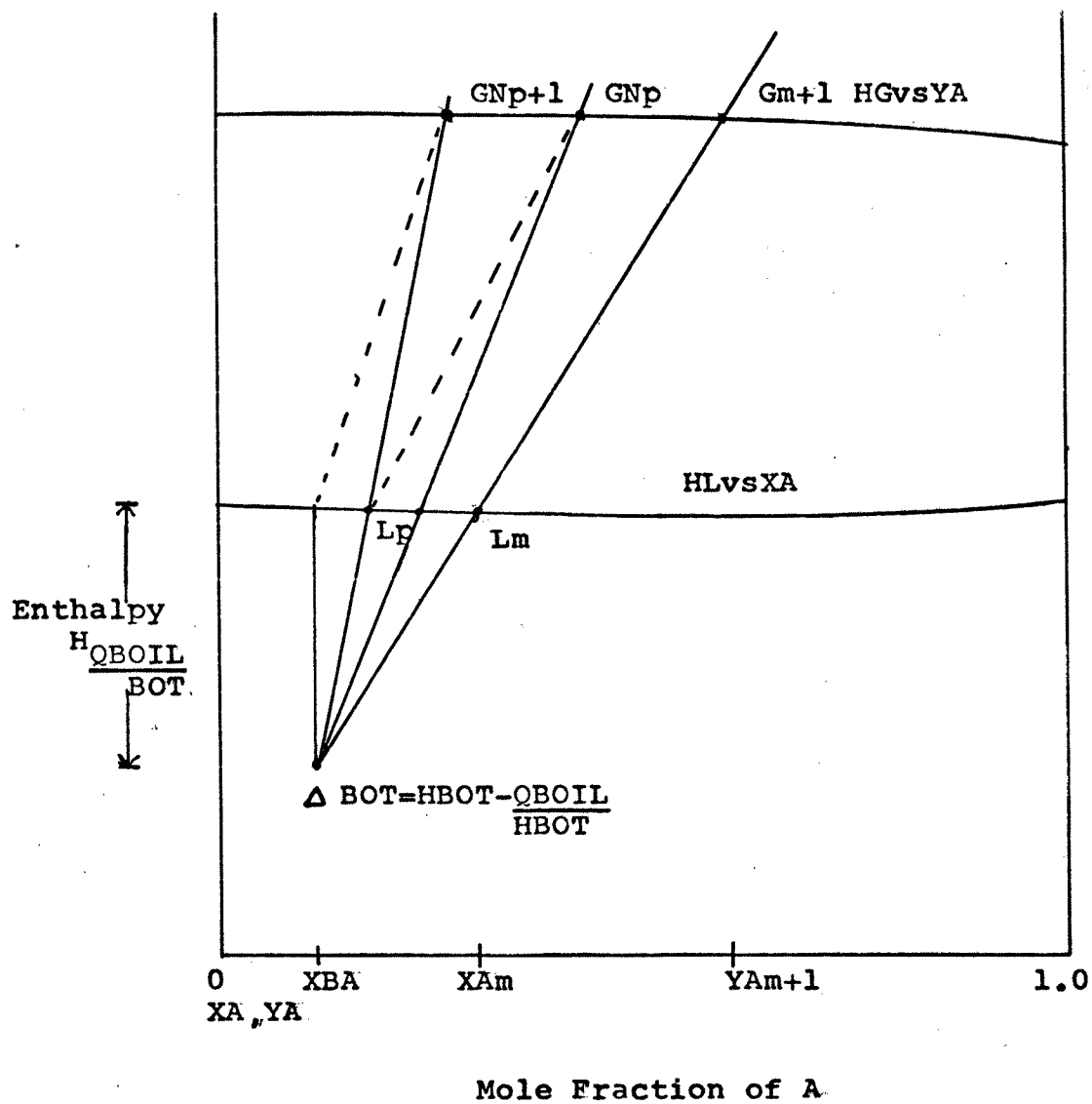


Figure 6
HXY Diagram for
Stripping Section

C. THE COMPLETE SYSTEM

If we go back to Figure 4 and consider the entire distillation plant, Section B, we can generate:

Material balances

$$\text{Equation (1) } \text{FEED} = \text{DIST} + \text{BOT}$$

$$\text{Equation (2) } \text{FEED}(\text{ZFA}) + \text{DIST}(\text{XDA}) + \text{BOT}(\text{XBA})$$

and the enthalpy balance

$$\text{Equation (23) } \text{QBOIL} = \text{DIST}(\text{HDIST}) + \text{BOT}(\text{HBOT}) + \text{QCOND} - \text{FEED}(\text{HFEED})$$

Utilizing the values of HDELD AND HDELB, defined by Equations (26) and (32) respectively, in Equation (23) we obtain

$$\text{FEED}(\text{HFEED}) = \text{DIST}(\text{HDELD}) + \text{BOT}(\text{HDELB}) \quad (35)$$

The elimination of FEED from the three (3) above equations allows us to obtain

$$\frac{\text{DIST}}{\text{BOT}} = \frac{\text{ZFA} - \text{XBA}}{\text{XDA} - \text{ZFA}} = \frac{\text{HFEED} - \text{HDELB}}{\text{HDELD} - \text{HFEED}} \quad (36)$$

Equation (36) represents a straight line on the Hxy diagram in Figure 7. This line is through points (HDELD, XDA) at Δ DIST, (HFEED, ZFA) at FD, and (HDELB, XBA) at Δ BOT.

We will call this line the overall operating line for the system.

The feed location shown in Figure 7 represents a feed condition of saturated liquid at its bubble point. This is only one case and the feed can be represented anywhere from liquid below its bubble point to super-heated vapor above the saturated-vapor curve.

Now that we have discussed the basic principles for tray determination in each section of the column, we will explain how total number of trays

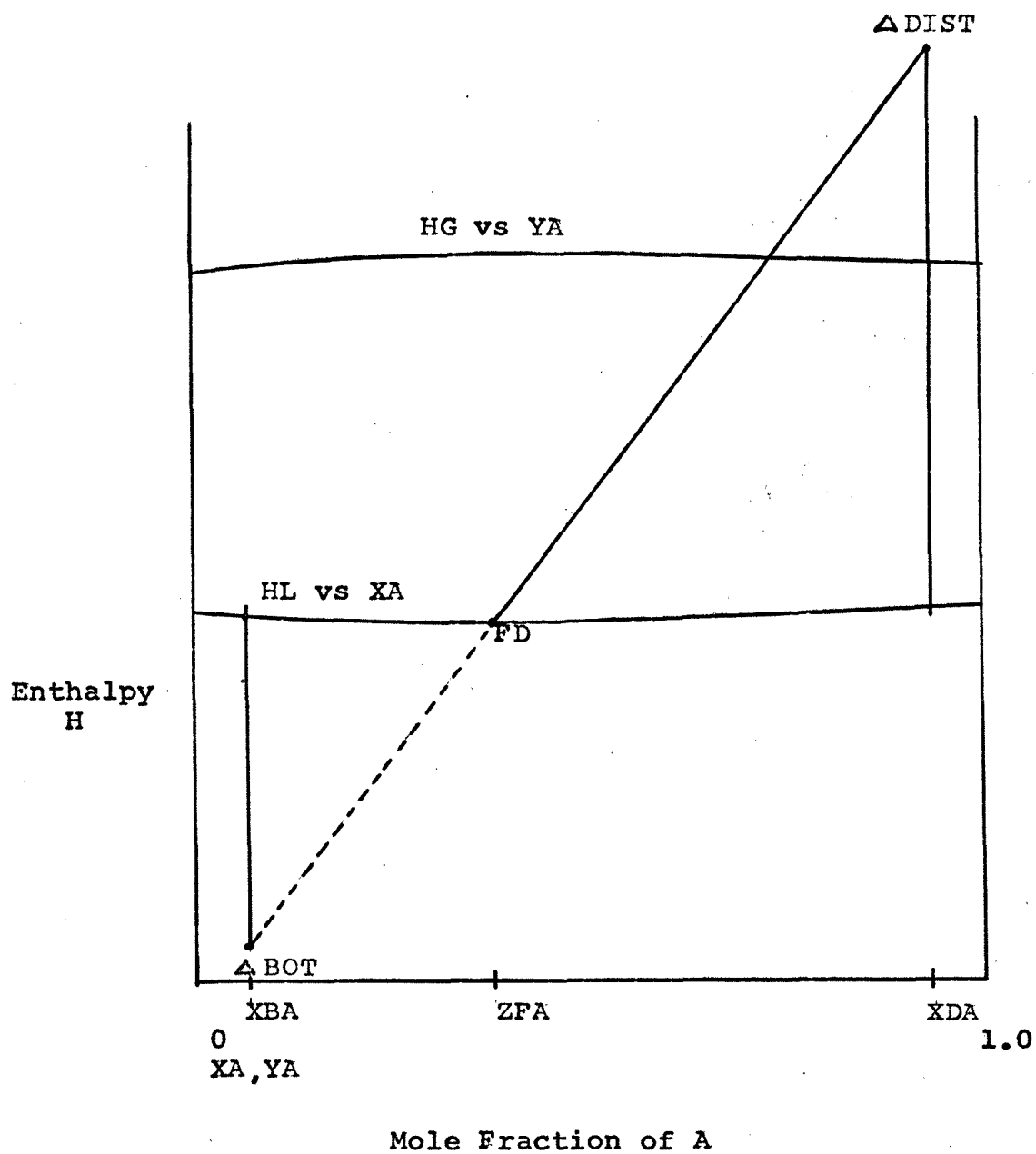


Figure 7
HXY Diagram with
Overall Operating Line

for the system is established. (Refer to Figure 8.)

Once we have established the location of FD on Hxy diagram, we determine the location of Δ DIST from the reflux ratio utilizing Equation (30). We then construct the overall operating line through Δ DIST and FD. This line establishes point Δ BOT where it intersects with XBA (Equation (36)). We now proceed, as discussed in Section IIIA, to construct a series of alternating tie lines and operating lines through Δ DIST commencing at point G1.

This is continued until we find the tray where the liquid concentration, point K, is less than the abscissa of the intersection of the overall operating line with the saturated liquid curve. This tray establishes the location for the introduction of the feed. This is a critical point for if the feed is introduced above or below it, the system will require additional trays to achieve the separation.

The feed tray separates the enriching section of the column from the stripping section of the column. When the feed tray is reached, we must change the construction of our operating lines from Δ DIST to Δ BOT. Line BOT1 represents this switch. We now determine the number of trays in the stripping section. This is done, as discussed in Section IIIB, by a series of tie lines and operating lines starting at point GB. The last tray is determined when we find the first tray where the liquid concentration, point P, is less than or equal to XBA.

The total number of trays required to achieve the separation is the number of tie lines commencing at point G1 and terminating at point P.

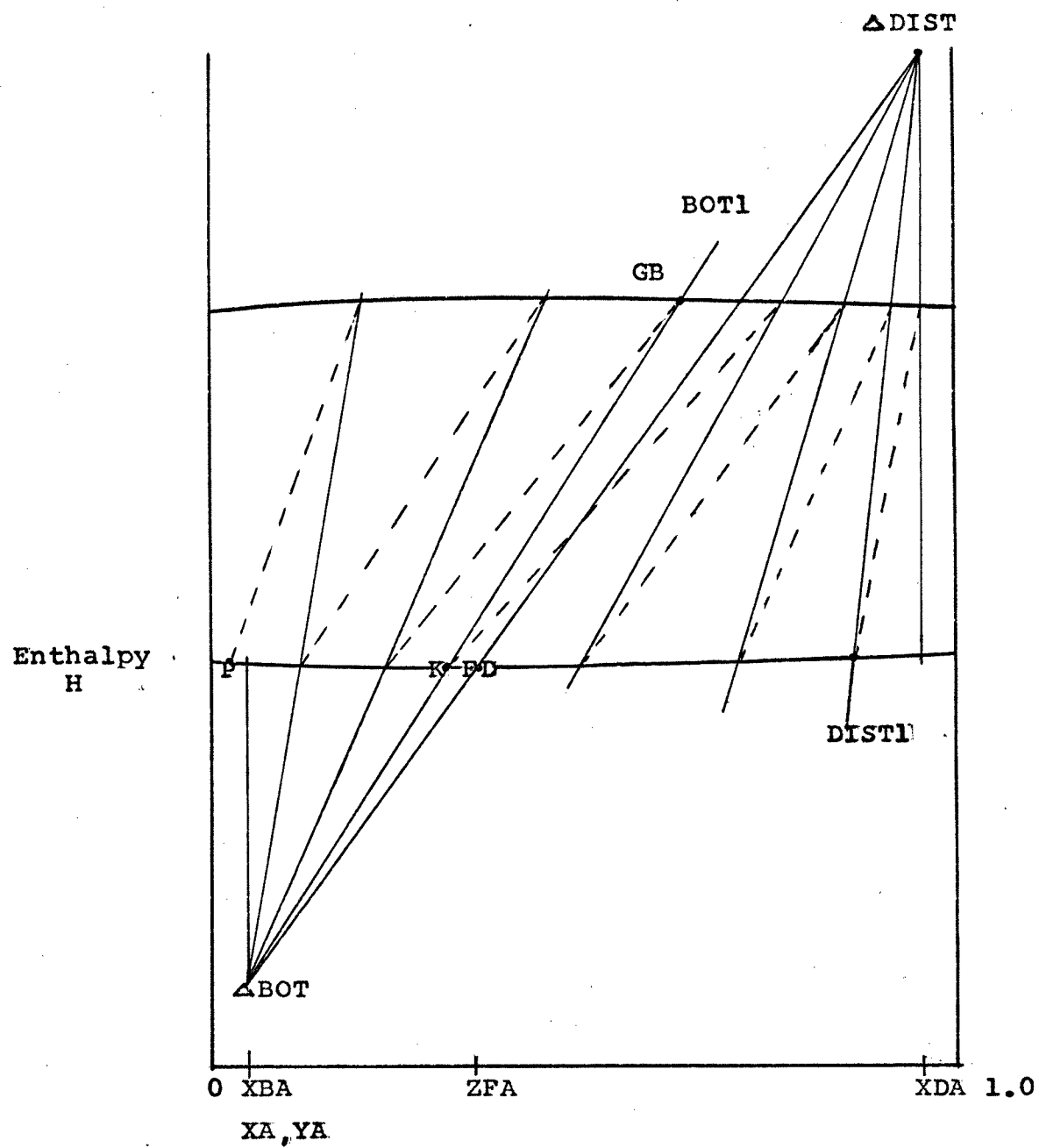


Figure 8
Pochon-Savarit
Solution

IV. LAGRANGE INTERPOLATION

The computer program utilizes Lagrange Interpolation for determination of the enthalpy data required for construction of the operating lines discussed previously. The Lagrange method allows for interpolation for unequally spaced data.

The Lagrange method lends itself to this type computer calculation, because it is less complex than other methods available. Other methods utilized for unequally-spaced arguments, such a determinant form or Aitken's method, require the setting up of matrices. Since the Lagrange method does not require matrices, it may be readily used with the smaller computers available today.

The method of Lagrange states that if we have three (3) sets of unequally spaced arguments

$$(X_1, Y_1), (X_2, Y_2), \text{ and } (X_3, Y_3)$$

we can determine for any X its corresponding Y value. This is accomplished utilizing the following equations

$$A_1 = \frac{(X-X_2)(X-X_3)}{(X_1-X_2)(X_1-X_3)} (Y_1) \quad (37)$$

$$A_2 = \frac{(X-X_1)(X-X_3)}{(X_2-X_1)(X_2-X_3)} (Y_2) \quad (38)$$

$$A_3 = \frac{(X-X_1)(X-X_2)}{(X_3-X_1)(X_3-X_2)} (Y_3) \quad (39)$$

$$Y = A_1 + A_2 + A_3 \quad (40)$$

Equation (40) represents the solution to the Lagrange interpolation.

V. PROGRAM DESCRIPTION

The computer program is written to allow as many sets of experimental data to be run within one execution as desired by the user. The only requirement is that the input data follow Appendices I and II. Should any set of data be read in missing a "Title" card, the program will terminate at that point with an appropriate error message printing out.

The program is divided into a main program consisting of three (3) distinct sections and five (5) subprograms. Each of these will be discussed briefly.

A. MAIN PROGRAM

1. MATERIAL BALANCE CALCULATIONS

This section utilized the equations developed in Section IIA. The data returned from this section includes:

1. Mole fraction of the feed
2. Mole fraction of the distillate
3. Mole fraction of the bottom
4. The distillate flow in pounds per hour
5. The bottoms flow in pounds per hour

2. ENTHALPY CALCULATIONS

Utilizing equations developed in Section IIB and III, this section returns the following data:

1. Enthalpy of the feed, BTU/lb-mole
2. Enthalpy of the distillate, BTU/lb-mole
3. Enthalpy of the distillate del point (Δ DIST), BTU/lb-mole
4. Condenser heat load, BTU/hr

5. Enthalpy of the bottom product, BTU/lb-mole
6. Enthalpy of the bottom del point (Δ BOT), BTU/lb-mole
7. Reboiler heat load, BTU/hr

3. POCHON-SAVARIT CALCULATIONS

The calculations in this section are basically the same as discussed in Section III. Since all the calculations are done mathematically, we are presented with problems that did not exist for a graphical solution. The values we obtained graphically for $HG(i+1)$ by construction of the operating from $HL(i)$ to Δ DIST must now be determined mathematically. This is accomplished by utilizing the Lagrange interpolation to get values of HG until we find the value on the same line as $HL(i)$ and Δ DIST. We compare the slope of the line Δ DIST-HG to the slope of the line Δ DIST- $HL(i)$. We consider the slopes equivalent when the dividend of the slope of our i^{th} iterative guess line and our initial guess line is less than 10^4 or when the increment ($YINC$) divided by the guess point ($YATS$) is less than 10^4 . This same type of check is used in the stripping section.

To determine when we change from the enriching section calculation to stripping section calculations, we again compare slopes. This time we call for the change when the slope of line Δ DIST-FD is greater or equal to the slope of line Δ DIST- $HL(i)$.

The last tray in the stripping section is reached when the $XL(i)$ value is less than or equal to XBA .

Since the guess point ($YATS$) on our curve range from 1 to .01 (or

less), a factor of 100 in order of magnitude, the iterative increment (Y1NC) is set to YATS/100 at all points along the curve. This speeds up the calculations in enriching section without detriment to the calculations in stripping section.

This portion of the program returns the following:

1. The total number of trays required including the reboiler.
2. The enthalpy and concentration of the liquid for each tray.
3. The enthalpy and concentration of the vapor for each tray.
4. The feed tray location.

B. SUBPROGRAMS

1. WHERE is a search routine to locate a variable in an ascending or descending array.
2. YLIN is a linear interpolation.
3. YLAGR is the Lagrange interpolation described in Section IV.
4. EL is used to calculate the enthalpy of the saturated liquid.
5. EV is used to calculate the enthalpy of the saturated vapor.

VI. DISCUSSION OF RESULTS

Appendix V contains sample computer program outputs to confirm the validity of the program. The printout for each system includes the system title and all the input variables as well as all the required output data. Each printout will be discussed briefly.

SYSTEM I: METHANOL - WATER

To be sure the program would give valid results, an example problem from Mass-Transfer Operations by Treybal, pages 326-329 was selected for System I. This problem requires the design of a methanol-water distillation plant. The design parameters for the system are:

The feed to the system will be supplied at a temperature of 136°F with a composition of fifty percent (50%) by weight of methanol at a rate of 5,000 pounds per hour. The system will produce a distillate containing ninety-five percent (95%) by weight methanol and a bottom product that is 1.0% by weight methanol. The reflux ratio for the system is 1.029.

All of the program calculations agree with text answers with the exception of the total number of trays required. The text answer is nine (9) trays including the reboiler and the program requires ten (10) trays including the reboiler.

This difference occurs in the stripping section. This is confirmed by the fact that the feed locations for both solutions are the same. The reason for the additional tray is believed to be related to the degree of accuracy of the computer calculation versus that of the graphical solution.

The values for XBA and the liquid concentrations leaving tray 9 and 10 are

0.00565, 0.006, and 0.001 respectively. Since completion of the program requires that the liquid concentration be less than or equal to XBA, ten (10) trays are required. If this were solved graphically, we would get nine (9) required trays because the difference between XBA and XA (9) would not be detected.

SYSTEM II: ETHANOL - WATER

This system requires the design of a plant for an ethanol - water distillation. The design parameters for this system include:

A feed to the system of a temperature of 177°F , with a composition of fifty-two percent (52%) by weight ethanol and a rate of 2,000 pounds per hour.

The system is to produce a distillate with a concentration of ninety-one percent (91%) ethanol and a bottom product composed of four percent (4%) by weight ethanol. The reflux ratio is specified at 3.00. The system requires ten (10) trays with the feed tray at stage 8. The system indicates we are getting very little separation in the enriching section per tray compared to that of the stripping section. This appears to be because of the azeotrope that occurs 10.57 mole percent ethanol.

These results are very similar to those obtained by direct graphical methods, but there is a great savings in time and labor with an increase in accuracy when utilizing this program. Essentially, this method evaluates only the necessary points on the HXY curves, thus a total picture of the system under study is not required.

VII. CONCLUSION

This program should be easily and widely used because it utilizes commonly available real data. Unlike the method of McCabe-Theile, it does not require equal molal overflow. The application of Lagrangian interpolation is relatively new with respect to machine solution of stage-to-stage calculations in chemical engineering. This procedure can easily be extended to solution of extraction problems expressed in a manner similar to that of the Pochon-Savarit method. This method is particularly useful because it can be used with unequally spaced data such as normally found or developed in a laboratory.

APPENDIX I

REQUIRED INPUT DATA

APPENDIX IREQUIRED INPUT DATA

| | <u>SYMBOL</u> | <u>UNITS</u> | <u>SOURCE</u> |
|--|---------------|---------------------------|---------------|
| 1. Equilibrium Data* | | | 5 |
| Mole fraction of A in liquid | XA | - | |
| Mole fraction of A in vapor | YA | - | |
| Liquid temperature for XA | TL | $^{\circ}\text{F}$ | |
| Vapor temperature for YA | TG | $^{\circ}\text{F}$ | |
| 2. Heat of solution | HSA | Kilojoule/g-mole | 4 |
| 3. Reference temperature for HSA | T0 | $^{\circ}\text{F}$ | 4 |
| 4. Molecular weight of A | MWA | lb/lb-mole | 5 |
| 5. Molecular weight of B | MWB | lb/lb-mole | 5 |
| 6. Heat of vaporization at normal boiling point, for A | LAMA1 | cal/g-mole | 6 |
| 7. Heat of vaporization at normal boiling point, for B | LAMB1 | cal/g-mole | 6 |
| 8. Critical temperature of A | TCA | $^{\circ}\text{K}$ | 8 |
| 9. Critical temperature of B | TCB | $^{\circ}\text{K}$ | 8 |
| 10. Boiling point of A | BPA | $^{\circ}\text{F}$ | 5 |
| 11. Boiling point of B | BPB | $^{\circ}\text{F}$ | 5 |
| 12. Specific heat of A | CPA** | BTU/lb $^{\circ}\text{F}$ | 9 |
| 13. Specific heat of B | CPB** | BUT/lb $^{\circ}\text{F}$ | 9 |
| 14. Feed rate | F | lbs/hour | *** |
| 15. Weight fraction of A in feed | WFA | | *** |

| | <u>SYMBOL</u> | <u>UNITS</u> | <u>SOURCE</u> |
|---|---------------|----------------|---------------|
| 16. Weight fraction of A in distillate | WDA | - | *** |
| 17. Weight fraction of A in bot- toms | WBA | - | *** |
| 18. Temperature of the feed | TF | ^o F | *** |
| 19. Reflux ratio | REFLX | - | *** |

*The equilibrium data and heats of solution used for these programs were obtained from the curves in Appendix III to facilitate the input data

**Since the specific heat is a function of temperature, the values for the liquids and vapor of each component are calculated for each temperature. The equations for these calculations are on the order of

$$CP = A + B \text{ TEMP} + C \text{ TEMP}^2 + D \text{ TEMP}^3$$

This common form enables us to read in to the program only the coefficients A, B, C, D for the liquid and vapor calculations of each component for a given set of calculations.

***The terms are specified for a given distillation problem.

APPENDIX II

INPUT DATA SHEET

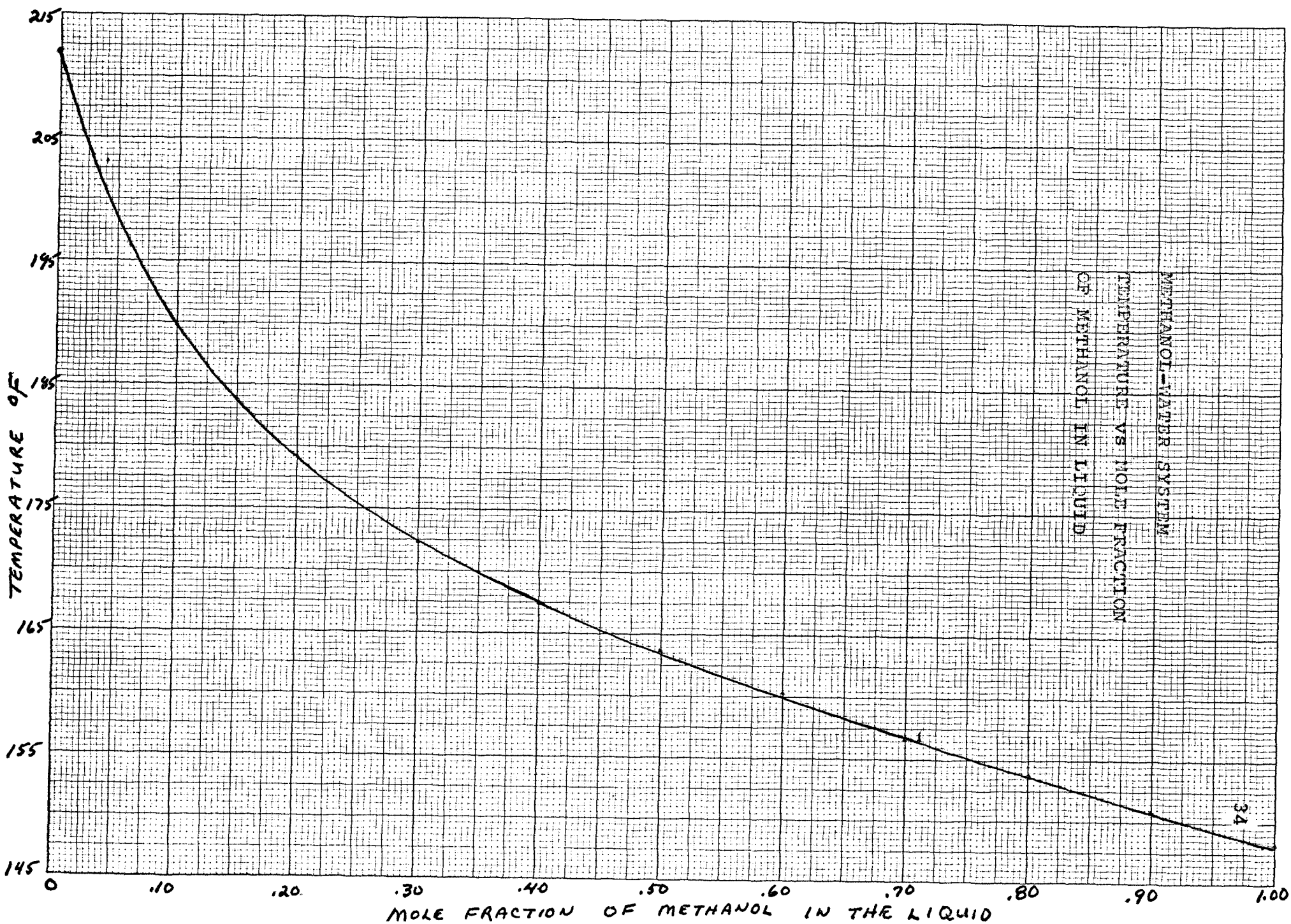
APPENDIX II
INPUT DATA SHEET

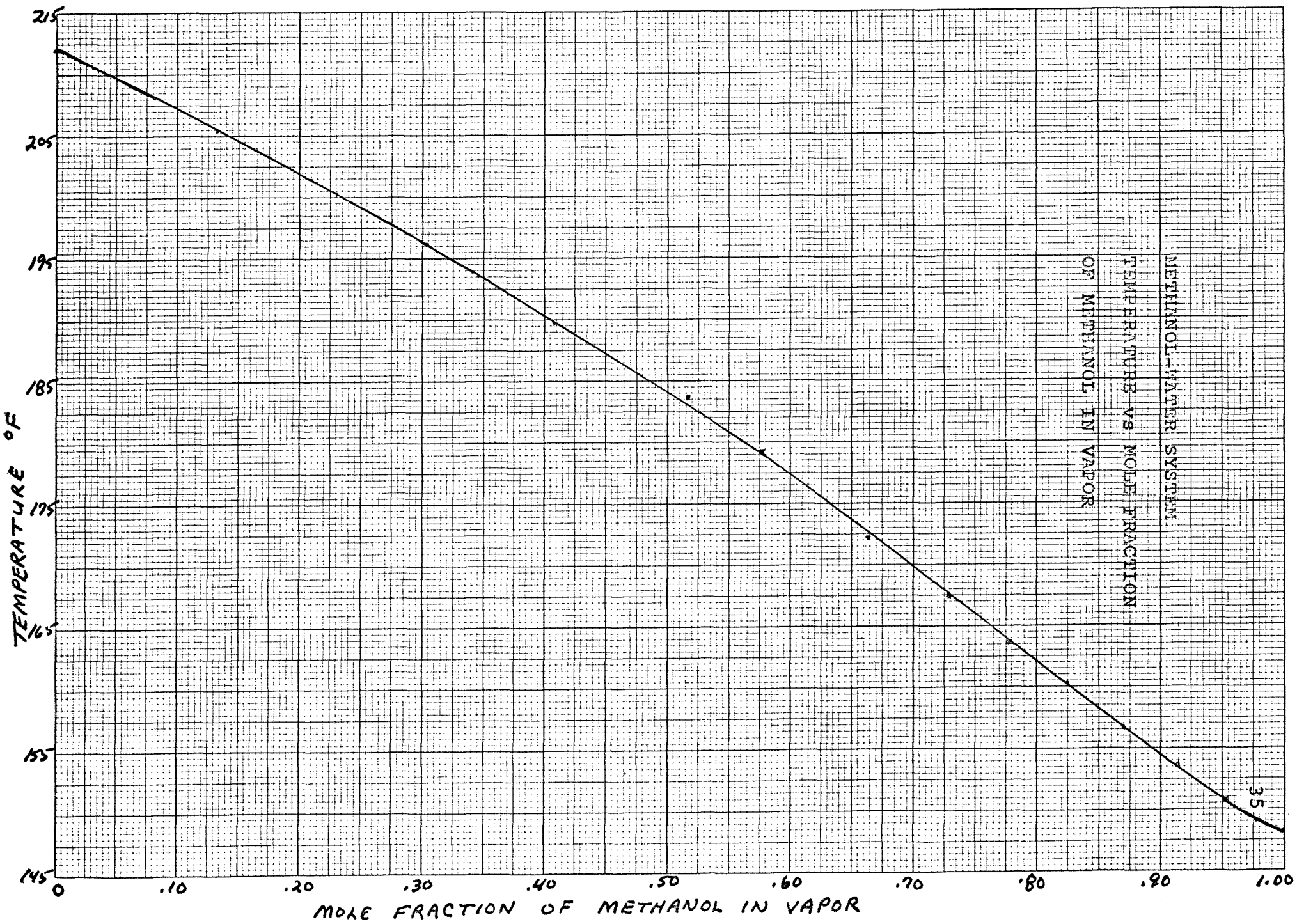
| <u>CARD NUMBER</u> | <u>INPUT</u> | <u>COLUMN NUMBER</u> |
|------------------------|--|--------------------------|
| 1 | Title Card | |
| | Titlebb | 1-8 |
| | Any user title for experiment | 9-80 |
| 2-21 | Table values for equilibrium data and heats of solution; 20 values for each XA(=YA), TL, HSA, TG | |
| | 1 card for each set of variables in XA ascending order (F10.0 format) | |
| | XA(=YA) | 1-10 |
| | TL | 11-20 |
| | HSA | 21-30 |
| | TG | 31-40 |
| 22 | Input variables (F10.0 format) | |
| | F, WFA, MWA, MWB, WDA, WBA, TF, REFLX | 1-80 |
| 24-27 | Specific heat coefficients (E20.6 format) | |
| 24 | AEL coefficients for specific of liquid A | |
| | Coefficient of constant | 1-20 |
| | Coefficient of linear term | 21-40 |
| | Coefficient of quadratic term | 41-60 |
| | Coefficient of cubic term | 61-80 |

| <u>CARD NUMBER</u> | <u>INPUT</u> | <u>COLUMN NUMBER</u> |
|------------------------|---|--------------------------|
| 25 | BEL coefficients for specific heat of liquid B | (Same as Card 24) |
| 26 | AEV coefficients for specific heat of vapor A | (Same as Card 24) |
| 27 | BEV coefficients for specific heat of vapor B | (Same as Card 24) |

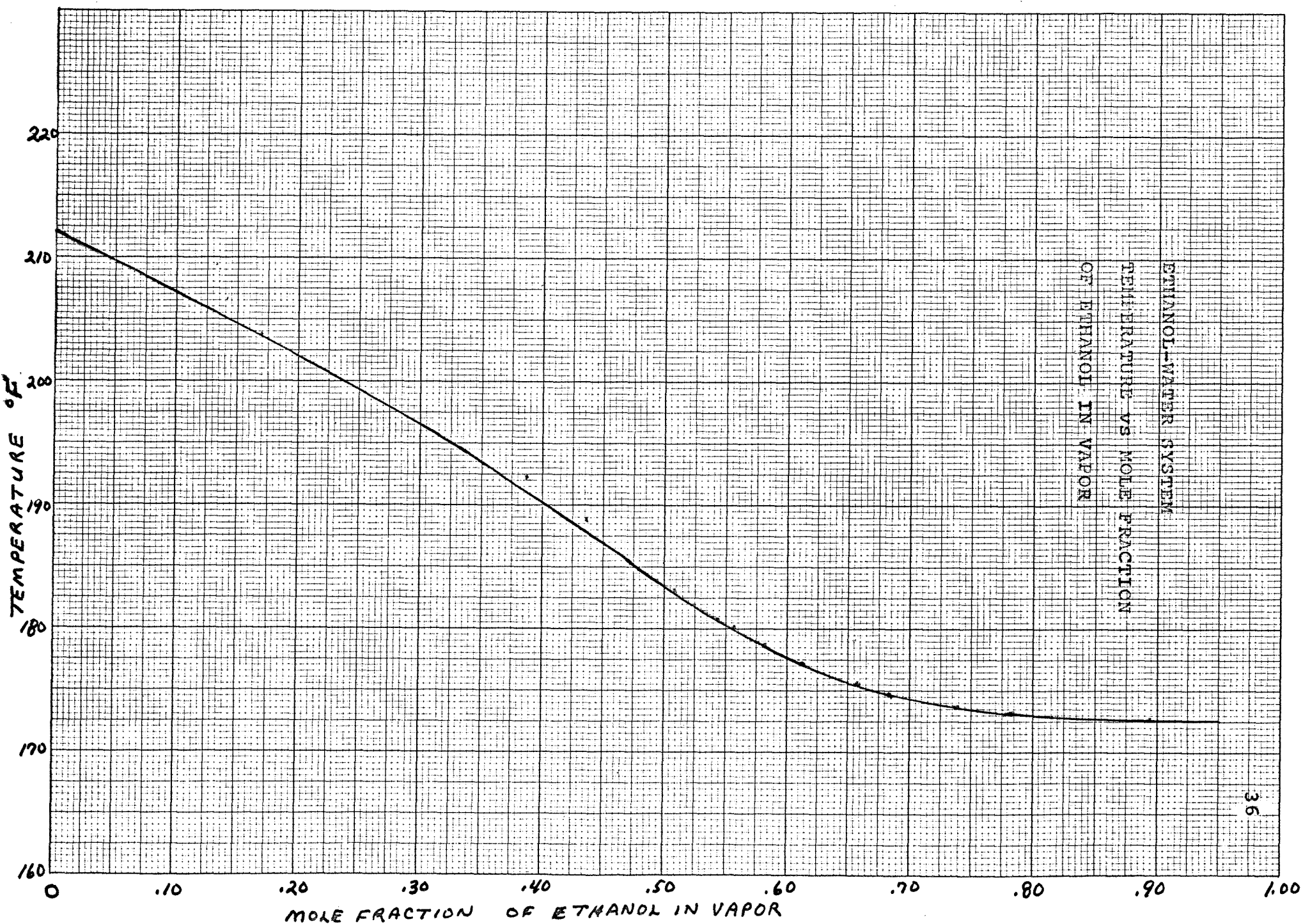
APPENDIX III

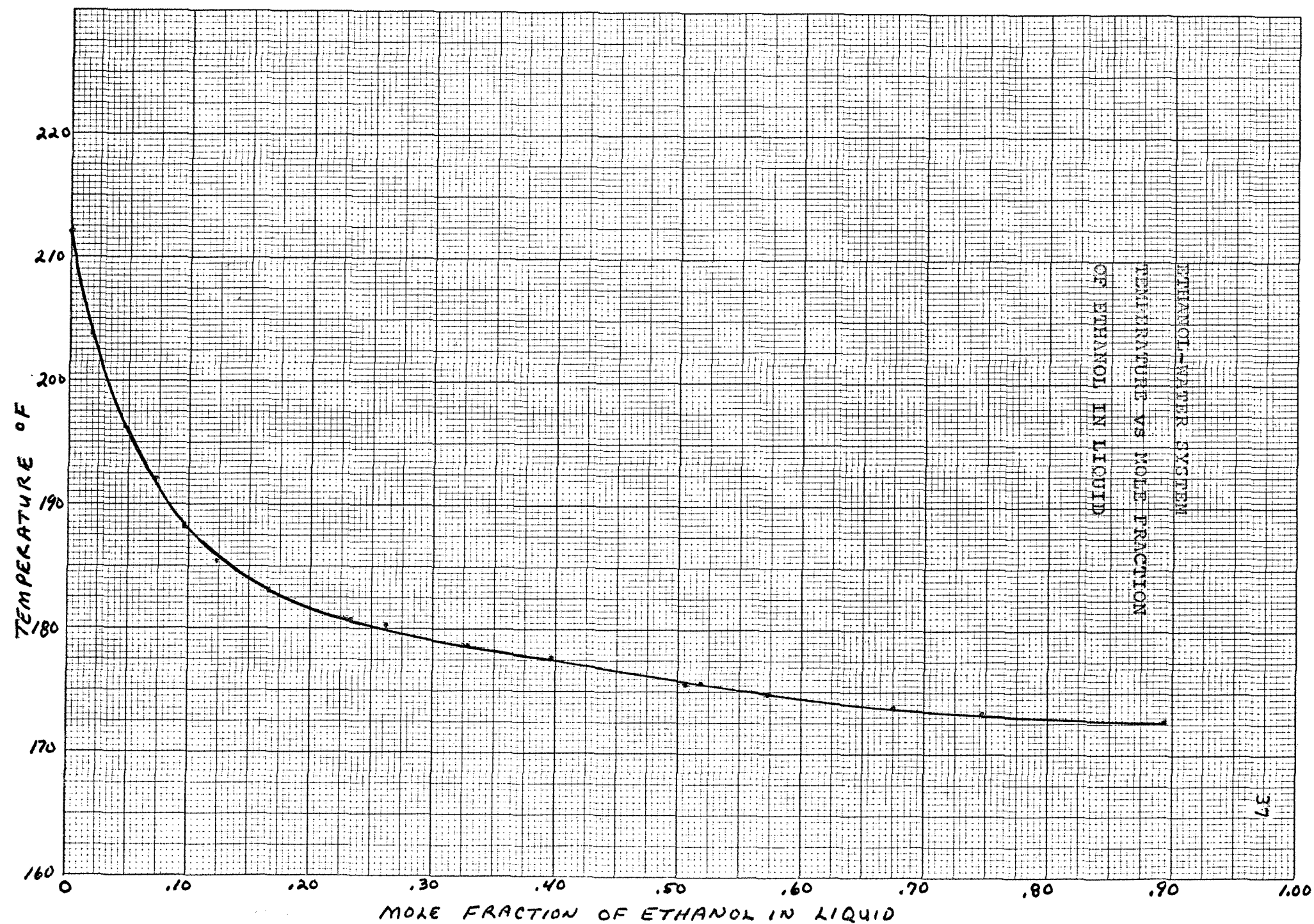
LIQUID - VAPOR EQUILIBRIUM DATA





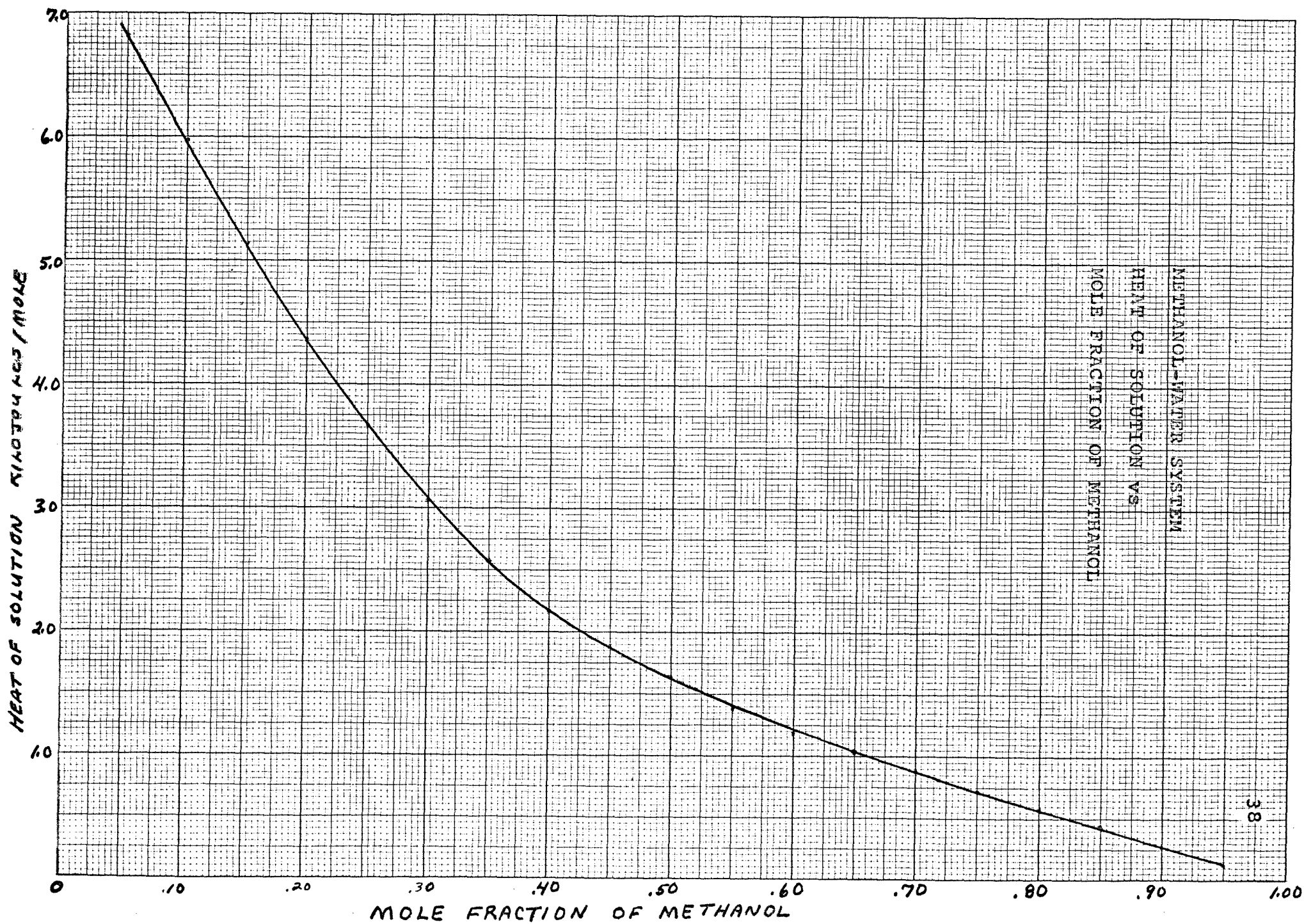
ETHANOL-WATER SYSTEM
TEMPERATURE VS MOLE FRACTION
OF ETHANOL IN VAPOR

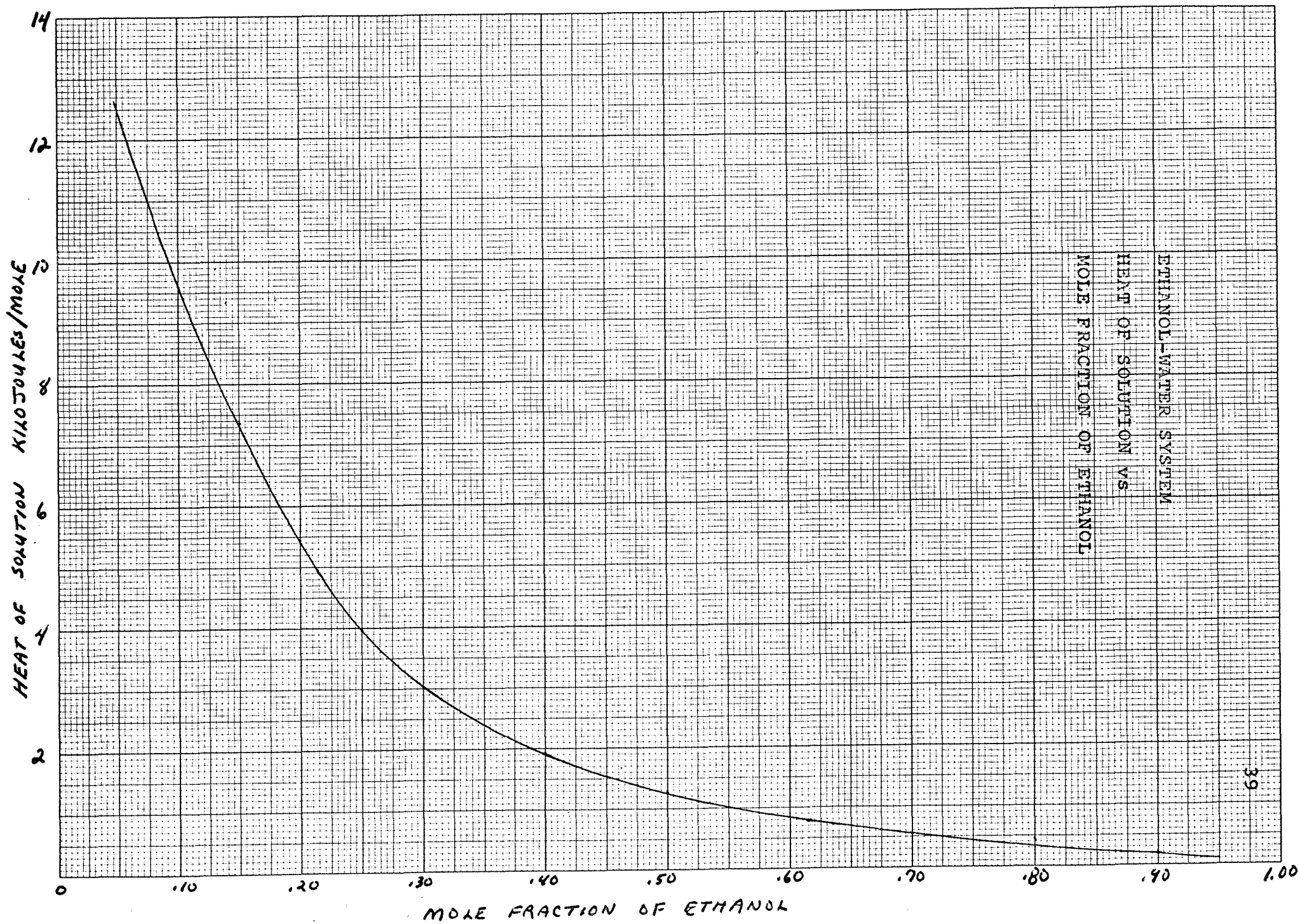




APPENDIX III

HEAT OF SOLUTION DATA





APPENDIX IV

COMPUTER PROGRAM

```

//B616      JOB (050557$*****.FFFF.0*20$003.05.0.99.1)      JOB 879
//S1 EXEC  FORTHCL,PARM='XREF'
XXFORT     PROC MEMBER=GO
***
***          FORTRAN H
***
***          PROCEDURE TO COMPILE AND LINK EDIT A FORTRAN SOURCE MODULE
***
XXFORT     EXEC PGM=FRTH,REGION=250K
***
XXCONTROLP DD DSN=SYS6.CONTROL(IEKAA00),DISP=SHR
XXMSGPRINT DD SYSOUT=A
XXSYSLIN   DD DSN=*&LOADSET,UNIT=SYSSQ,DISP=(MOD,PASS,DELETE),
XX          DCB=(RECFM=FB,LRECL=80,BLKSIZE=3200),
XX          SPACE=(CYL,(1,1),,CONTIG)
XXSYSPRINT DD SYSOUT=A
XXSYSPUNCH DD SYSOUT=B
XXSYSUT1   DD UNIT=SYSSQ,SPACE=(CYL,(1,1),,CONTIG)
XXSYSUT2   DD UNIT=SYSSQ,SPACE=(CYL,(1,1),,CONTIG)
***
***
//FORT.SYSIN DD *
IEF236I ALLOC. FOR B616      FORT      S1
IEF237I 343   ALLOCATED TO CONTROLP
IEF237I A45   ALLOCATED TO MSGPRINT
IEF237I 345   ALLOCATED TO SYSLIN
IEF237I A49   ALLOCATED TO SYSPRINT
IEF237I A11   ALLOCATED TO SYSPUNCH
IEF237I 345   ALLOCATED TO SYSUT1
IEF237I 345   ALLOCATED TO SYSUT2
IEF237I AA4   ALLOCATED TO SYSIN
IEF142I - STEP WAS EXECUTED - COND CODE 0004
IEF285I   SYS6.CONTROL      KEPT
IEF285I   VOL SER NOS= SYSLB2.
IEF285I   SYS75227.T073405.RV000.B616.LOADSET  PASSED
IEF285I   VOL SER NOS= DISK01.
IEF285I   SYS75227.T073405.RV000.B616.R0005906 DELETED
IEF285I   VOL SER NOS= DISK01.
IEF285I   SYS75227.T073405.RV000.B616.R0005907 DELETED
IEF285I   VOL SER NOS= DISK01.
IEF373I STEP /FORT      / START 75227.1219
IEF374I STEP /FORT      / STOP 75227.1220 CPU   0MIN 02.16SEC STOR VIRT 256K
XXLKED     EXEC PGM=IEWL,PARM=(MAP,LIST),REGION=130K,COND=(4,LT,FORT) 00000200
***
XXSYSLIB   DD DSN=SYS6.USERLIB,DISP=SHR      00000210
XX          DD DSN=SYS6.USERLIB,DISP=SHR      00000220
XX          DD DSN=SYS6.FORTLIB,DISP=SHR      00000230
XX          DD DSN=SYS7.FORTLIB,DISP=SHR      00000240
XXSYSLIN   DD DSN=*.FORT.SYSLIN,DISP=(OLD,DELETE) 00000250
XX          DD DDNAME=SYSIN                   00000260
//LKED.SYSLMOD DD DSN=RESEARCH.MODLIB(B616),DISP=SHR
X/SYSLMOD DD DSN=*&GOSET(&MEMBER),UNIT=SYSDA,DISP=(MOD,PASS,DELETE), 00000280
IEF653I SUBSTITUTION JCL - DSN=*&GOSET(GO),UNIT=SYSDA,DISP=(MOD,PASS,DELETE),
XX          SPACE=(CYL,(1,1,1),,CONTIG)      00000290
XXSYSPRINT DD SYSOUT=A                        00000300
XXSYSUT1   DD UNIT=SYSSQ,SPACE=(CYL,(1,1),,CONTIG) 00000310
IEF236I ALLOC. FOR B616      LKED      S1
IEF237I 521   ALLOCATED TO SYSLIB
IEF237I 521   ALLOCATED TO
IEF237I 343   ALLOCATED TO
IEF237I 521   ALLOCATED TO
IEF237I 345   ALLOCATED TO SYSLIN
IEF237I 13A   ALLOCATED TO SYSLMOD

```

```

IEF237I A42   ALLOCATED TO SYSPRINT
IEF237I 345   ALLOCATED TO SYSUT1
IEF142I - STEP WAS EXECUTED - COND CODE 0000
IEF285I   SYS6.USERLIB                                KEPT
IEF285I   VOL SER NOS= SYSLB1.
IEF285I   SYS6.USERLIB                                KEPT
IEF285I   VOL SER NOS= SYSLB1.
IEF285I   SYS6.FORTLIB                                KEPT
IEF285I   VOL SER NOS= SYSLB2.
IEF285I   SYS7.FORTLIB                                KEPT
IEF285I   VOL SER NOS= SYSLB1.
IEF285I   ,SYS75227.T073405.RV000.B616.LOADSET        DELETED
IEF285I   VOL SER NOS= DISK01.
IEF285I   RESEARCH.MODLIB                             KEPT
IEF285I   VOL SER NOS= DSK014.
IEF285I   SYS75227.T073405.RV000.B616.R0005910        DELETED
IEF285I   VOL SER NOS= DISK01.
IEF373I STEP /LKED      / START 75227.1220
IEF374I STEP /LKED      / STOP  75227.1221 CPU    0MIN 00.40SEC STOR VIRT 124K
//S2 EXEC PGM=B616
//STEPLIB DD DSN=RESEARCH.MODLIB.DISP=SHR
//FT06F001 DD SYSOUT=A
//FT05F001 DD *
//
IEF236I ALLOC. FOR B616      S2
IEF237I 13A   ALLOCATED TO STEPLIB
IEF237I A45   ALLOCATED TO FT06F001
IEF237I A43   ALLOCATED TO FT05F001
COMPLETION CODE - SYSTEM=322 USER=0000
IEF285I   RESEARCH.MODLIB                                KEPT
IEF285I   VOL SER NOS= DSK014.
IEF373I STEP /S2      / START 75227.1221
IEF374I STEP /S2      / STOP  75227.1226 CPU    0MIN 17.44SEC STOR VIRT  44K
IEF375I JOB  /B616    / START 75227.1219
IEF376I JOB  /B616    / STOP  75227.1226 CPU    0MIN 20.00SEC

```



```

C
C
C      FEED ENTHALPY CALCS.
ISN 0038      XATS=ZFA
C
C      CALL WHERE TO FIND WHERE IN TABLE VALUE FITS
C      WHERE RETURNS THE LAST I VALUE OF THE ARRAY <=THE ARG
C
ISN 0039      II=+1
ISN 0040      CALL WHERE(XA,NP,XATS,II)
C
C      DO LINEAR INTERP. TO GET TLT + HSAT
C
ISN 0041      I=II
ISN 0042      TLT=YLIN(XATS,XA(I),XA(I+1),TL(I),TL(I+1))
ISN 0043      HSAT=YLIN(XATS,XA(I),XA(I+1),HSA(I),HSA(I+1))
C
C      CALL EL TO RETURN ENTHALPY OF LIQUID =HL
C
ISN 0044      CALL EL(XATS,HSAT,TF,HL)
ISN 0045      IF((TF-TLT).GT.0.) GO TO 12
ISN 0047      GO TO 15
ISN 0048      12 YATS=ZFA
ISN 0049      II=+1
ISN 0050      CALL WHERE(YA,NP,YATS,II)
ISN 0051      TGT=YLIN(YATS,YA(II),YA(II+1),TG(II),TG(II+1))
ISN 0052      CALL EV(YATS,TGT,HG)
ISN 0053      HFEED=HG
C
C      .....
C      NOTE DIVISION CAN OCCUR IF TGT=TLT ---- THIS SHOULD NOT OCCUR
ISN 0054      IF((TF-TGT).LT.0.) HFEED=((HG-HL)/(TGT-TLT))*(TF-TLT) + HL
ISN 0056      GO TO 18
ISN 0057      15 HFEED=HL
ISN 0058      18 WRITE(6,604) HFEED
C
ISN 0059      I=1
C
C      ENTHALPY CALC. FOR HG1
C
ISN 0060      YATS=XDA
ISN 0061      II=+1
ISN 0062      CALL WHERE(YA,NP,YATS,II)
C
C      DO LINEAR INTERP TO GET TGT
C
ISN 0063      TGT=YLIN(YATS,YA(II),YA(II+1),TG(II),TG(II+1))
C
C      CALL EV TO RETURN ENTHALPY OF VAPOR = HG
C
ISN 0064      CALL EV(YATS,TGT,HG)
ISN 0065      HG1(I)=HG
C
C      CALC. ENTHALPY OF DISTILLATE
C
ISN 0066      XATS=XDA
ISN 0067      II=+1
ISN 0068      CALL WHERE(XA,NP,XATS,II)
ISN 0069      TLT=YLIN(XATS,XA(II),XA(II+1),TL(II),TL(II+1))
ISN 0070      HSAT=YLIN(XATS,XA(II),XA(II+1),HSA(II),HSA(II+1))

```

```

ISN 0071      CALL EL(XATS,HSAT,TLT,HL)
ISN 0072      HDIST=HL
ISN 0073      WRITE(6,606) HDIST
C
C
C      ENTHALPY OF DEL PT.
ISN 0074      HDELD=(REFLX*(HG1(I)-HDIST))+ HG1(I)
ISN 0075      WRITE(6,607) HDELD
C
C
C      CONDENSER HEAT LOAD
ISN 0076      QCOND=(HDELD-HDIST)*DIST
ISN 0077      WRITE(6,608) QCOND
C
C
C      ENTHALPY OF BOTTOMS
ISN 0078      XATS=XBA
ISN 0079      II=+1
ISN 0080      CALL WHERE(XA,NP,XATS,II)
ISN 0081      TLT=YLIN(XATS,XA(II),XA(II+1),TL(II),TL(II+1))
ISN 0082      HSAT=YLIN(XATS,XA(II),XA(II+1),HSA(II),HSA(II+1))
ISN 0083      CALL EL(XATS,HSAT,TLT,HL)
ISN 0084      HBOT=HL
ISN 0085      WRITE(6,610) HBOT
C
C
C      ENTHALPY OF BOT. DEL. PT.
ISN 0086      HDELB=(FEED*HFEED-DIST*HDELD)/BOT
ISN 0087      WRITE(6,611) HDELB
C
C
C      REBOILER HEAT LOAD
ISN 0088      QBOIL=(HBOT-HDELB)*BOT
ISN 0089      WRITE(6,612) QBOIL
C
C
C      WRITE(6,605) I,HG1(I),YATS
C
C
C
C      ENTHALPY CALCS. FOR ENRICHING & STRIPPING SECTION BY ITERATIVE TECHNIQUE
C      LFLAG=0      -- ENRICHING SECTION
C      LFLAG=2      -- STRIPPING SECTION
ISN 0091      LFLAG=0
C
ISN 0092      YTRY=YATS
ISN 0093      20 YATS=YTRY
ISN 0094      II=+1
ISN 0095      CALL WHERE(YA,NP,YATS,II)
ISN 0096      TGT=YLIN(YATS,YA(II),YA(II+1),TG(II),TG(II+1))
ISN 0097      21 TLT=TGT
ISN 0098      II=-1
ISN 0099      CALL WHERE(TL,NP,TLT,II)
ISN 0100      HSAT=YLIN(TLT,TL(II),TL(II+1),HSA(II),HSA(II+1))
ISN 0101      XATS=YLIN(TLT,TL(II),TL(II+1),XA(II),XA(II+1))
ISN 0102      25 CONTINUE
ISN 0103      CALL EL(XATS,HSAT,TLT,HL)
ISN 0104      IF(LFLAG.EQ.0) WRITE(6,6051) I,HL,XATS
ISN 0105      IF(LFLAG.EQ.2) WRITE(6,615) I,HL,XATS

```

```

C.....
C..... TEMP IN THIS(MAIN) PROGRAM INDICATES TEMPORARY ARGUMENT .....
C..... TEMP IN EL AND EV SUBROUTINES INDICATES TEMPERATURE .....
C.....
ISN 0108 IF(LFLAG.EQ.2) GO TO 28
ISN 0110 TEMP=(HDELD-HFEED)/(XDA-ZFA) - (HDELD-HL)/(XDA-XATS)
ISN 0111 IF(TEMP.GE.0.) GO TO 66
ISN 0113 GO TO 30
ISN 0114 28 IF((XATS-XBA).LE.(0.00)) GO TO 101

C
C
C SEARCH FOR NEXT HG1 POINT
C
ISN 0116 30 GET NEXT 3 YA TABLE VALUES < HG1(I)
ISN 0117 30 DO 35 J=1,19
ISN 0118 JJ=20-J
ISN 0120 IF(YA(JJ).LE. YATS ) GO TO 37
ISN 0120 35 CONTINUE
C
ISN 0121 JJ=1 IF FALL THRU
ISN 0123 37 IF(JJ.LE.3) JJ=3
ISN 0124 YAT1=YA(JJ)
ISN 0125 YAT2=YA(JJ-1)
ISN 0126 YAT3=YA(JJ-2)
ISN 0127 TGT1=TG(JJ)
ISN 0127 TGT2=TG(JJ-1)
ISN 0128 TGT3=TG(JJ-2)
ISN 0129 CALL EV(YAT1,TGT1,HGT1)
ISN 0130 CALL EV(YAT2,TGT2,HGT2)
ISN 0131 CALL EV(YAT3,TGT3,HGT3)
ISN 0132 YTRY=YATS
ISN 0133 YINC=YTRY/100.
ISN 0134 SAVE=-1.
ISN 0135 SAVET=0.

C
ISN 0136 45 YTRY=YTRY-YINC
ISN 0137 ANS=YLAGR(YTRY,YAT1,YAT2,YAT3,HGT1,HGT2,HGT3)
ISN 0138 IF(LFLAG.EQ.2) GO TO 46
ISN 0140 TEMP=(HDELD-HL)/(XDA-XATS) - (HDELD-ANS)/(XDA-YTRY)
ISN 0141 GO TO 47
ISN 0142 46 TEMP=(ANS-HDELB)/(YTRY-XBA) - (HL-HDELB)/(XATS-XBA)
ISN 0143 47 CONTINUE
ISN 0144 IF(SAVE.EQ.-1. .AND. SAVET.EQ.0.) SAVET=TEMP
ISN 0146 YINTR=YINC/YTRY
ISN 0147 IF(ABS(TEMP/SAVET).LT.1.E-4 .OR. ABS(YINTR).LT.1.E-4) GO TO 49
ISN 0149 IF((TEMP*SAVE).GT.0.) GO TO 45
ISN 0151 SAVE=TEMP
ISN 0152 48 YINC=-YINC/2.
ISN 0153 GO TO 45
ISN 0154 49 I=I+1
ISN 0155 HG1(I)=ANS
ISN 0156 IF(LFLAG.EQ.0) WRITE(6,605) I,HG1(I),YTRY
ISN 0158 IF(LFLAG.EQ.2) WRITE(6,6151) I,HG1(I),YTRY
ISN 0160 GO TO 20

C
ISN 0161 66 WRITE(6,609) I
ISN 0162 LFLAG=2
ISN 0163 GO TO 30

C
C
C
C

```

```

ISN 0164      101 WRITE(6,614) I
ISN 0165      GO TO 10

C
C
ISN 0166      500 FORMAT(20A4)
ISN 0167      501 FORMAT(4F10.0)
ISN 0168      502 FORMAT(8F10.0)
ISN 0169      503 FORMAT( 4E20.6 )
ISN 0170      6000 FORMAT('1',///,18X,'***** / BINARY DISTILLATION CALCULATION BY PONCH
10N-SAVARIT METHOD *****',//
220X,'***** ENTHALPY DATA CALCULATED USING LAGRANGE INTERPOLATION
3 *****',//
420X,'***** ',13A4,' *****',//
525X,'-----'//)

ISN 0171      600 FORMAT('0'////
1 5X,'XA=YA',5X,'TL',8X,'HSA',7X,'TG',//,
2 20(4F10.3,/) , //
3 ' F=',F10.3,5X,'WFA=',F10.3,5X,'MWA=',F10.3,5X,'MWB=',F10.3,//,
4 ' WDA=',F10.3,5X,'WBA=',F10.3,5X,'TF=',F10.3,5X,'REFLX=',F10.3,//
5 ' TO=',F10.3,5X,'LAMA1=',F10.3,5X,'LAMB1=',F10.3,5X,'TCA=',F10.3,
6. ///, ' TCB=',F10.3,5X,'BPA=',F10.3,5X,'BPB=',F10.3,//)

ISN 0172      601 FORMAT(10X,'OUTPUT FOR ',13A4,/,
110X,'-----'//
2--',//
3 10X,'MOLE FRACTION OF FEED = ',F5.3,/)

ISN 0173      602 FORMAT(10X,'MOLE FRACTION OF DISTILLATE = ',F5.3,/)
ISN 0174      603 FORMAT(10X,'MOLE FRACTION OF BOTTOMS = ',F7.5,/)
ISN 0175      6031 FORMAT(10X,'DISTILLATE (POUNDS/HOUR) = ',E14.6)
ISN 0176      6032 FORMAT(10X,'BOTTOMS (POUNDS/HOUR) = ',E14.6,/)
ISN 0177      604 FORMAT(10X,'ENTHALPY OF FEED = ',E14.6,/)
ISN 0178      605 FORMAT('0ENTHALPY OF VAPOR ENRICHING SECTION - STAGE ',I2,
1 ' = ',E14.6,5X,'YA=',F5.3)

ISN 0179      6051 FORMAT('0ENTHALPY OF LIQUID ENRICHING SECTION - STAGE ',I2,
1 ' = ',E14.6,5X,'XA=',F5.3,/)

ISN 0180      606 FORMAT(10X,'ENTHALPY OF DISTILLATE = ',E14.6,/)
ISN 0181      607 FORMAT(10X,'ENTHALPY OF DISTILLATE DEL POINT = ',E14.6,/)
ISN 0182      608 FORMAT(10X,'CONDENSER HEAT LOAD = ',E14.6,/)
ISN 0183      609 FORMAT(70X,'FEED TRAY LOCATION PLATE = ',I3,/)
ISN 0184      610 FORMAT(10X,'ENTHALPY OF BOTTOMS = ',E14.6,/)
ISN 0185      611 FORMAT(10X,'ENTHALPY OF BOTTOMS DEL POINT = ',E14.6,/)
ISN 0186      612 FORMAT(10X,'REBOILER HEAT LOAD = ',E14.6,/)
ISN 0187      614 FORMAT(///,75X,'TOTAL NUMBER OF IDEAL PLATES INCLUDING REBOILER=',
1 I3)

ISN 0188      615 FORMAT('0ENTHALPY OF LIQUID STRIPPING SECTION - STAGE ',I2,
1 ' = ',E14.6,5X,'XA=',F5.3,/)

ISN 0189      6151 FORMAT('0ENTHALPY OF VAPOR STRIPPING SECTION - STAGE ',I2,
1 ' = ',E14.6,5X,'YA=',F5.3)

ISN 0190      616 FORMAT('0AEL COEFFICIENTS - ',4E15.6,/,
1 ' BEL COEFFICIENTS - ',4E15.6,/,
2 ' AEV COEFFICIENTS - ',4E15.6,/,
3 ' BEV COEFFICIENTS - ',4E15.6,/, '1')

C
C
C      ERROR

ISN 0191      800 WRITE(6,801)
ISN 0192      801 FORMAT('1',///,'0***** ERROR - NO TITLE CARD FOR EXPERIMENT
1*')

C
ISN 0193      999 STOP

```

ISN 0194

END

LEVEL 21.6 (MAY 72)

OS/360 FORTRAN H

COMPILER OPTIONS - NAME= MAIN,OPT=00,LINECNT=62,SIZE=0000K,
SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF

```

ISN 0002      SUBROUTINE EL(XATS,HSAT,TLT,HL)
              C
              C
              C      EL  CALCS. ENTHALPY OF LIQUID = HL
ISN 0003      REAL*4 MWA,MWB,LAMA1,LAMB1,MOLA,MOLB,MWFAV,MWDAV,MWBAV
ISN 0004      REAL*4 MWAV
ISN 0005      COMMON F,WFA,MWA,MWB,WDA,WBA,TF,REFLX,TD,LAMA1,LAMB1,TCA,TCB,BPA,
              1      BPB
ISN 0006      COMMON /CPAB/ AEL(4),BEL(4),AEV(4),BEV(4)
              C
              C      DELHS= HEAT OF SOL.
ISN 0007      DELHS= -238.9*1.8*HSAT**XATS
              C
ISN 0008      MWAV=XATS*MWA + (1.-XATS)*MWB
ISN 0009      TEMP=(TLT+460.)/1.8
ISN 0010      CPA=AEL(1)+AEL(2)*TEMP+AEL(3)*TEMP**2+AEL(4)*TEMP**3
ISN 0011      CPB=BEL(1)+BEL(2)*TEMP+BEL(3)*TEMP**2+BEL(4)*TEMP**3
ISN 0012      CPM=XATS*CPA + (1.-XATS)*CPB
ISN 0013      HL=(CPM*(TLT-TD)*MWAV) + DELHS
ISN 0014      RETURN
ISN 0015      END

```

LEVEL 21.6 (MAY 72)

05/360 FORTRAN H

COMPILER OPTIONS - NAME= MAIN,OPT=00,LINECNT=62,SIZE=0000K,

SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF

```

      ISN 0002      SUBROUTINE EV(YAT ,TGT,HG)
                  C
                  C      EV CALCS. ENTHALPY OF VAPOR =HG
                  C
      ISN 0003      REAL*4 MWA,MWB,LAMA1,LAMB1,MOLA,MOLB,MWFAV,MWDAY,MWBAY
      ISN 0004      REAL*4 LAMA2,LAMB2
      ISN 0005      COMMON F,WFA,MWA,MWB,WDA,WBA,TF,REFLX,TO,LAMA1,LAMB1,TCA,TCB,BPA,
1      BPB
      ISN 0006      COMMON /CPAB/ AEL(4),BEL(4), AEV(4),BEV(4)
                  C
                  C
      ISN 0007      TRA1=(BPA+460.)/(1.8*TCA)
      ISN 0008      TRB1=(BPB+460.)/(1.8*TCB)
      ISN 0009      TRA2=(TGT+460.)/(1.8*TCA)
      ISN 0010      TRB2=(TGT+460.)/(1.8*TCB)
      ISN 0011      LAMA2=LAMA1*((1.-TRA2)/(1.-TRA1))**.38 *(1.8/MWA)
      ISN 0012      LAMB2=LAMB1*((1.-TRB2)/(1.-TRB1))**.38 *(1.8/MWB)
      ISN 0013      TEMP=(TGT+460.)/1.8
      ISN 0014      CPA=AEV(1)+AEV(2)*TEMP+AEV(3)*TEMP**2+AEV(4)*TEMP**3
      ISN 0015      CPB=BEV(1)+BEV(2)*TEMP+BEV(3)*TEMP**2+BEV(4)*TEMP**3
      ISN 0016      HG=  YAT * (  CPA*MWA*(TGT-TO) + LAMA2*MWA )
1      +(1.-YAT)*(  CPB*MWB*(TGT-TO) + LAMB2*MWB )
      ISN 0017      RETURN
      ISN 0018      END

```

LEVEL 21.6 (MAY 72)

OS/360 FORTRAN H

COMPILER OPTIONS - NAME= MAIN,OPT=00,LINECNT=62,SIZE=0000K,
SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF

```

ISN 0002      SUBROUTINE WHERE(ARRAY,N,ELEM,I)
              C
              C      WHERE WILL DETERMINE WHERE IN THE ARRAY ELEM FITS
              C      AND RETURN I OF THE LAST ARRAY ELEMENT <= ELEM.
ISN 0003      DIMENSION ARRAY(N)
              C
              C      ARRAY IS STRICTLY MONOTONIC INCREASING OR DECREASING
              C      DEPENDING ON I      IF I=+1, INCREASING ----- IF I=-1, DECREASING
ISN 0004      IF(I.LT.0) GO TO 50
              C
ISN 0006      DO 10 J=2,N
ISN 0007      IF(ARRAY(J).GT.ELEM) GO TO 20
ISN 0009      10 CONTINUE
ISN 0010      I=N
ISN 0011      RETURN
ISN 0012      20 I=J-1
ISN 0013      RETURN
              C
ISN 0014      50 CONTINUE
ISN 0015      DO 60 J=2,N
ISN 0016      IF(ARRAY(J).LT.ELEM) GO TO 70
ISN 0018      60 CONTINUE
ISN 0019      I=N
ISN 0020      RETURN
ISN 0021      70 I=J-1
ISN 0022      RETURN
              C
ISN 0023      END

```

LEVEL 21.6 (MAY 72)

OS/360 FORTRAN H

COMPILER OPTIONS - NAME= MAIN.OPT=00.LINECNT=62.SIZE=0000K,
 SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF

ISN 0002

FUNCTION YLAGR(X,X1,X2,X3,Y1,Y2,Y3)

C
C
C
C
C
C
C
C

YLAGR IS A NON-LINEAR LAGRANGE INTERPOLATION FUNCTION

YLAGR WILL RETURN THE Y VALUE ON THE Y1,Y2,Y3 SCALE
 CORRESPONDING TO THE X VALUE ON THE X1,X2,X3 SCALE.
 (I.E. GIVEN PTS. (X1,Y1),(X2,Y2),(X3,Y3) AND X ON THIS CURVE,
 GET Y)

ISN 0003

 $A1 = ((X-X2)*(X-X3)) / ((X1-X2)*(X1-X3)) * Y1$

ISN 0004

 $A2 = ((X-X1)*(X-X3)) / ((X2-X1)*(X2-X3)) * Y2$

ISN 0005

 $A3 = ((X-X1)*(X-X2)) / ((X3-X1)*(X3-X2)) * Y3$

ISN 0006

YLAGR=A1+A2+A3

ISN 0007

RETURN

ISN 0008

END

LEVEL 21.6 (MAY 72)

OS/360 FORTRAN H

```

      COMPILER OPTIONS - NAME=  MAIN,OPT=00,LINECNT=62,SIZE=0000K,
                           SOURCE,EBCDIC,NOLIST,NODECK,LOAD,MAP,NOEDIT,ID,XREF
ISN 0002      FUNCTION YLIN(X,X1,X2,Y1,Y2)
              C
              C      YLIN  IS A LINEAR INTERPOLATION FUNCTION
              C
              C      YLIN WILL RETURN THE Y VALUE ON THE Y1,Y2 SCALE
              C      CORRESPONDING TO THE X VALUE ON THE X1,X2 SCALE.
              C      (I.E. GIVEN PT.(X1,Y1),(X2,Y2) AND X ON THIS LINE - GET Y)
ISN 0003      YLIN=(Y2-Y1)/(X2-X1) * (X-X1)  +  Y1
ISN 0004      RETURN
ISN 0005      END

```

APPENDIX V

SAMPLE OUTPUTS

```

***** BINARY DISTILLATION CALCULATION BY PONCHON-SAVARIT METHOD *****
***** ENTHALPY DATA CALCULATED USING LAGRANGE INTERPOLATION *****
***** SYSTEM 1: COMPONENT A=METHANOL   COMPONENT B=WATER *****

```

| XA=YA | TL | HSA | TG |
|-------|---------|-------|---------|
| 0.0 | 212.000 | 7.700 | 212.000 |
| 0.050 | 199.000 | 6.838 | 209.500 |
| 0.100 | 190.000 | 5.989 | 207.200 |
| 0.150 | 183.800 | 5.114 | 204.600 |
| 0.200 | 179.200 | 4.357 | 202.000 |
| 0.250 | 175.500 | 3.666 | 199.100 |
| 0.300 | 172.500 | 3.055 | 196.400 |
| 0.350 | 170.000 | 2.591 | 193.300 |
| 0.400 | 167.600 | 2.218 | 190.300 |
| 0.450 | 165.500 | 1.896 | 187.200 |
| 0.500 | 163.600 | 1.632 | 184.000 |
| 0.550 | 161.900 | 1.398 | 181.000 |
| 0.600 | 160.100 | 1.197 | 177.500 |
| 0.650 | 158.500 | 1.017 | 173.600 |
| 0.700 | 157.000 | 0.862 | 170.000 |
| 0.750 | 155.400 | 0.716 | 166.000 |
| 0.800 | 153.900 | 0.569 | 162.000 |
| 0.850 | 152.400 | 0.419 | 158.400 |
| 0.900 | 150.800 | 0.272 | 154.500 |
| 0.950 | 149.500 | 0.134 | 151.000 |

```

F= 5000.000   WFA= 0.500   MWA= 32.040   MWB= 18.020
WDA= 0.950    WBA= 0.010   TF= 136.000   REFLX= 1.029
TO= 67.500    LAMA1= 8430.000   LAMB1= 9717.000   TCA= 513.000
TCB= 647.000   BPA= 148.000   BPB= 212.000

```

```

AEL COEFFICIENTS - 0.582480E+00 -0.375646E-03 -0.167844E-05 0.106214E-07
BEL COEFFICIENTS - 0.213974E+01 -0.968137E-02 0.268536E-04 -0.242139E-07
AEV COEFFICIENTS - 0.189431E+00 0.361729E-03 0.548825E-06 -0.443884E-09
BEV COEFFICIENTS - 0.452219E+00 -0.129224E-03 0.417008E-06 -0.200401E-09

```

OUTPUT FOR SYSTEM 1: COMPONENT A=METHANOL COMPONENT B=WATER

MOLE FRACTION OF FEED = 0.360

MOLE FRACTION OF DISTILLATE =0.914

MOLE FRACTION OF BOTTOMS =0.00565

DISTILLATE(POUNDS/HOUR) = 0.260638E+04

BOTTOMS (POUNDS/HOUR) = 0.239362E+04

ENTHALPY OF FEED = 0.996142E+03

ENTHALPY OF DISTILLATE = 0.170925E+04

ENTHALPY OF DISTILLATE DEL POINT = 0.313272E+05

CONDENSER HEAT LOAD = 0.250309E+07

ENTHALPY OF BOTTOMS = 0.258734E+04

ENTHALPY OF BOTTOMS DEL POINT = -0.183865E+05

REBOILER HEAT LOAD = 0.277379E+07

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR ENRICHING SECTION - STAGE | 1 = | 0.163066E+05 | YA=0.914 |
| ENTHALPY OF LIQUID ENRICHING SECTION - STAGE | 1 = | 0.168723E+04 | XA=0.814 |

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR ENRICHING SECTION - STAGE | 2 = | 0.164300E+05 | YA=0.864 |
| ENTHALPY OF LIQUID ENRICHING SECTION - STAGE | 2 = | 0.168173E+04 | XA=0.689 |

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR ENRICHING SECTION - STAGE | 3 = | 0.165814E+05 | YA=0.802 |
| ENTHALPY OF LIQUID ENRICHING SECTION - STAGE | 3 = | 0.168633E+04 | XA=0.552 |

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR ENRICHING SECTION - STAGE | 4 = | 0.167428E+05 | YA=0.736 |
| ENTHALPY OF LIQUID ENRICHING SECTION - STAGE | 4 = | 0.169819E+04 | XA=0.412 |

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR ENRICHING SECTION - STAGE | 5 = | 0.169069E+05 | YA=0.670 |
| ENTHALPY OF LIQUID ENRICHING SECTION - STAGE | 5 = | 0.173396E+04 | XA=0.306 |

FEED TRAY LOCATION PLATE = 5

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR STRIPPING SECTION - STAGE | 6 = | 0.172365E+05 | YA=0.538 |
| ENTHALPY OF LIQUID STRIPPING SECTION - STAGE | 6 = | 0.187420E+04 | XA=0.173 |

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR STRIPPING SECTION - STAGE | 7 = | 0.178461E+05 | YA=0.304 |
| ENTHALPY OF LIQUID STRIPPING SECTION - STAGE | 7 = | 0.222230E+04 | XA=0.066 |

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR STRIPPING SECTION - STAGE | 8 = | 0.183517E+05 | YA=0.113 |
| ENTHALPY OF LIQUID STRIPPING SECTION - STAGE | 8 = | 0.248506E+04 | XA=0.021 |

| | | | |
|---|-----|--------------|----------|
| ENTHALPY OF VAPOR STRIPPING SECTION - STAGE | 9 = | 0.185765E+05 | YA=0.033 |
|---|-----|--------------|----------|

ENTHALPY OF LIQUID STRIPPING SECTION - STAGE 9 = 0.258273E+04 XA=0.006

ENTHALPY OF VAPOR STRIPPING SECTION - STAGE 10 = 0.186479E+05 YA=0.007

ENTHALPY OF LIQUID STRIPPING SECTION - STAGE 10 = 0.261636E+04 XA=0.001

TOTAL NUMBER OF IDEAL PLATES INCLUDING REBOILER= 10

***** BINARY DISTILLATION CALCULATION BY PONCHON-SAVARIT METHOD *****

***** ENTHALPY DATA CALCULATED USING LAGRANGE INTERPOLATION *****

***** SYSTEM 2: COMPONENT A=ETHANOL COMPONENT B=WATER *****

| XA=YA | TL | HSA | TG |
|-------|---------|--------|---------|
| 0.0 | 212.000 | 16.000 | 212.000 |
| 0.050 | 196.000 | 12.540 | 209.500 |
| 0.100 | 188.000 | 9.856 | 207.100 |
| 0.150 | 184.000 | 7.407 | 204.500 |
| 0.200 | 181.600 | 5.428 | 202.000 |
| 0.250 | 180.100 | 3.972 | 199.400 |
| 0.300 | 179.000 | 3.038 | 196.500 |
| 0.350 | 178.400 | 2.385 | 193.500 |
| 0.400 | 177.500 | 1.900 | 190.200 |
| 0.450 | 176.700 | 1.523 | 187.000 |
| 0.500 | 176.000 | 1.251 | 183.500 |
| 0.550 | 175.200 | 1.004 | 180.500 |
| 0.600 | 174.500 | 0.824 | 177.800 |
| 0.650 | 174.000 | 0.691 | 175.800 |
| 0.700 | 173.530 | 0.590 | 174.440 |
| 0.750 | 173.250 | 0.478 | 173.620 |
| 0.800 | 172.960 | 0.410 | 173.030 |
| 0.850 | 172.820 | 0.289 | 172.860 |
| 0.900 | 172.700 | 0.176 | 172.700 |
| 0.950 | 172.500 | 0.088 | 172.500 |

F= 2000.000 WFA= 0.520 MWA= 46.050 MWB= 18.020
WDA= 0.910 WBA= 0.040 TF= 177.000 REFLX= 3.000
TO= 32.000 LAMA1= 9220.000 LAMB1= 9717.000 TCA= 516.000
TCB= 647.000 BPA= 173.000 BPB= 212.000

REL COEFFICIENTS - 0.504351E+00 -0.481584E-03 -0.921631E-06 0.114379E-07
BEL COEFFICIENTS - 0.213974E+01 -0.968137E-02 0.268536E-04 -0.242139E-07
REV COEFFICIENTS - 0.131120E+00 0.918566E-03 -0.235957E-06 -0.719165E-10
BEV COEFFICIENTS - 0.452219E+00 -0.129224E-03 0.417000E-06 -0.200401E-09

OUTPUT FOR SYSTEM 2: COMPONENT A=ETHANOL COMPONENT B=WATER

MOLE FRACTION OF FEED = 0.298

MOLE FRACTION OF DISTILLATE =0.798

MOLE FRACTION OF BOTTOMS =0.01604

DISTILLATE(POUNDS/HOUR) = 0.110345E+04
 BOTTOMS (POUNDS/HOUR) = 0.896551E+03

ENTHALPY OF FEED = 0.312547E+04

ENTHALPY OF DISTILLATE = 0.427635E+04

ENTHALPY OF DISTILLATE DEL POINT = 0.643590E+05

CONDENSER HEAT LOAD = 0.164125E+07

ENTHALPY OF BOTTOMS = 0.313950E+04

ENTHALPY OF BOTTOMS DEL POINT = -0.313332E+05

REBOILER HEAT LOAD = 0.167337E+07

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR ENRICHING SECTION - STAGE | 1 = | 0.192970E+05 | YA=0.798 |
| ENTHALPY OF LIQUID ENRICHING SECTION - STAGE | 1 = | 0.425532E+04 | XA=0.784 |

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR ENRICHING SECTION - STAGE | 2 = | 0.192947E+05 | YA=0.788 |
| ENTHALPY OF LIQUID ENRICHING SECTION - STAGE | 2 = | 0.422270E+04 | XA=0.763 |

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR ENRICHING SECTION - STAGE | 3 = | 0.192918E+05 | YA=0.772 |
| ENTHALPY OF LIQUID ENRICHING SECTION - STAGE | 3 = | 0.416531E+04 | XA=0.730 |

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR ENRICHING SECTION - STAGE | 4 = | 0.192871E+05 | YA=0.747 |
| ENTHALPY OF LIQUID ENRICHING SECTION - STAGE | 4 = | 0.408411E+04 | XA=0.686 |

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR ENRICHING SECTION - STAGE | 5 = | 0.192802E+05 | YA=0.714 |
| ENTHALPY OF LIQUID ENRICHING SECTION - STAGE | 5 = | 0.398303E+04 | XA=0.629 |

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR ENRICHING SECTION - STAGE | 6 = | 0.192711E+05 | YA=0.672 |
| ENTHALPY OF LIQUID ENRICHING SECTION - STAGE | 6 = | 0.382616E+04 | XA=0.550 |

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR ENRICHING SECTION - STAGE | 7 = | 0.192565E+05 | YA=0.613 |
| ENTHALPY OF LIQUID ENRICHING SECTION - STAGE | 7 = | 0.350584E+04 | XA=0.414 |

| | | | |
|--|-----|--------------|----------|
| ENTHALPY OF VAPOR ENRICHING SECTION - STAGE | 8 = | 0.192247E+05 | YA=0.514 |
| ENTHALPY OF LIQUID ENRICHING SECTION - STAGE | 8 = | 0.283177E+04 | XA=0.177 |

FEED TRAY LOCATION PLATE = 8

| | | | |
|---|-----|--------------|----------|
| ENTHALPY OF VAPOR STRIPPING SECTION - STAGE | 9 = | 0.191071E+05 | YA=0.254 |
|---|-----|--------------|----------|

ENTHALPY OF LIQUID STRIPPING SECTION - STAGE 9 = 0.296176E+04 XA=0.040
ENTHALPY OF VAPOR STRIPPING SECTION - STAGE 10 = 0.189898E+05 YA=0.051
ENTHALPY OF LIQUID STRIPPING SECTION - STAGE 10 = 0.320362E+04 XA=0.008

TOTAL NUMBER OF IDEAL PLATES INCLUDING REBOILER= 10

NOMENCLATURE

| | |
|-------|--|
| BOT | bottom product, pounds per hour |
| BPA | natural boiling point of A, $^{\circ}\text{F}$ (A is the more volital component.) |
| BPB | natural boiling point of B, $^{\circ}\text{F}$ |
| CPA | specific heat of A, $\text{BTU/lb-}^{\circ}\text{F}$ |
| CPB | specific heat of B, $\text{BTU/lb-}^{\circ}\text{F}$ |
| CPM | specific heat of the mixture of the two (2) components, $\text{BTU/lb-}^{\circ}\text{F}$ |
| DELHS | heat of solution at T0 and the prevailing concentration, BTU/lb-mole |
| DIST | distillate, lb-mole/hour |
| F | feed, lbs/hour |
| FEED | feed, lb-moles/hour |
| G | vapor flow rate, lb-moles/hr |
| Gm | vapor flow rate at any tray m in the stripping section, lb-moles/hr |
| Gn | vapor flow rate at any tray n in the enriching section, lb-moles/hr |
| HBOT | enthalpy of the bottom product, BTU/lb-mole |
| HDELB | enthalpy of the bottom del point, BTU/lb-mole |
| HDELD | enthalpy of the distillate del point, BTU/lb-mole |
| HDIST | enthalpy of the distillate, BTU/lb-mole |
| HFEED | enthalpy of the feed, BTU/lb-mole |

| | |
|-------|---|
| HG | enthalpy of the vapor, BTU/lb-mole |
| HG(i) | enthalpy of the vapor at tray i, BTU/lb-mole |
| HL | enthalpy of the liquid, BTU/lb-mole |
| HL(i) | enthalpy of the liquid at tray i, BTU/lb-mole |
| HSA | heat of solution, kilojoules/g-mole A |
| LAMA | latent heat of vaporization of A at its natural boiling point, cal/g-mole |
| LAMB | latent heat of vaporization of B at its natural boiling point, cal/g-mole |
| L | liquid flow rate, lb-moles/hour |
| Lm | liquid flow rate at any tray m in the stripping section, lb-moles/hour |
| Ln | liquid flow rate at any tray n in the enriching section, lb-moles/hour |
| MOLA | lb-moles of A in the feed |
| MOLB | lb-moles of B in the feed |
| MWA | molecular weight of A, lbs/lb-mole |
| MWAV | average molecular weight of component mixture, lbs/lb-mole |
| MWB | molecular weight of B, lbs/lb-mole |
| MWBAV | average molecular weight of bottom product, lbs/lb-mole |
| MWDAV | average molecular weight of the distillate, lbs/lb-mole |
| MWFAV | average molecular weight of the feed, lbs/lb-mole |
| QBOIL | reboiler heat load, BTU/hour |
| QCOND | condenser heat load, BTU/hour |
| REFLX | reflux ratio, lb-mole reflux/lb-mole distillate |

| | |
|-------|---|
| TCA | critical temperature of A, $^{\circ}\text{K}$ |
| TCB | critical temperature of B, $^{\circ}\text{K}$ |
| TEMP | In main program, it is used as a temporary value used in the check equations. In the enthalpy calculation, it is the temperature in the CP calculations, $^{\circ}\text{K}$ |
| TF | feed temperature, $^{\circ}\text{F}$ |
| TG | dew point temperature, $^{\circ}\text{F}$ |
| TL | bubble point temperature, $^{\circ}\text{F}$ |
| TR | reduced temperature |
| WBA | weight fraction of A in bottom product |
| WBOT | bottom product flow, lbs/hour |
| WDA | weight fraction of A in the distillate |
| WDIST | distillate flow, lbs/hour |
| WFA | weight fraction of A in the feed |
| XA | mole fraction of A in the liquid |
| XBA | mole fraction of A in the bottom product |
| XDA | mole fraction of A in the distillate |
| YA | mole fraction of A in the vapor |
| ZFA | mole fraction of the feed |

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