COMPUTERIZED COMPUTATION OF COUNTER-CURRENT EXTRACTION PROBLEMS FOR TERNARY LIQUID SYSTEMS

BY

ALBERT WARREN PATTERSON, JR.

A THESIS

PRESENTED IN PARTIAL FULFILLMENT OF

THE REQUIREMENTS FOR THE DEGREE

OF

MASTER OF SCIENCE IN CHEMICAL ENGINEERING

AT

NEWARK COLLEGE OF ENGINEERING

Newark, New Jersey
June, 1972

APPROVAL OF THESIS

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FACULTY COMMITTEE

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ACKNOWLEDGEMENTS

The author wishes to express his appreciation to Dr. J.E. McCormick for his helpful assistance and thoughtful review of this work.

Also, the author expresses his appreciation to Hoffmann La Roche, Inc. for permitting him to use its facilities.

ABSTRACT

A Fortran computer program has been developed that will calculate the number of theoretical equilibrium stages required for a countercurrent liquid-liquid extraction design problem. It also furnishes a complete stagewise material balance. Further utility can be found by using it for optimization studies. The program can be utilized for three-component systems that form one pair of partially miscible liquids, the most frequently occuring situation. The program was written for the General Electric Mark I Time-Sharing System.

The program has a practical advantage in that isothermal liquid equilibria data are used directly for calculation purposes. No use is made of theoretically derived equations of the Margules or Redlich-Kister type to predict distribution coefficients, rather equilibria data is correlated in the region of interest by using a three coefficient interpolating polynomial. The empirical correlation proposed by D.B. Hand is utilized to derive tie line equations.

Some of the features of the program include the user's option of either specifying the mole or weight fraction of solute in the raffinate or the percentage overall recovery of solute in the extract. The latter option would be a time-consuming iterative procedure when attempted by hand computation. An especially valuable feature for optimization studies is the storage of equilibria data in permanent files so that parametric cases can be run without the bother of having to input a large volume of data for each case.

The program is arranged so as to be used by a person with little or no knowledge of computer programing. With this in mind a stepwise procedure for using the program is presented along with solutions to sample problems.

Sample problems presented for the ternary system acetone-water-1,1,2-trichloroethane show good agreement with graphical procedures.

To my loving wife, Joan

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I. INTRODUCTION

Today, separations utilizing the liquid-liquid extraction technique are extremely important in the chemical and petroleum industry. The theoretical or ideal stage forms the basis for most industrial designs, and thus is the fundamental unit considered during chemical engineering process development. In the theoretical stage, intimate contact between the two phases is maintained for a sufficient period of time so that distribution equilibrium occurs. This is to say that the extract and raffinate are equilibrium solutions.

When ternary systems are considered, the interrelationships among the phase equilibria, the number of theoretical stages, concentrations and weights of the various streams are most easily represented on a diagram of the phase equilibria. While several types of coordinate systems can be used, the most common for ternary equilibrium data is the triangular diagram either of the equilateral or right isosceles type. For convenience the right triangle will be utilized in the following discussions since it enables all points to be described on rectilinear coordinates.

The use of graphical procedures for solving countercurrent, multiple contact design problems involving ternary systems is usually straightforward as long as sufficient distribution and tie line data are available. Treybal[1] has presented a quite complete coverage of the methods employed. These graphical methods are considered very much satisfactory for the majority of the design problems which may be encountered wherein it is necessary to determine the number of theoretical equilibrium stages required to obtain a specified separation. However, often this approach becomes time consuming. For instance, when the engineer wants to consider several parametric cases required for optimization studies, it is often necessary to make numerous graphical constructions using several scales in order to obtain satisfactory accuracy. Furthermore, in one type of design problem the percent recovery of the solute is specified. If this is the case, a graphical-computational trial and error solution is necessary.

In addition, the graphical method often necessitates replotting data several times on various types of coordinates and scales to obtain accurate results for even the most elementary extraction design problem.

Scope of Thesis

It is believed that by appropriate mathematical formulations and development of a Fortran computer program that the above mentioned inconveniences of the graphical method can be eliminated. In addition, the computer will be able to store liquid equilibria data for any number of ternary systems in a readily accessible form for computation.

The intent of this thesis is the following:

(1) to develop mathematical relationships to describe and interrelate tie lines, concentrations, weights and various construction lines with the phase equilibria isotherm.

(2) to develop a computer program in the Fortran language that will employ the above mentioned mathematical relationships in order to solve practical design problems utilizing available phase solubility and equilibrium data;

(3) to test the above method by way of sample problems and compare the results with the graphical method;

(4) to present a stepwise procedure for easy use of the program.

As can be seen, the desirable features of the graphical procedure will be maintained, but its shortcomings will be eliminated.

The desirability of using experimentally determined equilibrium data should be emphasized. Souders[2] has stated that probably the most important factor in the successful design of a separation process is the adequacy of the equilibrium data. He goes on to say, the best possible equilibrium data are those determined experimentally on the actual materials used in the process. "As useful as generalizations and correlations are in assessment and preliminary selection of separation processes, actual experiment is the final arbiter. For safe design, experimental data obtained in the laboratory or pilot plant is usually required."

All developments and discussions will be confined to ternary systems forming one pair of partially miscible liquids, the most frequently occuring case. Furthermore, it will be assumed that equilibrium data are available to graphically describe the phase isotherm and establish a tie line correlation (as proposed by Hand) of the form,[3]

$$\frac{X_{CB}}{X_{BB}} = k\left[\frac{X_{CA}}{X_{AA}}\right]^{r} \qquad (1)$$

where X_{CB} and X_{BB} are the weight fractions of components C and B respectively in the "B" rich phase, while X_{CA} and X_{AA} are the weight fractions of C and A in the "A" rich phase.

The system acetone-water-1,1,2-trichloroethane at 25 degrees Centigrade was chosen for sample problem purposes.

Previous Work

Several computational methods for solving countercurrent extraction problems have been proposed using either graphical or analytical techniques.[4] The methods proposed by Smith and Brinkley,[5] by Hanson, Duffin, and Sommerville,[6] and by Hartland,[7] utilize the same basic approach for solving extraction problems. In general, the methods are iterative procedures based upon calculations made possible through a set of initial assumptions for solution. Corrections of the assumptions follow until hopefully, the final converged solution of the problem is found.

Roche,[8] has proposed an algorithm which will solve both the material balance and equilibrium relationships simultaneously to obtain a valid solution to the general countercurrent extraction problem assuming the number of ideal equilibrium stages are known.

II. THEORY

Liquid Equilibria

Ternary liquid equilibria are usually reported in the literature on equilateral triangular coordinates where the apexes represent pure components A, B, and C, the solute, the carrier, and the solvent respectively. A binary mixture is represented by a point anywhere on the perimeter of the triangle. Its composition is comprised of the pure components at the end of that side. Any point inside the triangle represents a ternary mixture. This method of representation has been described in various references which should be consulted for further detail.[9] Furthermore, the data can be replotted on a right triangular diagram, constructing in essence a rectangular coordinate system.

When ternary equilibria data for components A, B, C are presented on a right triangular diagram (see Figure 1), the weight fractions (X_B and X_C) of components B and C of any specific mixture can be read directly from the diagram. The weight fraction of A is determined by the difference from 1.0. As is the case when the equilateral triangle is used for representing solubility data, all mixtures of components represented by points outside the phase isotherm curve D-K-P-J-G are single liquid phase solutions, while those mixtures within the area bounded by the curve form two immiscible liquid phases. A mixture with an overall composition of H will form two liquid phases of compositions K and J. The point H is on the tie

FIGURE 1
TERNARY LIQUID EQUILIBRIA

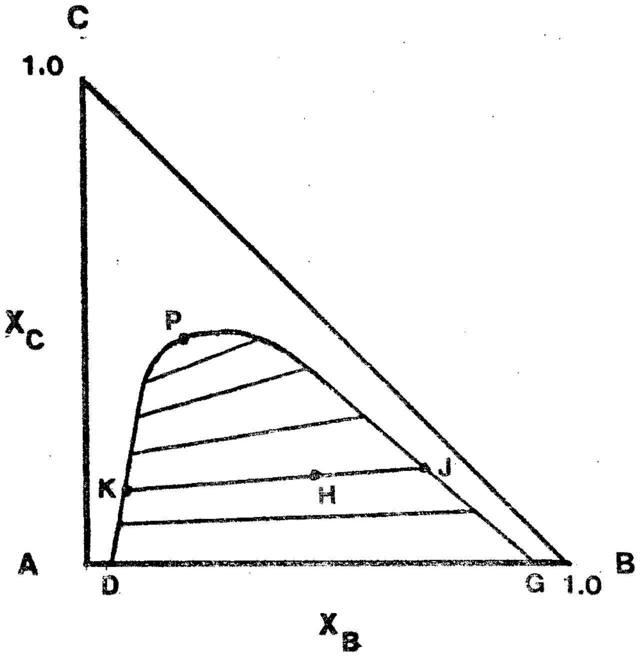
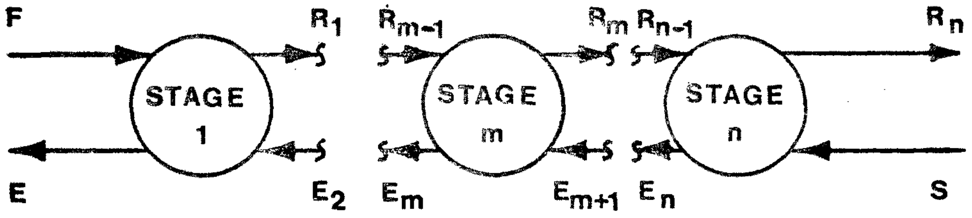


FIGURE 2
COUNTERCURRENT MULTIPLE CONTACT



line connecting points K and J. In reality, the area of immiscibility contains an infinite number of tie lines which relate the compositions of respective pairs of two phase solutions that are formed.

Stagewise Solvent Extraction

When a system consists of, or can be reduced to the equivalent three components, the two to be separated and the solvent, it can be classified as a single solvent system. For classification purposes, either stagewise or continuous contact may exist depending upon the arrangement of the equipment. Stagewise contact implies that the solvent and mixture to be separated are intimately contacted, given time to approach equilibrium, and separated. Such is the case when mixer-settlers are employed. On the other hand continuous contact connotes the use of tower, column, or centrifugal designs where the solvent and mixture to be separated are continuously in contact within the equipment. Equilibrium is not usually approached.

Fundamental data and concepts are usually developed utilizing stagewise contact techniques. Once this data is available, scale-up techniques are employed. Stage efficiencies are taken into account to develop practical industrial scale processes utilizing continuous contact equipment.

Countercurrent Multiple Contact Extraction

Stagewise single-solvent extraction can be performed in several ways, depending upon the arrangement of the stages, each yielding different results. For instance, extractions can usually be classified as single contact, differential, crosscurrent multiple contact, and countercurrent multiple contact. Perhaps the most interesting to study from a chemical process point of view is the last case.

When single-solvent extraction is considered utilizing the countercurrent multiple-contact technique, a cascade of stages is involved where the extracting solvent (S) and solution to be extracted (F) enter at opposite ends of the cascade. Therefore, the extracts (E_n, E_2, E_1 etc.) and raffinates (R_1, R_2, R_n etc.) flow countercurrently. See Figure 2.[10] While the afore-mentioned process is necessarily continuous, it can be simulated by a laboratory batchwise technique.[11] For the purposes of clarification and formulae development, the general graphical procedure for solving a simple countercurrent extraction design problem will be reviewed.

<u>Graphical method</u>. Refer to Figure 3.[12] Assume that the location of F, R_n, and S are known (ie. their weight as well as composition). M, representing the mixture of feed and solvent, is in the two-phase region. Its magnitude and location can be determined by calculating its composition by material balances.

An overall balance is:

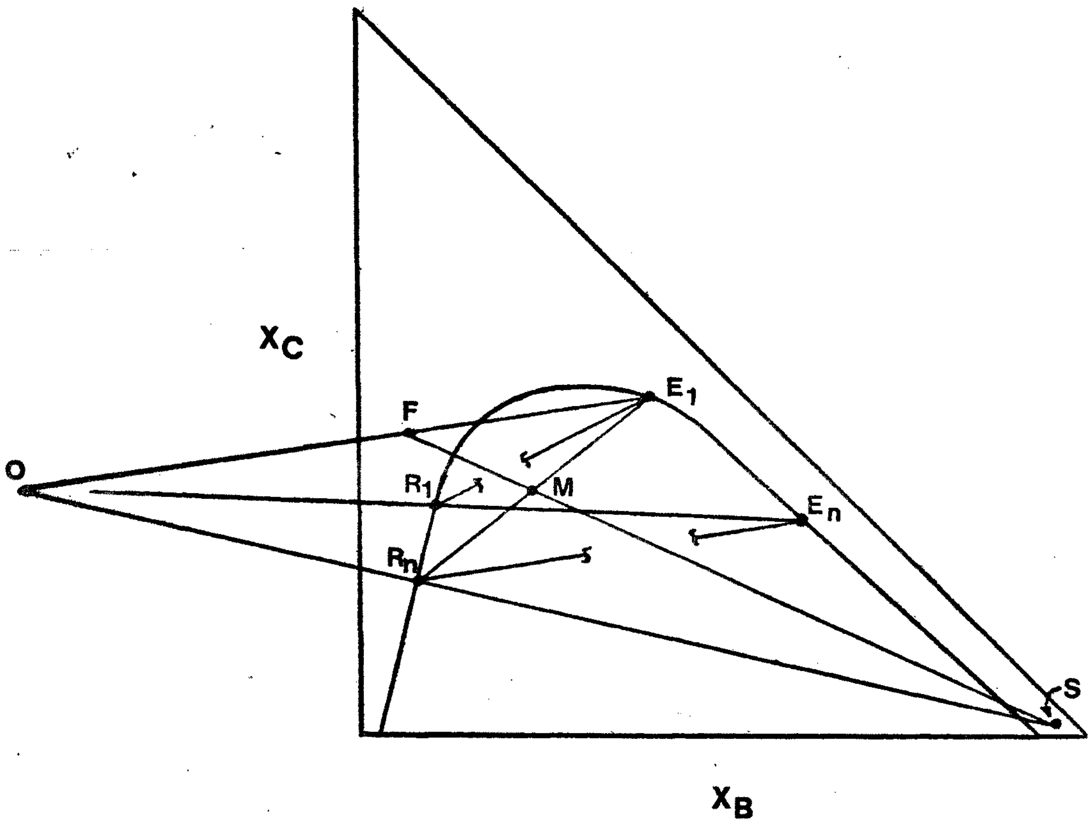
$$M = F+S \qquad (2)$$

A C balance gives:

$$FX_{CF} + SX_{CS} = MX_{CM} \qquad (3)$$

FIGURE NO. 3
COUNTERCURRENT EXTRACTION

A TYPICAL GRAPHICAL CONSTRUCTION



where X_{CF} is the fraction of component C in the feed stream, while X_{CS} is the fraction of component C in the solvent. M is the magnitude of the mix point and X_{CM} is the weight fraction of C in the mixture.

Therefore:

$$X_{CM} = \frac{X_{CF} + SX_{CS}}{M} \tag{4}$$

A B balance yields

$$FX_{BF} + SX_{BS} = MX_{BM} \tag{5}$$

therefore,

$$X_{BM} = \frac{FX_{BF} + SX_{BS}}{M} \tag{6}$$

Once point M, the mix point, is determined, the extract E_1 can be located by extending line R_nM to its intersection with the B-rich solubility curve. By material balance the value of E_1 can be determined.

$$E_1 + R_n = F + S = M \tag{7}$$

A series of material balances are used to relate E_{m+1} and R_m. A brief development follows. A material balance around stages 1 through m is

$$F + E_{m+1} = E_1 + R_m \qquad (8)$$

or

$$F - E_1 = R_m - E_{m+1} = O \qquad (9)$$

where O is the net flow between stages. It is the operating or delta point and is a constant for a given extraction problem. Point O can be located by extending lines EF and SR_n until they intersect. A material balance around the m^{th} stage is

$$R_{m-1} + E_{m+1} = R_m + E_m \qquad (10)$$

or

$$R_{m-1} - E_m = R_m - E_{m+1} = O \qquad (11)$$

From the above equations 9 and 11 it can be seen that any extract E_{m+1} can be located graphically by extending line OR_m to its intersection with the B-rich solubility curve. The extract from stage m, E_m, and the raffinate R_m will be in equilibrium and located on the solubility curve at opposite ends of a tie line. Accordingly, starting from E_1, R_1 may be located at the opposite end of the tie line through E_1. E_2 is found by extending line OR_1 to its intersection with the B-rich side of the solubility curve and R_2 by the tie line through E_2. This procedure is continued until R_m meets the requirements set forth in the specific problem. Thus the number of theoretical equilibrium stages required to achieve a specified separation can be estimated.

Analytical method. In order to solve the graphical problem solely by analytical methods it will be necessary to calculate the composition of all the required points by using material balances in terms of the B and C components since the coordinate system is based on them. Furthermore, it will be necessary to express the solubility curve in a mathematical form as a function of X_B and X_C. For the purposes of the proposed calculation method, the solubility data will be interpolated by using a three coefficient polynomial in the local region of interest having the form

$$P\ (X_C) = A_1 X_B^2 + A_2 X_B + A_3 \tag{12}$$

The three solubility data points nearest the intersection point of the solubility curve and the construction line or tie line will be used to evaluate the constants A_1, A_2, and A_3. The technique developed to determine which data points to use will be discussed later.

As previously stated the mix point M can be located by equations 2, 4 and 6.

Often the design problem may state only the required concentration of the solute C in the raffinate, X_{CRN}. If this is the case, X_{BRN} must be found on the solubility curve in order to locate R_n. This is accompliched by solving the following equation for X_{BRN}.

$$X_{CRN} = A_1 (X_{BRN})^2 + A_2 (X_{BRN}) + A_3 \tag{13}$$

The line R_nME_1 now can be described mathematically and the unknowns X_{BE1} and X_{CE1} inserted.

$$X_{CE(1)} = \left[\frac{X_{CM} - X_{CRN}}{X_{BM} - X_{BRN}}\right] X_{BE(1)} + \left[X_{CM} - X_{BRN}\right] \left[\frac{X_{CM} - X_{CRN}}{X_{BM} - X_{BRN}}\right] \tag{14}$$

Equation 14 is now solved simultaneously with the applicable B-rich phase interpolating polynomial (Equation 15) for $X_{BE(1)}$ and $X_{CE(1)}$, the coordinates of point E_1.

$$X_{CE(1)} = A_1 (X_{BE(1)})^2 + A_2 (X_{BE(1)}) + A_3 \tag{15}$$

Point O can be determined by solving simultaneously the equations for lines E_1FO and SR_nO for X_{OB} and X_{OC}. Line E_1FO is

$$X_{OC} = \left[\frac{X_{CE(1)} - X_{CF}}{X_{BE(1)} - X_{BF}}\right] X_{OB} + \left[X_{CE(1)} - X_{BF}\right]\left[\frac{X_{CE(1)} - X_{CF}}{X_{BE(1)} - X_{BF}}\right] \tag{16}$$

While line SR_nO is

$$X_{OC} = \left[\frac{X_{CS} - X_{CRN}}{X_{BS} - X_{BRN}}\right] X_{OB} + \left[X_{CS} - X_{BRN}\right]\left[\frac{X_{CS} - X_{CRN}}{X_{BS} - X_{BRN}}\right] \tag{17}$$

Raffinate R_1 can now be located by solving the intersection of tie line E_1R_1 with the appropriate solubility polynomial. Using the Hand tie line correlation of the form

$$\frac{X_{CB}}{X_{BB}} = k\left[\frac{X_{CA}}{X_{AA}}\right]^r \qquad (1)$$

with previously determined constants k and r the proper set of known values can be inserted.

$$\frac{X_{CE(1)}}{X_{BE(1)}} = k\left[\frac{X_{CR(1)}}{X_{AR(1)}}\right]^r \qquad (18)$$

Since

$$X_{AR(1)} + X_{BR(1)} + X_{CR(1)} = 1.0$$

$$X_{AR(1)} = 1.0 - X_{BR(1)} - X_{CR(1)} \qquad (19)$$

Equation 19 is substituted into equation 18 to yield

$$\frac{X_{CE(1)}}{X_{BE(1)}} = k\left[\frac{X_{CR(1)}}{1.0 - X_{BR(1)} - X_{CR(1)}}\right]^r \qquad (20)$$

The applicable solubility interpolating polynomial in the A-rich phase is

$$X_{CR(1)} = A_1\,(X_{BR(1)})^2 + A_2\,(X_{BR(1)}) + A_3 \qquad (21)$$

Thus, $X_{BR(1)}$ and $X_{CR(1)}$ can be calculated by solving Equations 20 and 21 simultaneously.

E_2 can now be located by finding the intersection of line OR_1E_2 (Equation 22) with the B-rich solubility interpolating polynomial (Equation 23).

$$X_{CE(2)} = \left[\frac{X_{OC} - X_{CR(1)}}{X_{OB} - X_{BR(1)}}\right] X_{BE(2)} + \left[X_{OC} - X_{BR(1)}\right]\left[\frac{X_{OC} - X_{CR(1)}}{X_{OB} - X_{BR(1)}}\right] \quad (22)$$

$$X_{CE(2)} = A_1 \left(X_{BE(1)}\right)^2 + A_2 \left(X_{BE(2)}\right) + A_3 \quad (23)$$

Following the same procedure the remaining extract and raffinate compositions can be calculated.

The calculation of the magnitudes of the extracts and raffinates will complete the description of all streams. E_1 and R_n can be calculated by combining Equation 7 with the C balance.

$$X_{CE(1)} E_1 + X_{CRN} R_n = X_{CM} M \quad (24)$$

Then,

$$E_1 = \frac{M\left(X_{CM} - X_{CRN}\right)}{X_{CE(1)} - X_{CRN}} \quad (25)$$

$$R_n = \frac{X_{CM} M - X_{CE(1)} E_1}{X_{CRN}} \quad (26)$$

The overall material balance for any stage m, Equation 10, can be rearranged to yield

$$E_{m+1} = R_m + E_m - R_{m-1} \tag{27}$$

And a C balance for stage m gives

$$R_{m-1} X_{CR(m-1)} + E_{m+1} X_{CE(m+1)} = R_m X_{CR(m)} + E_m X_{CE(m)} \tag{28}$$

By combining Equations 27 and 28

$$R_m = \frac{R_{(m-1)} (X_{CR(m-1)} - X_{CE(m+1)}) + E_m (X_{CE(m+1)} - X_{CE(m)})}{X_{CR(m)} - X_{CE(m+1)}} \tag{29}$$

Thus R_1 can be calculated using Equation 29 by setting m-1 = F and m = 1. E_2 is found from Equation 27 where m = 1. By letting m = 2, R_2 and E_3 can be calculated from Equations 29 and 27. The remaining extracts and raffinates are calculated in a similar manner knowing their component concentrations.

III. PROGRAM DEVELOPMENT

Representation of Solubility Data

An important consideration in the development of the Fortran program was how to mathematically describe the solubility curve of the ternary liquid system. As stated in the previous section, it was decided to describe the data using a three coefficient polynomial, a parabola.

$$P(X_C) = A_1(X_B)^2 + A_2(X_B) + A_3 \qquad (12)$$

Thus, by polynomial interpolation between available data points, the entire curve can be described in small sections. The use of more sophisticated, though empirical, equations such as the two constant Margules Equation[13] or the three constant Redlich and Kister Equation[14] was considered. However, the approach taken was to assume that laboratory data was available, and why not use it directly.

A first approach using linear interpolation between data points proved satisfactory, however, more accuracy was obtained by using polynomial interpolation. Hastland has previously proposed a linear approximation technique.[15] A comparison of results obtained using linear versus parabolic interpolation is presented in a later section.

By utilizing Equation 12, therefore, the intersections of tie lines and construction lines with the solubility curve could be determined analytically. The subprogram, ATER1 was written for this purpose. The constants A_1, A_2, A_3 are determined by substituting three sets of data points (B_i, C_i) into the equation as follows

$$C_1 = A_1 B_1^2 + A_2 B_1 + A_3$$
$$C_2 = A_1 B_2^2 + A_2 B_2 + A_3$$
$$C = A_1 B_2^2 + A_2 B_3 + A_3 \qquad (13)$$

This set of simultaneous linear equations can be solved by ant of the usual means. A subprogram, SEMQ, employing a modified Grauss-Jordan elimination technique to the augmented matrix of the above linear system was written to determine A_1, A_2, and A_3 in the present work.

The only problem that remains in order to conclude the discussion of the solubility curve is how the three sets of data points are chosen in the region of intersection. The approach used here was to test each successive set of the data points starting from the X_B axis by calculating the intersection of the interpolating tie line or construction line. The coordinates of the point of intersection were accepted only if they fell within the bounds of the data points used. Otherwise, the calculated intersection point was rejected and the next set of three successive data points were teated. Refer to Figure 4A and 4B. The iteration method begins on the applicable side of the solubility curve, the A-rich side or the B-rich side.

FIGURE 4A REJECTED INTERSECTION

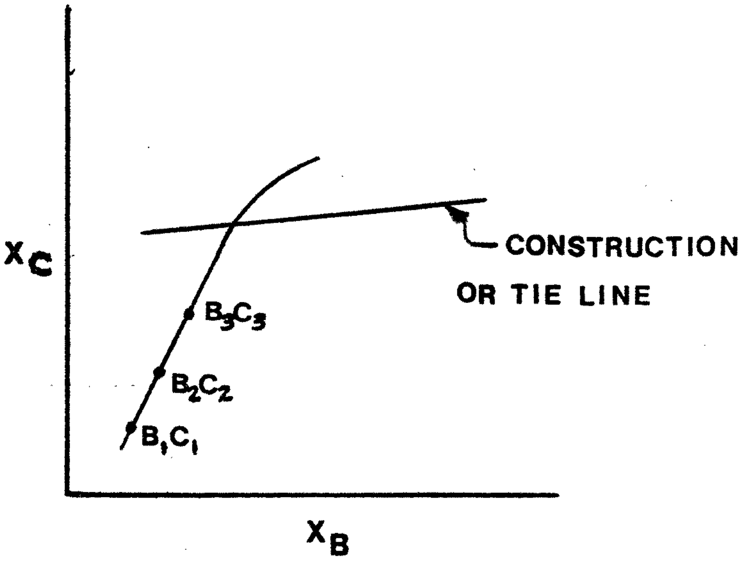
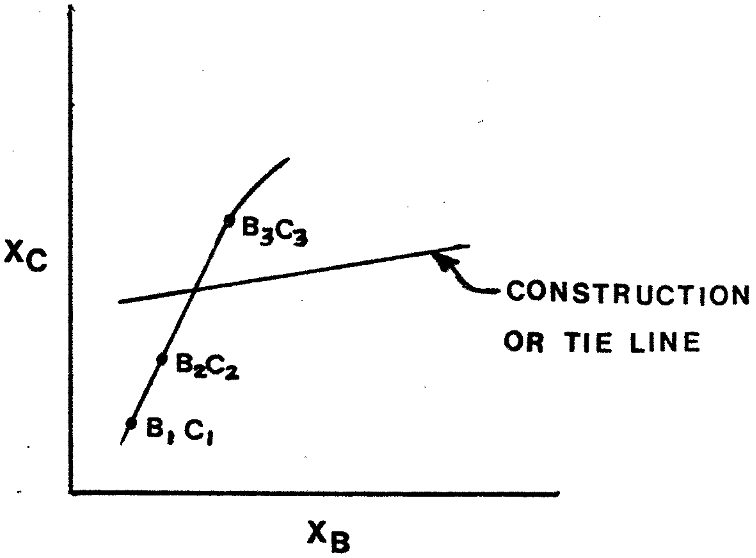


FIGURE 4B ACCEPTED INTERSECTION



The Program

The Fortran program consists of the following subdivisions: (1) the MAIN Program, (2) subprogram ATER1, (3) subprogram FDXCE1, and (4) subprogram SMEQ. Each subdivision will be discussed separately in the following sections.

The main program. Refer to the Flow Charts (Figure numbers 5 and 6). Utilizing the appropriate equations that were developed in the chapter on theory, the main program calculates the number of theoretical equilibrium stages required for a specified separation. It is necessary for the user to specify the following:

(1) a. the weight fraction of the socute in the raffinate, X_{CRN} or
    b. the percent recovery of solute C in the extract.

(2) the composition (X_{BF}, X_{CF}) and the magnitude (F) of the feed stream.

(3) the composition (X_{BS}, X_{CS}) and the magnitude (S) of the solvent stream.

(4) the constants (k,r) for the tie-line correlation (Equation 1).

(5) solubility data as a function of the weight fraction of B, X_B and the weight fraction of C, X_C.

The program will then procede to calculate n, the number of ideal stages rounded to the nearest higher integer value. In addition, the location of the mix point, M, and the operating point, O, will be given as an output. Furthermore, a complete component

FIGURE NO. 5-1

CCEXTG - MAIN PROGRAM
SIMPLIFIED FLOW CHART

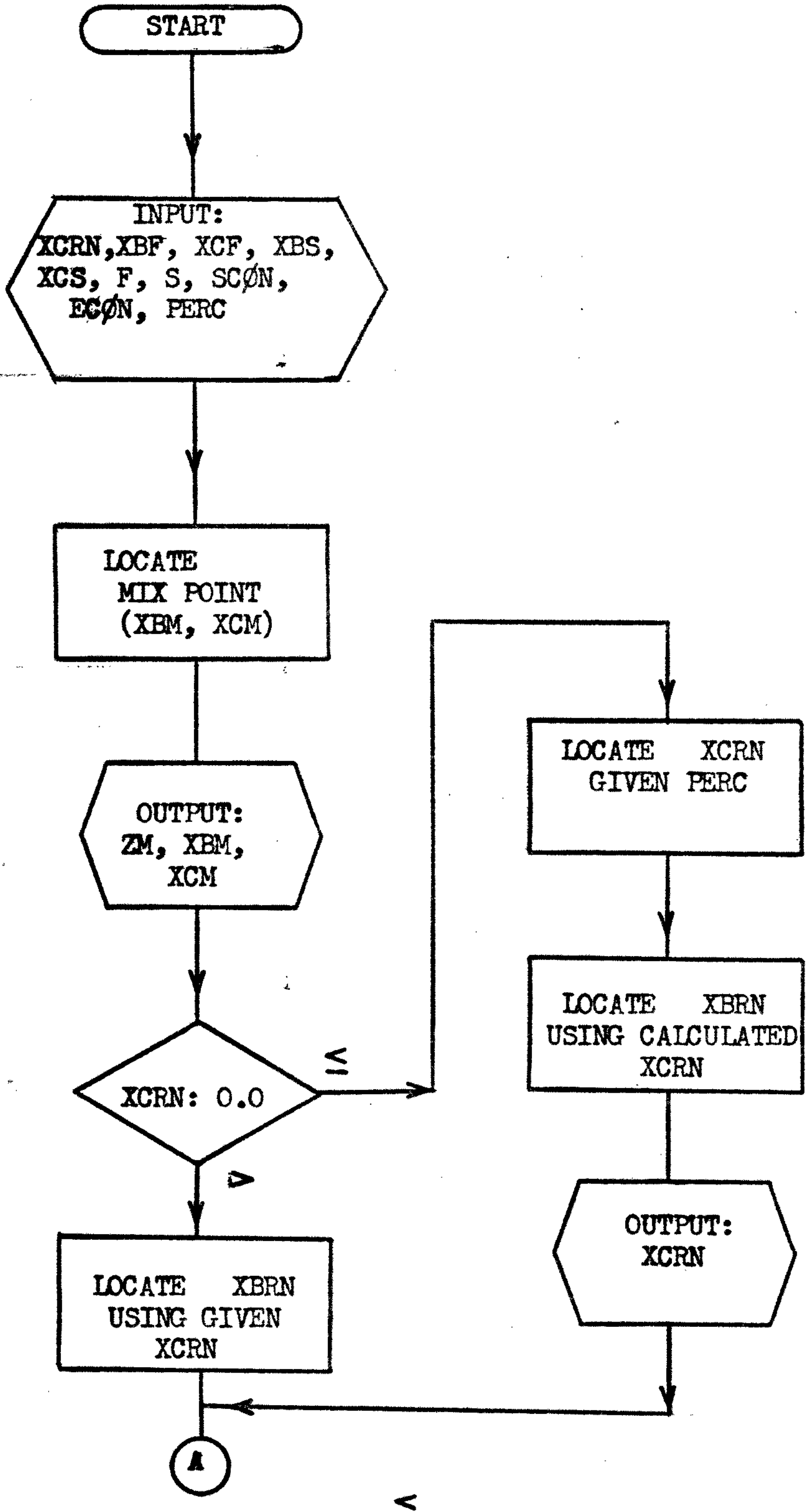


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FIGURE NO. 5-2

CCEXTG - MAIN PROGRAM SIMPLIFIED FLOW CHART (CONT.)

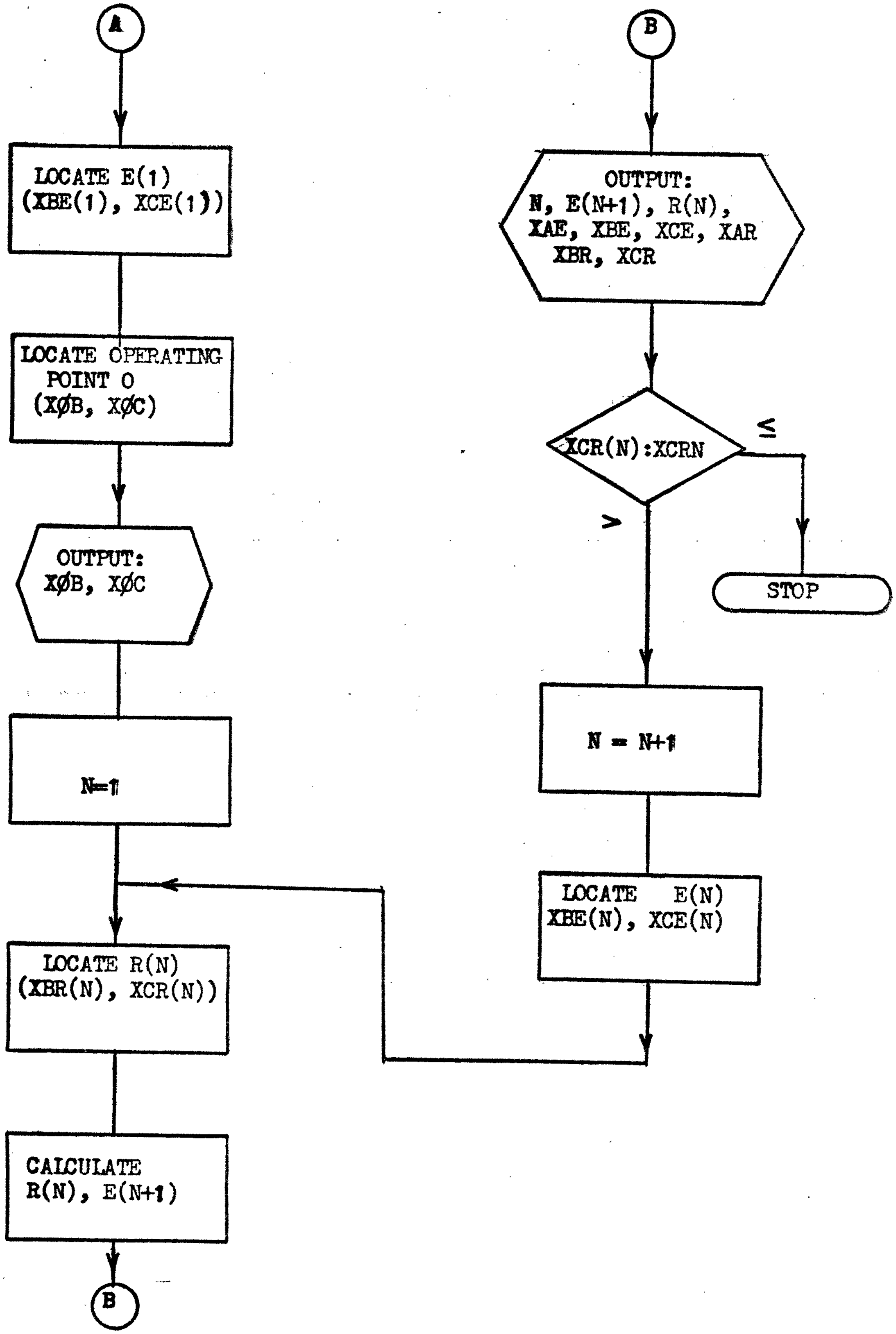


FIGURE NO. 6-1

CCEXTG - MAIN PROGRAM
DETAILED FLOW CHART

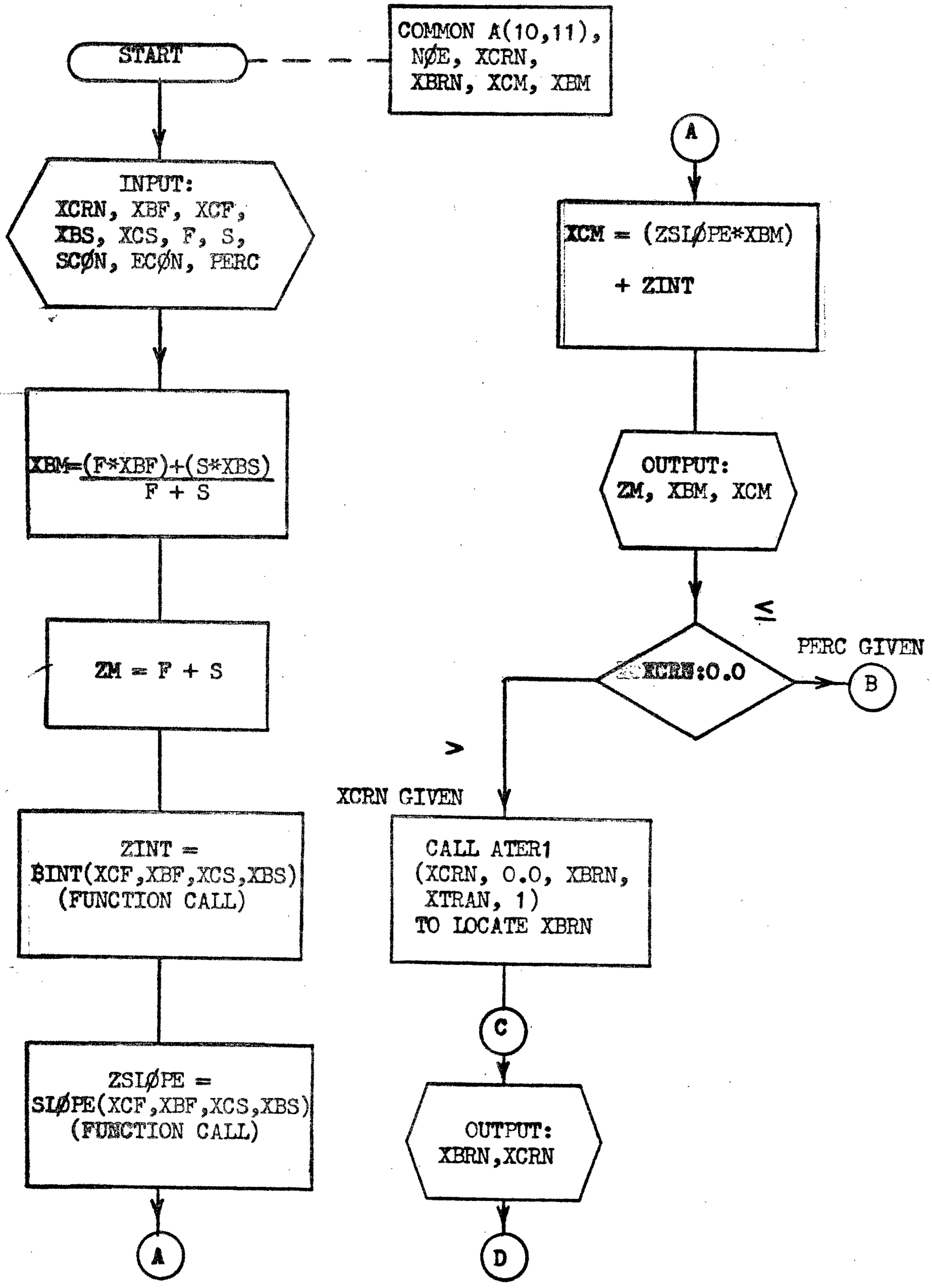


FIGURE NO. 6-2

CCEXTG - MAIN PROGRAM
DETAILED FLOW CHART (CONT.)

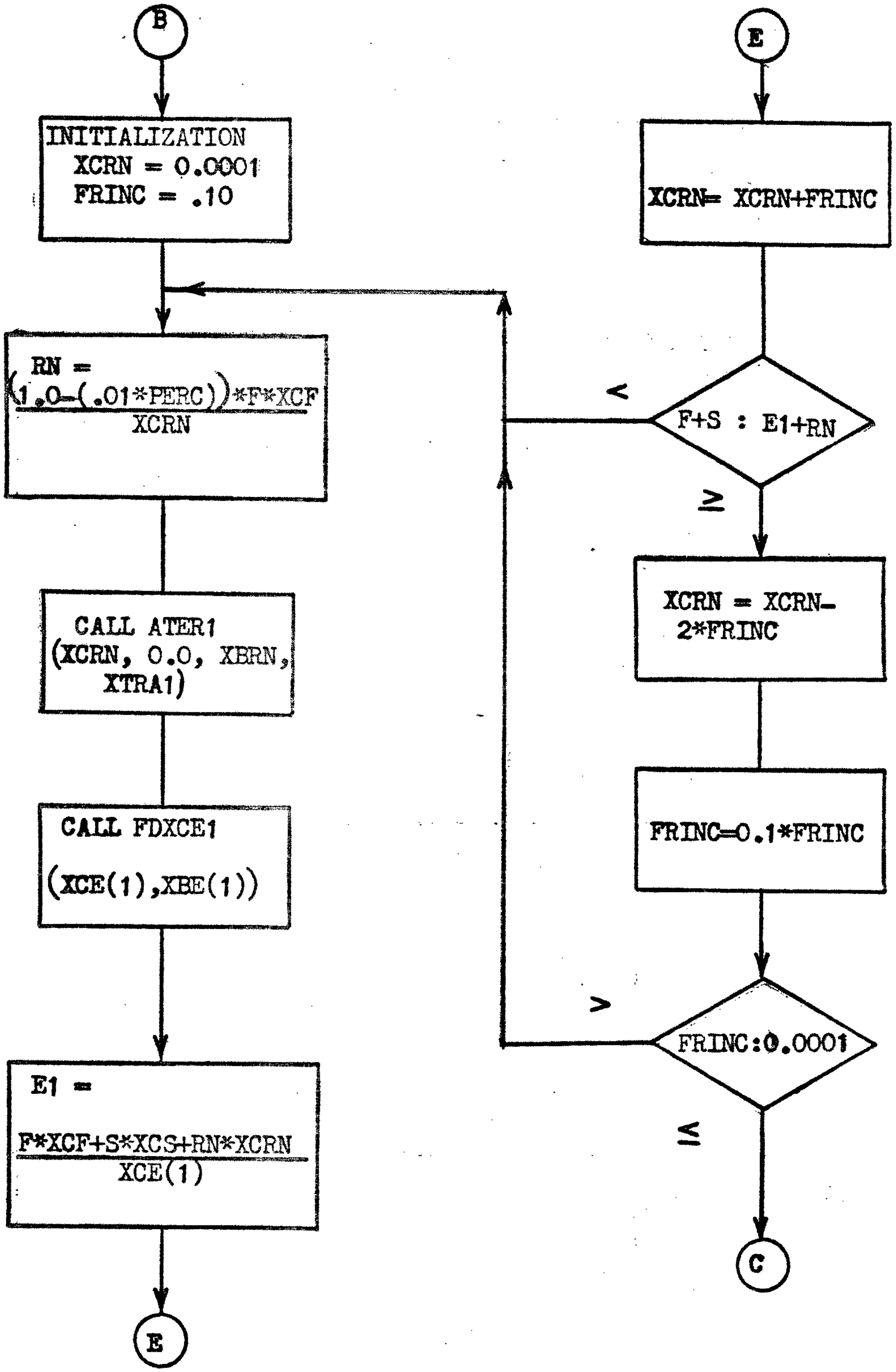


FIGURE NO. 6-3

CCEXTG - MAIN PROGRAM (CONT.)

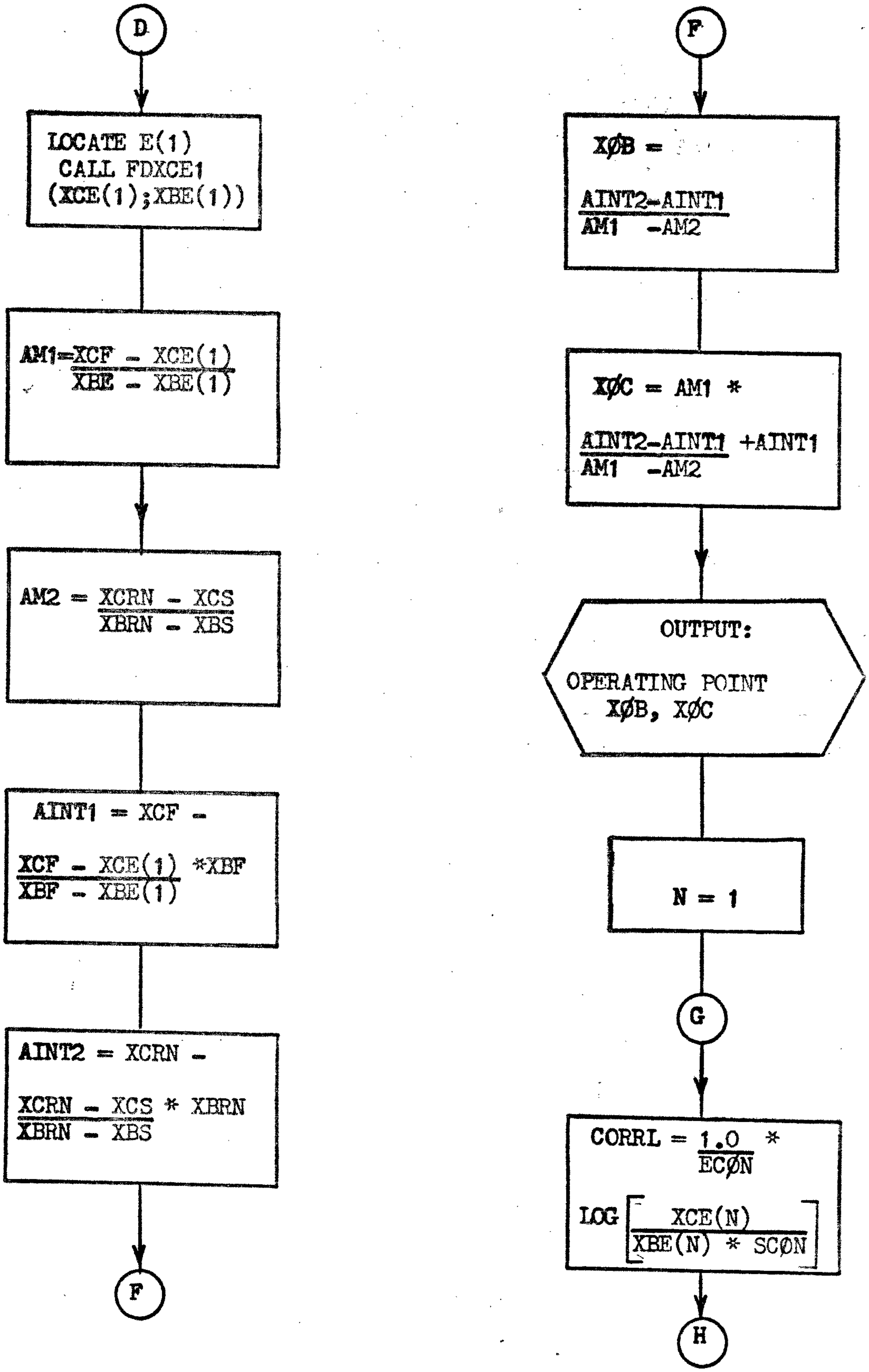
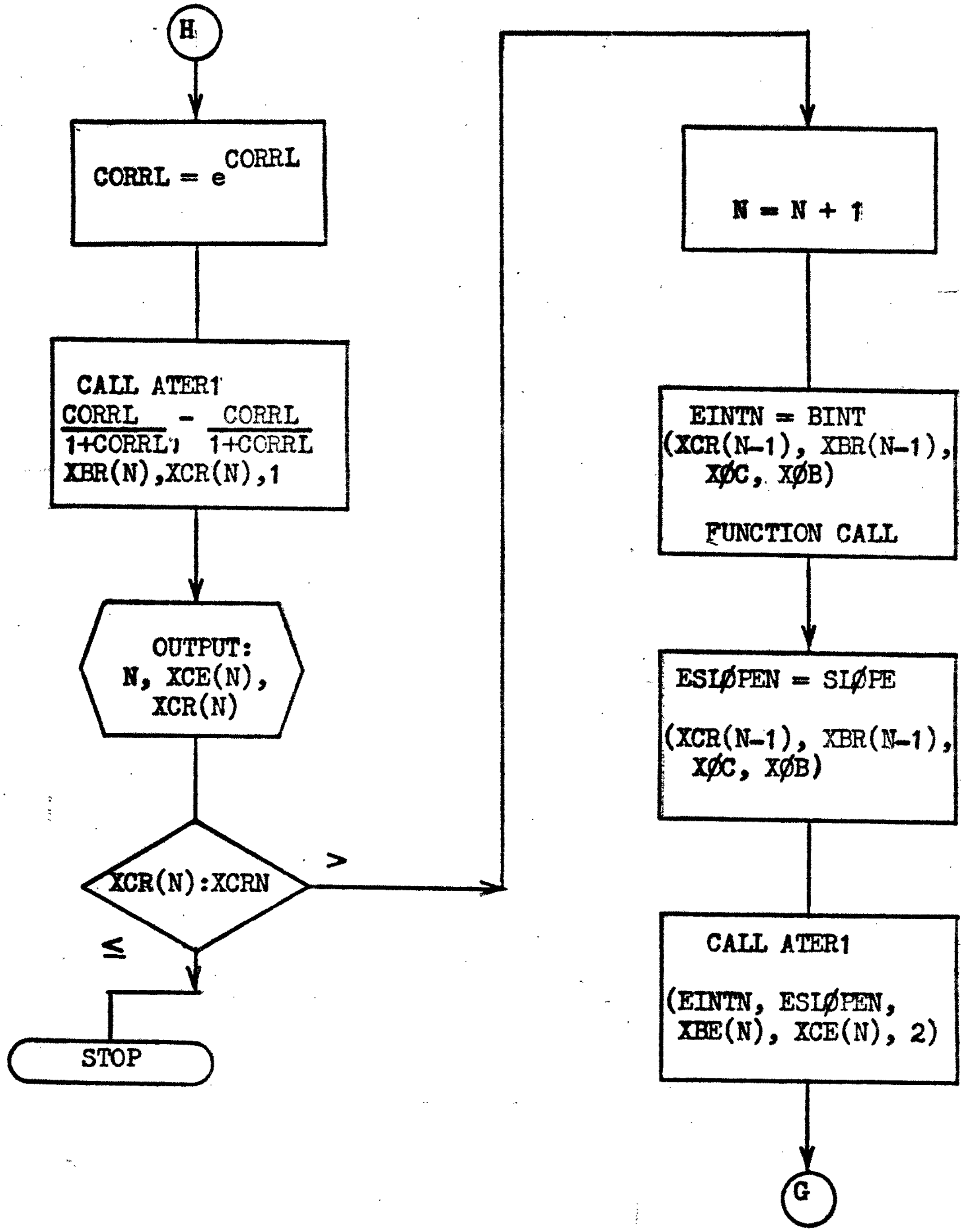


FIGURE NO. 6-4

ØCEXTG - MAIN PROGRAM (CONT.)



material balance is calculated for each ideal stage giving the compositions as well as the magnitudes of each extract and raffinate.

Essentially the program calculates M, the mix point, using Equations 2, 4, and 6. Then the weight fraction of the carrier in the raffinate, X_{BRN}, is found by solving Equation 13. The extract E_1 is located by using Equations 14 and 15. The operating point 0 is now determined by solving Equations 16 and 17 for X_{OC} and X_{OB}. R_1 is now located from E_1 by solving the Hand tie line correlation (Equation 20) simultaneously with Equation 21. E_2 is located from R_1 and the operating point 0 by Equations 22 and 23. In a similar manner, the extracts and raffinates continue to be located until the weight fraction of the solute in the raffinate, X_{CRN}, meets the specified requirements of the problem. The program is completed when the magnitudes of all the extracts and raffinates are calculated using overall stage material balances along with C component balances (Equations 25, 26, 27, and 29).

Subprogram ATER1. The subprogram ATER1 functions as the solubility data interpolating routine for the program. Refer to the flow chart for ATER1 (Figure 7). This routine does the following: (1) Determines the set of applicable solubility data points to use for the interpolating parabola, (2) Calculates the constants for Equation 12 with the aid of another subprogram, SEMQ, and (3) determines the intersection of the above described interpolating parabola with a tie line or construction line. The coordinates for the point of intersection are then supplied to the main program.

FIGURE NO.7-1

SUBPROGRAM ATER1
DETAILED FLOW CHART

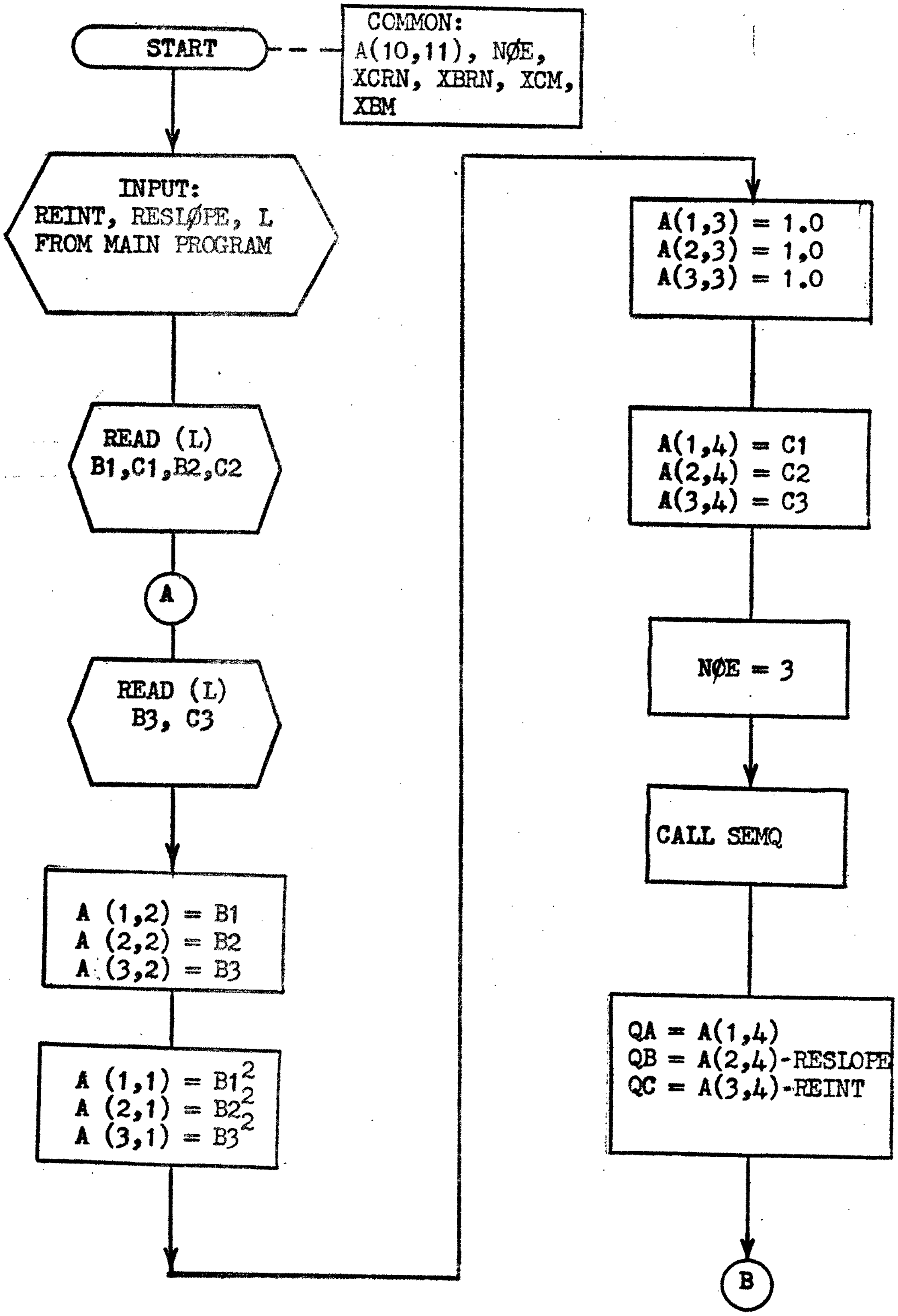
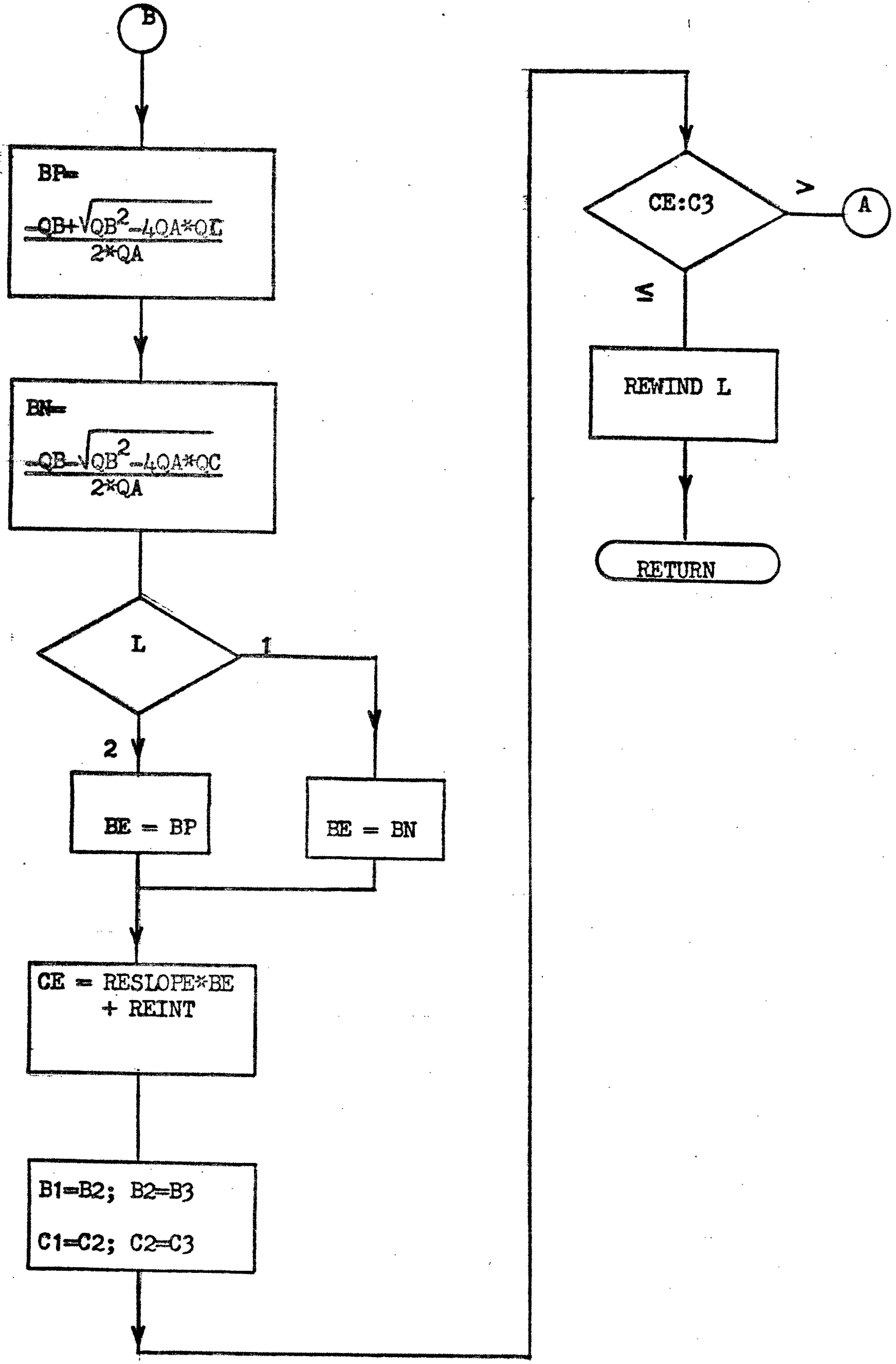


FIGURE NO. 7-2

SUBPROGRAM ATER1 (CONT.)



ATER1 accesses solubility data from permanent external files which have been established by the user prior to running the main program. The names SLAWT1 and SLAWT2 have been given to these files in the sample problem, however the user can furnish any names he wishes. The solubility data thus becomes a permanent part in the user's catalog of files and can be accessed any number of times without having to re-enter large volumes of data. Furthermore, the user may want to store solubility data for several ternary liquid systems. If this is the case, the user can utilize any one of these data files by merely changing one line in the program.

Subprogram FDXCE1. This subprogram determines the coordinates of E_1 by finding the intersection of the line R_nM with the solubility curve. Refer to Figure 8. It was advantageous to use a subprogram for this calculation since it is utilized several times within the main program.

Subprogram SEMQ. SEMQ is a second-order subprogram in that it is called exclusively by subprogram ATER1. Refer to Figure Number 9. SEMQ is a general subprogram that solves a set of up to ten linear simultaneous equations. The Gauss-Jordan elimination method[16] is used to reduce the augmented matrix to the diagonal form. In order to minimize round-off errors common to this technique, a modification was devised. For example, if a pivot element is not zero but is small, it may contain a large relative error. A search is made at each elimination step for the element of greatest magnitude in the pivot column, and the rows are exchanged so as to use it as the pivot element.

FIGURE NO. 8

SUBPROGRAM FDXCE1 DETAILED FLOW CHART

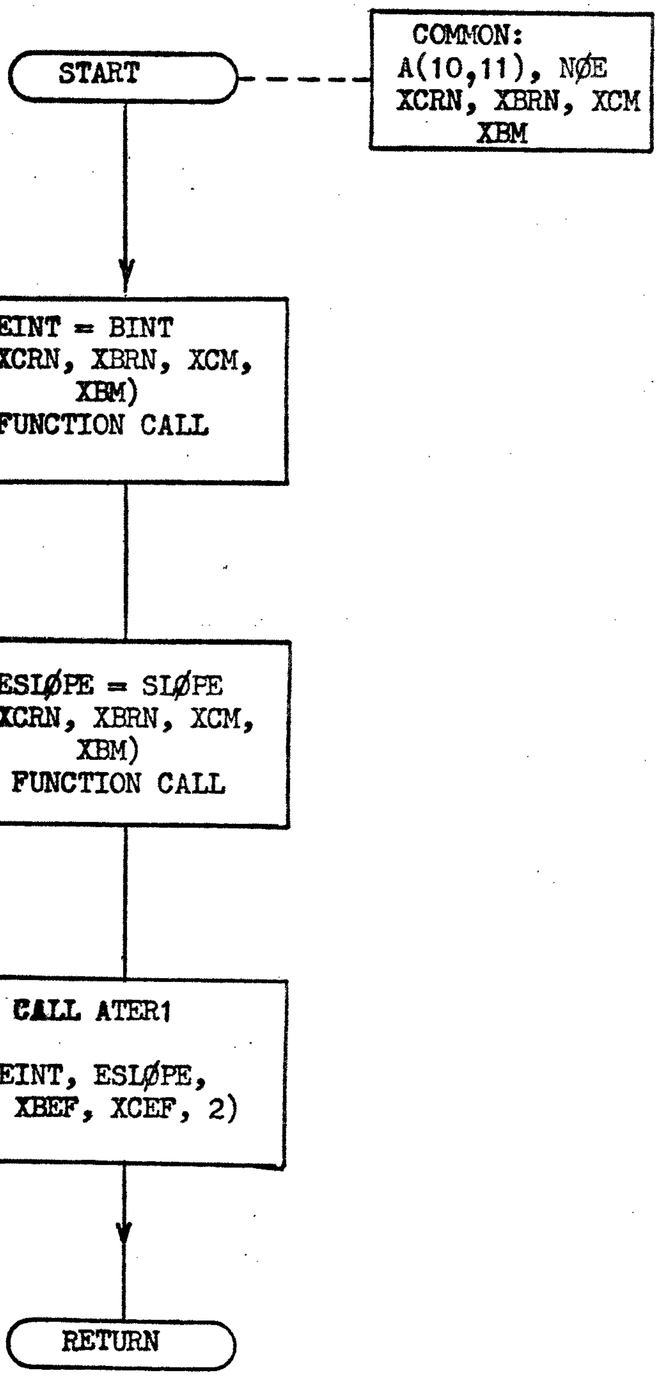


FIGURE NO. 9-1

SUBPROGRAM SEMQ
DETAILED FLOW CHART

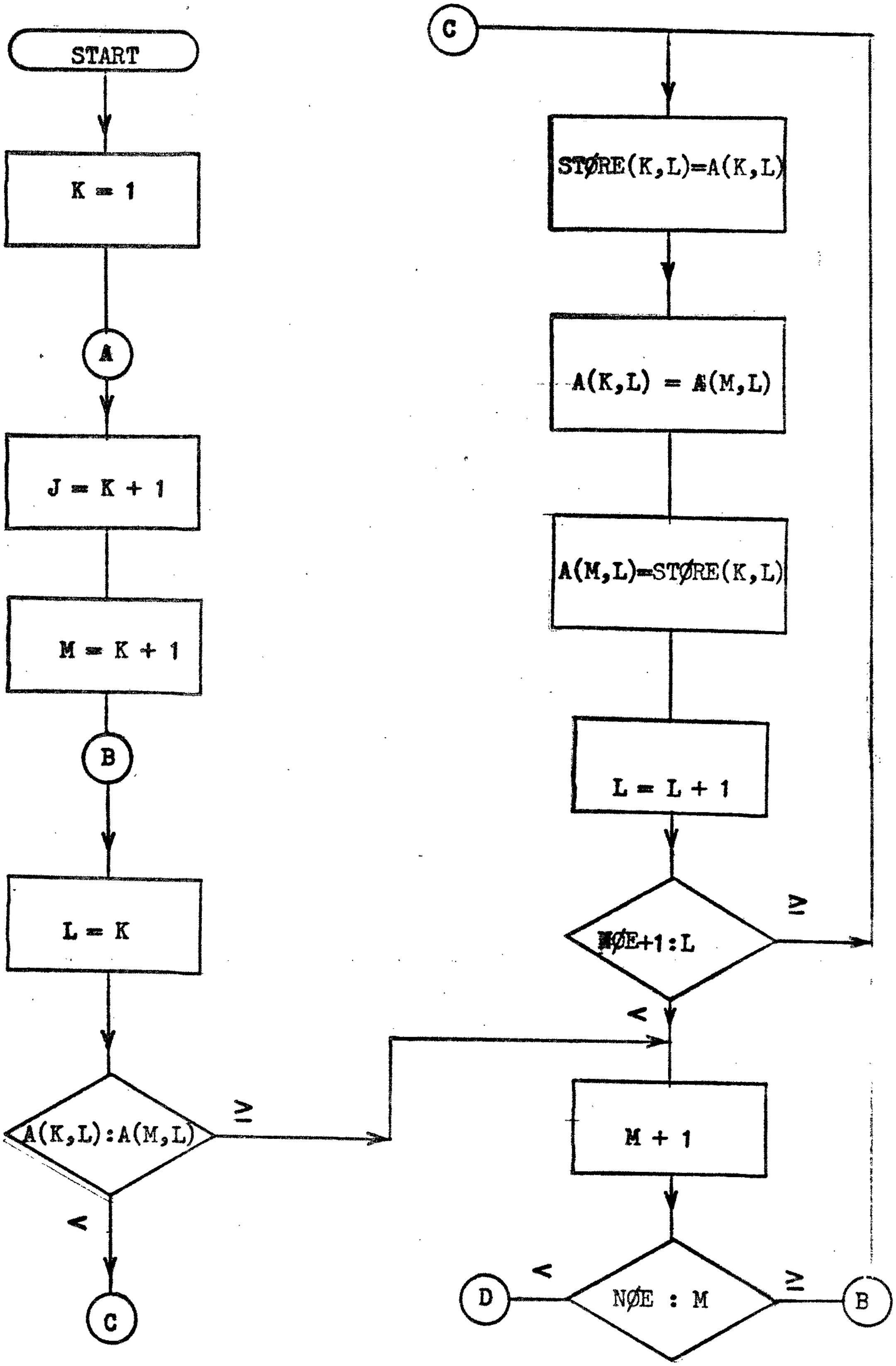
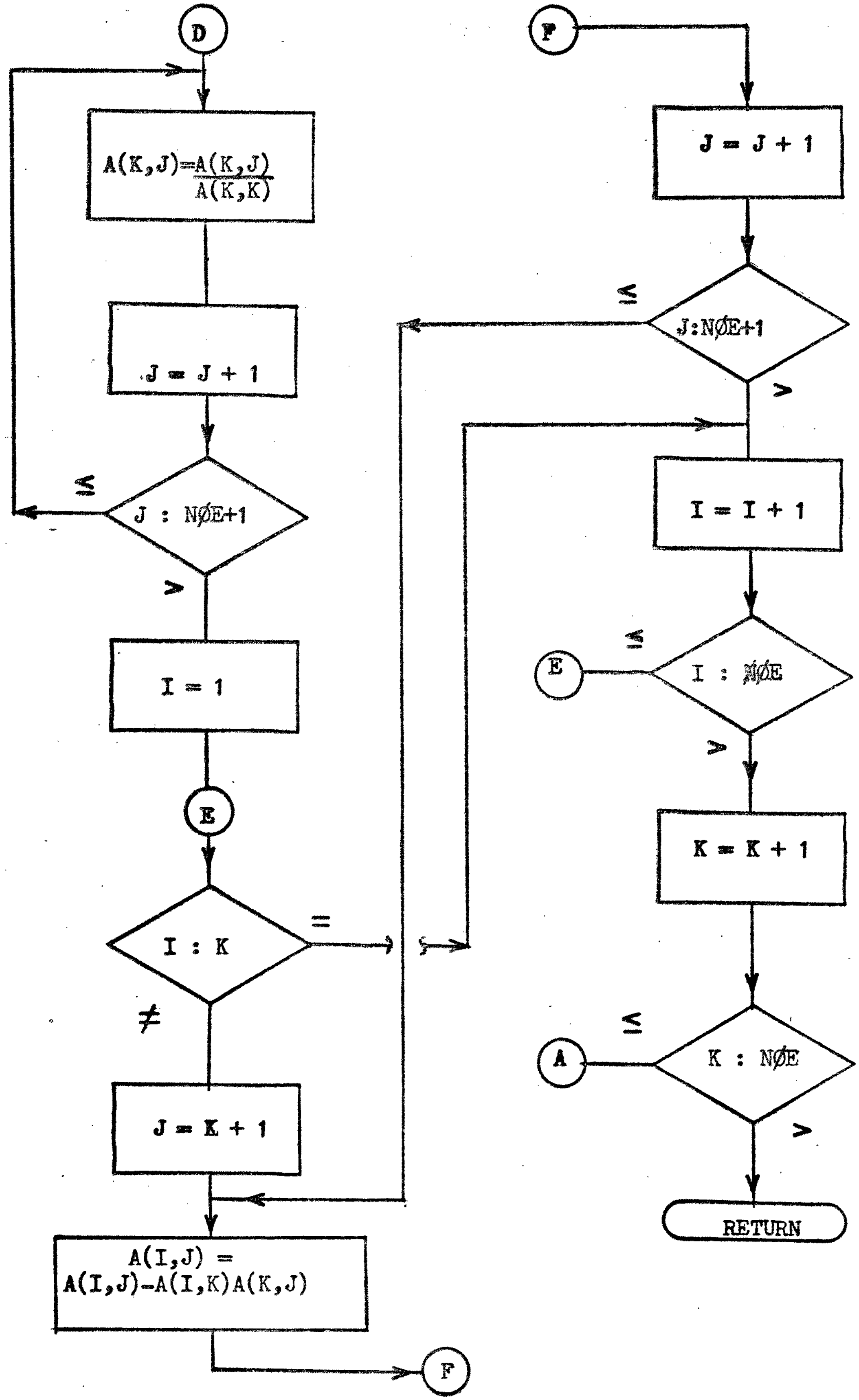


FIGURE NO. 9-2

SUBPROGRAM SEMQ (CONT.)



IV. SAMPLE PROBLEMS

Perhaps the best method that can be used to explain the functioning of the program is by way of sample problems. The sample problem chosen was one which has been previously solved by Treybal using the graphical procedure.[17]

The program was written in time sharing Fortran language utilizing the General Electric Mark I Time Sharing Service.[18] The system is accessed via a teletype terminal which may or may not be equipped with a paper tape reader and punch. The solubility data for the sample solvent system, Acetone - Water - 1,1,2 - Trichloroethane, is available in the literature.[19] The following procedure assumes the program, CCEXTG, has been previously stored in the user's catalog of saved programs, but it will be necessary to establish solubility data files.

External Data Files

Files must be established for the solubility data if the data has not been previously stored. The user can give the files any six character names consisting of letters and digits. The names of these files will be specified in, and used by, the main program. The data will be stored as pairs of coordinate points (X_B, X_C) on the solubility curve. The first file (SLAWT1 in the sample problem) stores the data points starting at the X_B axis on the A-rich side, for example the following three sets of data points: .0044, .0000; .0052, .0482; .0065, .1172. The second file (SLAWT2 in the sample problem) stores the solubility data point pairs starting at the X_B axis on the B-rich side:.9989, .0011; .9473, .0501; .9011, .0953. The files need not have equal numbers of sets of data points. The data can most conveniently be prepunched off line on paper tape then fed into the terminal via a paper tape reader as is shown on the following pages.

The user must first call and log-on the computer. The first computer request is for a file name, old or new. In the example, the keyboard input from the user is underlined. After the first file name is entered, the data are entered off the punch tape. This file may or may not be SAVED. A new file name is entered and the second set of data are transmitted to the computer via punched tape. Again, the file may or may not be put on SAVE.

The next keyboard response, OLD CCEXTG, recalls the actual program for use. The first requirement is identification of the appropriate data files, in this case SLAWT1 and SLAWT2. This is actually the first statement of CCEXTG and is line number 100. The form required is:

```
100    $FILE    SLAWT1,    SLAWT2
REPLACE
```

REPLACE is used as a matter of safety to insure that other data files stored in memory are not used inadvertently, causing erroneous results.

The user should then type RUN. The program title, time and data are then printed out.

Procedure for Establishing Data Files

```
NEW
NEW FILE NAME--SLAWT1   (Any name can be used.  Six character maximum)
READY.

TAPE
READY   (Operator should start tape reader.)

10      .0044,.0000,.0052,.0482,.0065,.1172,.0070,.1446
20      .0078,.1882,.0092,.2454,.0102,.2718
30      .0117,.3225,.0172,.3717,.0218,.4185
40      .0435,.4718,.0677,.5188,.0963,.5499
50      .1000,.5504,.1539,.5833,.2071,.5998
70      .3167,.5855,.3831,.5485,.4388,.5112
80      .4878,.4721,.5488,.4214,.6006,.3783
90      .6417,.3396,.6752,.3104,.7036,.2821
100     .7572,.2329,.7958,.1966,.8465,.1476
110     .9011,.0953,.9473,.0501,.9939,.0000
120     ENDFILE


SAVE
READY.

NEW
NEW FILE NAME--SLAWT2
READY.

TAPE
READY   (Operator should start tape reader.)

10      .9939,.0011,.9473,.0501,.9011,.0953
20      .8465,.1476,.7958,.1966,.7572,.2329
30      .7036,.2821,.6717,.3104,.6417,.3396
40      .6006,.3783,.5488,.4214,.4878,.4721
50      .4388,.5112,.3831,.5485,.3167,.5855
60      .2639,.6026,.2404,.6059,.2320,.6017
70      .2071,.5998,.1539,.5833,.1000,.5504
80      .0963,.5499,.0677,.5188,.0435,.4718
90      .0218,.4185,.0172,.3717,.0117,.3225
100     .0102,.2718,.0092,.2454,.0078,.1882
110     .0070,.1436,.0065,.1172,.0052,.0482,.0044,.0000
120     ENDFILE


SAVE
```

(Now it is necessary to insert the names of the data files (SLAWT1 and SLAWT2) into the program CCEXTG.)

```
ØLD CCEXTG
READY.

100 $FILE SLAWT1,SLAWT2
REPLACE
READY.
```

In this computer system, the program will ask a series of questions calling for various data as input. These must be supplied in the proper sequence and are as follows:

Problem Input

First line. Problem name. The problem name can consist of any 72 printable characters, including blanks.

Second line.

1. XCRN. The specified weight fraction of solute C to be contained in the final raffinate. If the percent recovery of solute C is specified, enter 0.0 for XCRN.
2. XBF, XCF. The X_B and X_C coordinate of the feed entering stage 1.
3. XBS, XCS. The X_B and X_C coordinates of the solvent entering stage n.
4. F, S. The weights of the feed and solvent respectively.
5. SCØN, ECØN. The constants k and r in the Hand tie line correlation equation for the specific ternary system.
6. PERC. The percent recovery of the solute C. (ie., the percent of C recovered in the extract flowing from stage 1). If XCRN is specified, enter 0.0 for the value of PERC.

Problem Output

1. Problem name.
2. The calculated values of XCRN if PERC is specified
3. The weights and compositions of the feed and solvent streams
4. The weight and composition of the feed solvent mixture. (Mix Point)

5. The coordinates of the operating point, 0

6. The weights and fractional compositions of the extracts and raffinates from stages one through n. Stage n is the first integer stage which satisfies the input specification for XCRN or PERC.

Two sample problems follow. In the first problem XCRN will be specified.(a value of 0.0 will be inserted for PERC), while in the second sample problem, the corresponding value of PERC will be specified (a value of 0.0 will be inserted for XCRN). The input values for the sample problems are as follows:

XCRN = 0.1 or 0.0
XBF = 0.0
XCF = 0.5
XBS = 1.0
XCS = 0.0

F = 100.0
S = 30.0
SCON = 1.841
ECON = 1.057
PERC = 0.0 or 90.2

In the example the first line of user input is

SAMPLE PROBLEM 1 XCRN IS SPECIFIED

While the second line consists of the user assigned values of

XCRN, XBF, XCF, XBS, XCS, F, S, SCON, ECON, PERC

After these data are accepted, the program continues automatically and prints the appropriate.output.

```
RUN

CCEXTG   19:52   09 MON 03/27/72

IN SMEO
IN .FIRST

? SAMPLE PROBLEM 1       XCRN IS SPECIFIED
? 0.1,0.0,0.5,1.0,0.0,100.0,30.0,1.341,1.057,0.0




SAMPLE PROBLEM 1       XCRN IS SPECIFIED


STREAM                 WEIGHT    X(A)     X(B)     X(C)


FEED                   100.000   .5000    .0000    .5000
SOLVENT                30.0000   .0000   1.0000    .0000
MIX POINT              130.000            .2308    .3846
OPERATING POINT                         -1.5469    .2563


STAGE    1

EXTRACT                30.8026   .0746    .3675    .5579
RAFFINATE              88.6312   .5319    .0249    .4432


STAGE    2

EXTRACT                69.4338   .0456    .4595    .4948
RAFFINATE              73.8494   .6154    .0141    .3705
```

```
STAGE    3

EXTRACT               54.6519    .0269    .5625    .4107
RAFFINATE             64.0984    .6982    .0108    .2910


STAGE    4

EXTRACT               44.9009    .0173    .6768    .3059
RAFFINATE             56.4201    .7841    .0082    .2076


STAGE    5

EXTRACT               37.2227    .0072    .8103    .1826
RAFFINATE             50.4036    .8737    .0065    .1198


STAGE    6

EXTRACT               31.2062    .0020    .9622    .0358
RAFFINATE             203.289    .9710    .0048    .0242




AT LINE NO. 85: STOP  END


USED      46.67 UNITS.
```

```
RUN

CCEXTG   19:59   09 MØN 03/27/72

IN SMEQ
IN .FIRST

? SAMPLE PRØBLEM 2       PERC IS SPECIFIED
? 0.0,0.0,0.5,1.0,0.0,100.0,30.0,1.841,1.057,90.2




SAMPLE PRØBLEM 2       PERC IS SPECIFIED
/XCRN=            .0991


STREAM                  WEIGHT    X(A)     X(B)     X(C)


FEED                    100.000   .5000    .0000    .5000
SØLVENT                 30.0000   .0000   1.0000    .0000
MIX PØINT               130.000            .2308    .3846
ØPERATING PØINT                          -1.5524    .2545

STAGE   1

EXTRACT                 80.8693   .0747    .3672    .5581
RAFFINATE               88.6754   .5316    .0250    .4434

STAGE   2

EXTRACT                 69.5446   .0458    .4589    .4954
RAFFINATE               73.9246   .6148    .0142    .3710
```

```
STAGE    3

EXTRACT                54.7939    .0272    .5611    .4117
RAFFINATE              64.1916    .6972    .0108    .2920


STAGE    4

EXTRACT                45.0609    .0176    .6745    .3079
RAFFINATE              56.5231    .7826    .0082    .2092


STAGE    5

EXTRACT                37.3924    .0073    .8067    .1860
RAFFINATE              50.5331    .8713    .0066    .1221


STAGE    6

EXTRACT                31.4024    .0023    .9563    .0414
RAFFINATE              174.871    .9673    .0049    .0278




AT LINE NO. 85: STOP  END


USED    131.00 UNITS.
```

V. DISCUSSION

To the best of the author's knowledge, this is the first computerized attempt at ternary liquid extraction problems using the parabolic interpolation approach to represent solubility data. It is believed that considerable accuracy can be achieved using such a method.

Note in particular that the Hand coefficients (k,r) must have been developed prior to using CCEXTG. This approach was chosen because many systems have considerable data scatter. In addition, there are some special systems that have two sets of Hand coefficients, ie. the direction in which the tie lines slope change as the concentration of component "C" is increased. With minor modification to CCEXTG, the above situation can be accommodated. Since this was the first work using this interpolation approach, the main effort was directed toward overall program development leaving refinements for the future.

Comparison of Graphical Method Versus Computerized Calculation

Using sample problem 1 as a basis, the results obtained using the computer program(parabolic interpolation) versus the results obtained by Treybal using the graphical method are compared. (See Table 1). The values for XCE and XCR for each ideal stage are compared for graphical and the computerized method. As can be seen, the results obtained differ by only 1.6 percent.

Comparison of Linear versus Parabolic Interpolation

In order to evaluate the merits of using parabolic interpolation of the solubility data, it will be necessary to compare results obtained using parabolic interpolation with those obtained using linear interpolation of data. A very early version of the program used linear interpolation. These results are abailable for comparison.

Again using the sample problem 1 as a basis for comparison, the values obtained for XCE and XCR using linear versus parabolic interpolation are compared. (See Table II). The values differ by an average of 13 percent. It is obvious that better results are obtained using parabolic interpolation.

Economic Analysis

When considering computer computation, the cost of solving a problem should not be overlooked. In order to present an estimation of the cost of solving a problem using the program CCEXTG, the two sample problems were considered typical. The cost of solving these problems can be calculated by using the number of computer resource units (CRU's) printed at the end of the problem by the computer. In Mark I time-sharing, the cost of a CRU is \$.05. In addition to the above cost, a terminal connect time charge must be added of \$8.50 per hour.[20] Cost calculations for the two sample problems follow:

Sample problem 1. XCRN is specified.

\$ .05/CRU	X 46.67	CRU's	=	\$ 2.34
\$8.50/ Hr.	X 0.1	Hr.	=	0.85
		Total Cost	=	\$ 3.19

TABLE I

COMPARISON OF GRAPHICAL AND COMPUTERIZED METHODS

	GRAPHICAL METHOD	COMPUTERIZED METHOD	ABSOLUTE DIFFERENCE	PERCENTAGE DIFFERENCE
STAGE No. 1				
XCE	0.557	0.558	0.001	0.18
XCR	0.438	0.443	0.005	1.14
STAGE No. 2				
XCE	0.489	0.495	0.006	1.22
XCR	0.363	0.376	0.013	3.58
STAGE No. 3				
XCE	0.403	0.411	0.008	1.98
XCR	0.287	0.291	0.004	1.39
STAGE No. 4				
XCE	0.300	0.306	0.006	2.00
XCR	0.206	0.206	0.002	0.97
STAGE No. 5				
XCE	0.180	0.183	0.003	1.66
XCR	0.120	0.120	0.000	0.00
STAGE No. 6				
XCE	0.038	0.036	0.002	5.26
XCR	0.025	0.024	0.001	4.00
Average			0.004	1.65

TABLE II

COMPARISON OF LINEAR VERSUS PARABOLIC INTERPOLATION OF SOLUBILITY DATA

	LINEAR VALUES	PARABOLIC VALUES	ABSOLUTE DIFFERENCE	PERCENTAGE DIFFERENCE
STAGE NO. 1				
XCE	0.557	0.558	0.001	0.18
XCR	0.440	0.443	0.003	0.68
STAGE No. 2				
XCE	0.491	0.495	0.004	0.81
XCR	0.366	0.376	0.010	2.73
STAGE No. 3				
XCE	0.404	0.411	0.007	1.73
XCR	0.285	0.291	0.006	2.10
STAGE No. 4				
XCE	0.297	0.306	0.009	3.03
XCR	0.201	0.208	0.007	3.48
STAGE No. 5				
XCE	0.171	0.183	0.012	7.01
XCR	0.112	0.120	0.008	7.14
STAGE No. 6				
XCE	0.022	0.036	0.014	70.00
XCR	0.015	0.024	0.009	60.00
		Average	0.008	13.00

<u>Sample problem 2.</u> PERC is specified.

$ .05/CRU	X	131.00	CRU's	=	$ 6.55
$8.50/Hr.	X	0.1	Hr.	=	0.85
			Total Cost	=	$ 7.40

As can be seen, the cost is well within reason when compared to the engineer's man-hours required to solve such a problem with equivalent accuracy.

VI. CONCLUSIONS AND RECOMMENDATIONS

The following conclusions are presented:

1. A Fortran computer program has been developed that will calculate the number of ideal stages required for a specified ternary countercurrent liquid extraction problem. Furthermore, the program calculates the weights and compositions of all extracts and raffinates.

2. The above program utilizes experimentally found solubility data to describe the phase equilibria isotherm. This is accomplished by the use of an interpolating parabola. Data has been presented that proves the use of parabolic interpolation is far superior to using linear interpolation for this purpose. The results obtained using linear interpolation differ from those found by parabolic interpolation by 13 percent.

3. The necessary relationships to describe and interrelate all tie lines, concentrations, weights, and construction lines with the phase equilibria isotherm have been developed.

4. The Fortran program has been tested and compared to published graphical solutions of extraction problems. The computer calculated values are within 2 percent of the graphically found values.

5. A stepwise procedure for the use of the program has been presented.

6. An economic cost analysis of using the program to solve typical extraction problems shows that costs are quite reasonable.

It is recommended that the following investigations be considered for future work:

1. Utilize the proposed computer program on additional solvent systems to further test the parabolic interpolation method for solubility data.

2. Conduct a study wherein the number of solubility data points are successively reduced to determine the effect on the accuracy of the calculation method.

3. Conduct an optimization study for an extraction design problem utilizing the computer program wherein feed rates and/or compositions of feed streams are adjusted to determine the best operating conditions.

4. Expand the capability of the calculation method to accommodate four-component systems. Possibly a four-coefficient polynomial can be employed to represent the solubility data.

5. Incorporate a subprogram into CCEXTG that will calculate the values of k and r for the tie line correlation.

APPENDIX

TEXT NOMENCLATURE

A	Component A, the main component of the carrier
B	Component B, the main component of the extracting solvent
C	Component C, the solute
E	Extract solution weight
F	Feed solution weight
k	A constant
M	Mix point
m	Any stage in the cascade
n	Total number of stages in the cascade or the last stage
O	Operating point
R	Raffinate solution weight
r	A constant
S	Extracting solvent weight
X	Weight or mole fraction

Subscripts:

A,B,C	Components A,B,C
E	Extract
F	Feed
M	Mix point
O	Operating point
R	Raffinate
S	Solvent
1,2,etc.	Stage 1,2,etc.

MAIN PROGRAM NOMENCLATURE

AINT1, AINT2	Programing variable
AM1, AM2	Programing variable
CORRL	Tie line correlation variable
E1	Weight of extract from stage 1
ECØN	Exponential constant, tie line correlation
E(M)	Weight of extract from stage M
F	Weight of feed
FRINC	Incremental variable used in XCRN search routine
EINTN	Programing variable
ESLØPEN	Programing variable
PERC	Percent recovery of component A in extract, E_1
N	Stage number
R(M)	Weight of raffinate from stage M
RN	Weight of raffinate from last stage
S	Weight of solvent
SCØN	Constant, tie line correlation
XØB, XØC	Coordinates of the operating point
XAE(N), XBE(N), XCE(N)	Fraction of A, B, C in extract from stage N
XAF, XBF, XCF	Fraction of A, B, C, in feed
XAS, XBS, XCS	Fraction of A, B, C in solvent
XBRN, XCRN	Fraction of B, C in specified raffinate
XAR(N), XBR(N), XCR(N)	Fraction of A, B, C, in raffinate from stage N
ZM	Mix point magnitude, F+S
ZINT, ZSLØPE	Programing variable
XTRAN, XTRA	Programing variable

```
CCEXTG  20:09   09 MØN 03/27/72

100        $FILE SLAWT1,SLAWT2
110
120        SUBRØUTINE FDXCE1(XCEF,XBEF)
130        CØMMØN A(10,11),NØE,XCRN,XBRN,XCM,XBM
140C       FINDS E(1) BY EXTENDING LINE RN-M
150        EINT=BINT(XCRN,XBRN,XCM,XBM)
160        ESLØPE=SLØPE(XCRN,XBRN,XCM,XBM)
170        CALL ATER1(EINT,ESLØPE,XBEF,XCEF,2)
180        RETURN
190
200        SUBRØUTINE ATER1(REINT,RESLØPE,BE,CE,L)
210C       INTERPØLATIØN ØF SØLUBILITY DATA
220C       A RICH PHASE FØR L=1; B RICH PHASE FØR L=2
230C        USES GREGØRY-NEWTØN METHØD.
240C       SØLVES FØR INTERSECTIØN WITH STRAIGHT LINE HAVING
250C       SLØPE=RESLØPE+INTERCEPT=REINT
260        CØMMØN A(10,11),NØE,XCRN,XBRN,XCM,XBM
270        READ (L) B1,C1,B2,C2
280     20 CØNTINUE
290        READ (L) B3,C3
300        A(1,2)=B1;A(2,2)=B2;A(3,2)=B3
310        A(1,1)=B1**2.0;A(2,1)=B2**2.0;A(3,1)=B3**2.0
320        A(1,3)=1.0;A(2,3)=1.0;A(3,3)=1.0
330        A(1,4)=C1;A(2,4)=C2;A(3,4)=C3
340        NØE=3
350        CALL SMEQ
360        QA=A(1,4)
370        QB=A(2,4)-RESLØPE
380        QC=A(3,4)-REINT
390        BP=(-QB+SQRT(ABS(QB**2.0-(4.0*QA*QC))))/(2.0*QA)
400        BN=(-QB-SQRT(ABS(QB**2.0-(4.0*QA*QC))))/(2.0*QA)
410        GØ TØ(1,2) L
420      1 BE=BP
430        GØ TØ 6
440      2 BE=BN
450      6 CE=(RESLØPE*BE)+REINT
460        B1=B2;B2=B3;C1=C2;C2=C3
470        IF(CE-C3) 30,30,20
480     30 CØNTINUE
490        REWIND L
510        RETURN
530
1000        FUNCTIØN SLØPE(Y1,X1,Y2,X2)
1010        SLØPE=(Y1-Y2)/(X1-X2)
1020        RETURN
1030        CØNTINUE
1040        FUNCTIØN BINT(Y1,X1,Y2,X2)
1050        BINT=Y1-(((Y1-Y2)/(X1-X2))*X1)
1060        RETURN
1070        END
1080
```

```
1090C     MAIN PRØGRAM
1100
1110      CØMMØN A(10,11),NØE,XCRN,XBRN,XCM,XBM
1120      DIMENSIØN XCR(20),XBR",XBE",XCE",XAR",XAE",F",R"
1130      INTEGER PRØB(72)
1140 180  FØRMAT(72A1)
1150 181  FØRMAT(//////)
1160 182  FØRMAT(///"STREAM",13X,"WEIGHT    X(A)    X(B)    X(C)")
1170 183  FØRMAT(//"FEED",12X,G10.6,3F8.4)
1180 184  FØRMAT("SØLVENT",9X,G10.6,3F8.4)
1190 185  FØRMAT(//"STAGE  ",I2)
1200 186  FØRMAT(/"EXTRACT",9X,G10.6,3F8.4)
1210 187  FØRMAT("RAFFINATE",7X,G10.6,3F8.4)
1220 188  FØRMAT("MIX PØINT",7X,G10.6,8X,2F8.4)
1230 189  FØRMAT("ØPERATING PØINT ",13X,2F8.4)
1240      INPUT 180,PRØB
1250      INPUT,XCRN,XBF,XCF,XBS,XCS,F,S,SCØN,ECØN,PERC
1260      PRINT 181
1270      PRINT 180,PRØB
1280C     FIND MIX PØINT
1290
1300      XAF=1.0-XBF-XCF
1310      XAS=1.0-XBS-XCS
1320      XBM=((F*XBF)+(S*XBS))/(F+S)
1330      ZM=F+S
1340      ZINT=BINT(XCF,XBF,XCS,XBS)
1350      ZSLOPE=SLOPE(XCF,XBF,XCS,XBS)
1360      XCM=(ZSLOPE*XBM)+ZINT
1370C     DECIDE IF XCRN IS GIVEN ØR MUST BE FØUND
1380
1390      IF(XCRN-0.0)110,110,100
1400 100  CØNTINUE
1410C     FINDS XBRN IF XCRN IS GIVEN
1420
1430      CALL ATER1(XCRN,0.0,XBRN,XTRAN,1)
1440      GØ TØ 150
1450 110  CØNTINUE
1460
```

```
1470C     FINDS XCRN IF NØT GIVEN-USES ITERATIØN METHØD
1480
1490C     INITIALZATIØN
1500      XCRN=0.0001;FRINC=.10
1510 120  CØNTINUE
1520      RN=((1.0-(.01*PERC))*F*XCF)/XCRN
1530C     FINDS XBRN FØR ASSUMED XCRN
1540      CALL ATER1(XCRN,0.0,XBRN,XTRA,1)
1550      CALL FDXCE1(XCE(1),XBE(1))
1560      E1=((F*XCF)+(S*XCS)-(XCRN*RN))/XCE(1)
1570      XCRN=XCRN+FRINC
1580      IF(F+S-E1-RN)120,130,130
1590 130  CØNTINUE
1600      XCRN=XCRN-(2.0*FRINC)
1610      FRINC=.1*FRINC
1620      IF(FRINC-.0001)140,140,120
1630 140  CØNTINUE
1640      PRINT,"/XCRN=",XCRN
1650      GØ TØ 100
1660 150  CØNTINUE
1670
1680C     FIND E(1) GIVEN RN-M
1690      CALL FDXCE1(XCF(1),XBE(1))
1700      AM1=(XCF-XCE(1))/(XBF-XBE(1))
1710      AM2=(XCRN-XCS)/(XBRN-XBS)
1720      AINT1=XCF-(((XCF-XCE(1))/(XBF-XBE(1)))*XBF)
1730      AINT2=XCRN-(((XCRN-XCS)/(XBRN-XBS))*XBRN)
1740      XØB=(AINT2-AINT1)/(AM1-AM2)
1750      XØC=(AM1*(AINT2-AINT1)/(AM1-AM2))+AINT1
1760
1770C     FIND RAFFINATE CØMPØSITIØN,R(N)
1780C     INTERSECTIØN ØF TIE LINE WITH SØLUBILITY CURVE
1790
1800      N=1
1810  70  CØNTINUE
1820      CØRRL=1.0/ECØN*(LØG(XCE(N)/(XBE(N)*SCØN)))
1830      CØRRL=EXP(CØRRL)
1840C     TIE LINE; XCA=-CØRRL/(1+CØRRL)*XBA+CØRRL/(1+CØRRL)
1850      CALL ATER1(CØRRL/(1.0+CØRRL),-CØRRL/(1.0+CØRRL),XBR(N),XCR(N),
1860      XAR(N)=1.0-XBR(N)-XCR(N)
1870      XAE(N)=1.0-XBE(N)-XCE(N)
1880      IF (XCR(N)-XCRN) 90,90,80
1890
```

```
1900C    FIND E(N) BY EXTENDING R(N)-Ø TØ INTERSECTIØN
1910C    WITH SØLUBILITY CURVE
1920
1930 80  N=N+1
1940     EINTN=BINT(XCR(N-1),XBR(N-1),XØC,XØB)
1950     ESLØPEN=SLØPE(XCR(N-1),XBR(N-1),XØC,XØB)
1960     CALL ATER1(EINTN,ESLØPEN,XBE(N),XCE(N),2)
1970     GØ TØ 70
1980
1990C    CALCULATE EXTRACTS + RAFFINATES
2000
2010 90  E(1)=ZM*(XCM-XCRN)/(XCE(1)-XCRN)
2020     RN=((XCM*ZM)-(XCE(1)*E(1)))/XCRN
2030     R(1)=(F*(XCF-XCE(2))+(E(1)*(XCE(2)-XCE(1))))/
2040     +(XCR(1)-XCE(2))
2050     E(2)=R(1)+E(1)-F
2060     DØ 160,M=2,N
2070     R(M)=(R(M-1)*(XCR(M-1)-XCE(M+1))+(E(M)*(XCE(M+1)-
2080     +XCE(M))))/(XCR(M)-XCE(M+1))
2090     E(M+1)=R(M)+E(M)-R(M-1)
2100 160 CØNTINUE
2110     PRINT 182
2120     PRINT 183,F,XAF,XBF,XCF
2130     PRINT 184,S,XAS,XBS,XCS
2140     PRINT 188,ZM,XBM,XCM
2150     PRINT 189,XØB,XØC
2160     DØ 170,M=1,N
2170     PRINT 185,M
2180     PRINT 186,E(M),XAE(M),XBE(M),XCE(M)
2190     PRINT 187,R(M),XAR(M),XBR(M),XCR(M)
2200 170 CØNTINUE
2210     $USE SMEQ
2220     STØP
2230     END
```

```
SMEQ     19:39   09 TUE 03/21/72

85        SUBRØUTINE SMEQ
90C       GAUSS-JØRDAN METHØD
100       CØMMØN A(10,11),NØE,XCRN,XBRN,XCM,XBM
105       DIMENSIØN STØRE(10,11)
140       K=1
150   10  CØNTINUE
160       J=K+1
170       M=K+1
180   12  L=K
190       IF (ABS(A(K,L))-ABS(A(M,L))) 13,14,14
195   13  STØRE(K,L)=A(K,L)
200       A(K,L)=A(M,L)
205       A(M,L)=STØRE(K,L)
210       L=L+1
220       IF(NØE+1-L) 14,13,13
230   14  M=M+1
240       IF(NØE-M) 20,12,12
250   20   A(K,J)=A(K,J)/A(K,K)
260       J=J+1
270       IF(J-(NØE+1)) 20,20,30
280   30  I=1
290   40  CØNTINUE
300       IF(I-K) 50,70,50
310   50  J=K+1
320   60  A(I,J)=A(I,J)-(A(I,K)*A(K,J))
330       J=J+1
340       IF(J-(NØE+1)) 60,60,70
350   70  I=I+1
360       IF(I-NØE) 40,40,80
370   80  K=K+1
380       IF(K-NØE) 10,10,90
390   90  CØNTINUE
430       RETURN
440       END
```

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