ALGORITHMS FOR FRACTIONATOR CALCULATIONS

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PREFACE

A critical evaluation of the Ball-Rose relaxation procedure for predicting fractionator performance was made. A computer program that handles columns which have from one to three feeds, up to three side draws and/or three sidestream strippers and a maximum of six intercoolers was employed in this study. The solutions obtained by machine calculations were compared with both published and private problem solutions to verify the reliability of the Ball-Rose technique. The ratio of the time interval to the tray holdup's effect on the program's ability in reaching convergence was also studied.

I should wish to express my appreciation for the assistance and guidance offered me by Professors J. H. Erbar and R. N. Maddox, both of whom gave so generously of their time and whose suggestions and encouragement were of great value. I would also thank the National Science Foundation whose traineeship grant made this work possible. In addition, I am also grateful to the Oklahoma State University Computing Center for the use of its computing facilities.

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CHAPTER I

INTRODUCTION

Countercurrent flow, mass transfer columns are primary unit operations in the chemical industry and as such have found extensive usage in the separation of complex hydrocarbon mixtures. Owing to the importance, a variety of methods for solving the equations simulating the specific types of these columns has been proposed and newer, more reliable methods are constantly being searched for.

The design of separation equipment has generally been based on the steady-state solution of the equations describing an equilibrium tray model. Due to the complexity of the describing equations and large number of hand calculations, numerous short-cut methods have previously been utilized by the design engineer.

The advent of large capacity, high speed digital computers has made tray-by-tray solutions practical. Interstage flow rates, stage temperatures, and compositions throughout the column are now readily accessible. With these newer methods, the design engineer in finalizing the design of process units need not rely so heavily on the short cut methods, with their inaccurate and sometimes invalid approximations.

The engineering scope of this study considers the Ball-Rose calculation method and its ability to describe the complex absorption system, the reboiled absorber. This procedure attempts to determine the steady-state conditions existing in a column through a transient approach. A system of simultaneous material balance equations is solved for each component on each tray. The advantages of the technique lie in its lack of assumptions designating key component splits, individual component product rates and in its ability to handle trace components throughout the column.

The method's reliability and limitations in approaching the converged solution for various absorber configurations was studied. In order to evaluate the technique and its convergence routine, a program written for the IBM 7040 was utilized. A guide for the best range of the program's convergence accelerator, the ratio of the time interval to the tray holdup, is presented.

CHAPTER II

LITERATURE SURVEY

A) Absorption Processes

The countercurrent contacting of a vapor and a liquid stream is termed gaseous absorption. The heavier stream is employed to remove certain components from the lighter gas stream. The rate of mass transfer is dependent on the relative concentration differences of the gaseous components in both streams as well as the degree of contacting.

The simple absorber column (Figure 1) consists of two feeds; the lean oil, which is usually free of gaseous components, enters the top of the column and the vapor stream rich with the desired components enters through the bottom. The unabsorbed gaseous stream, the lean gas, exits at the top of the column while the solvent rich oil, now abundant in accumulated vapors, leaves as the bottoms product.

An important variation of the simple absorber is the combination of an absorber and an exhausting section with the addition of another feed to form a reboiled absorber column (Figure 2).

The top portion of the reboiled absorber serves as an absorber; the lean oil removes the heavier, less volatile gaseous components from the ascending vapor stream. The

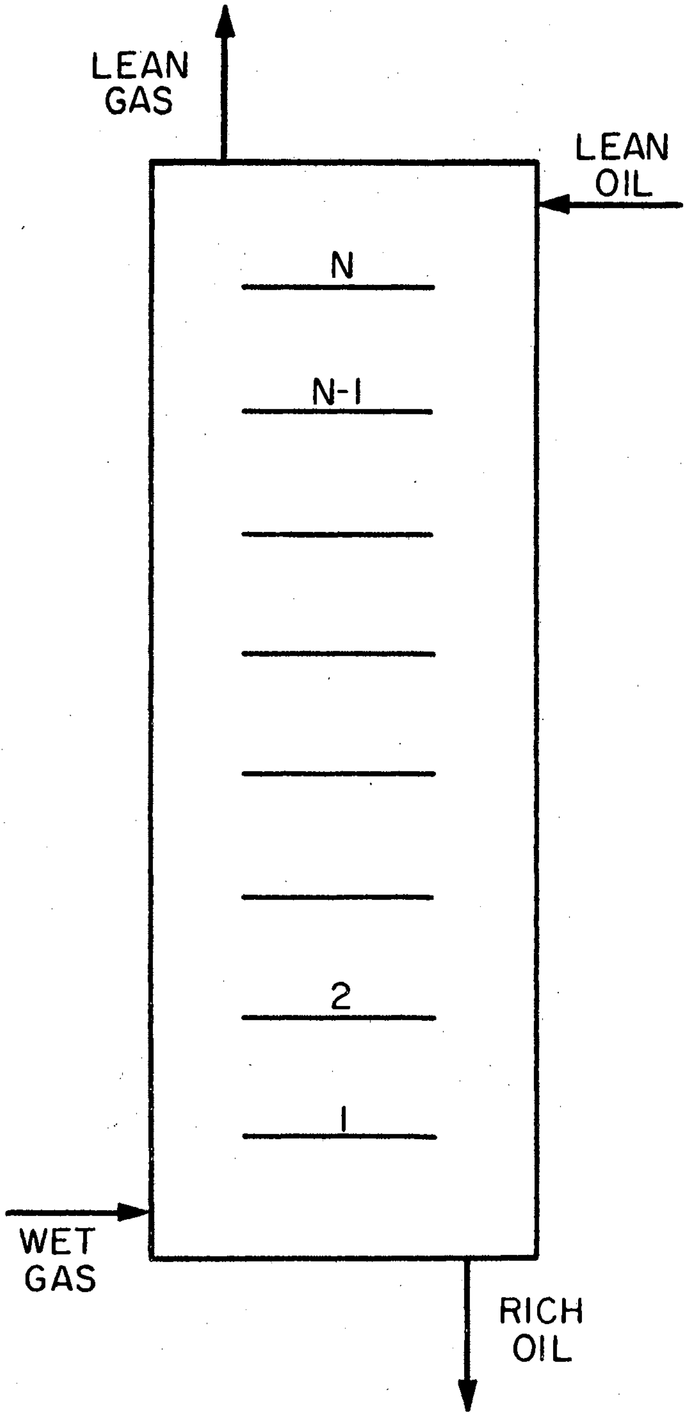

Figure 1. A "Simple" N Tray Absorption Column

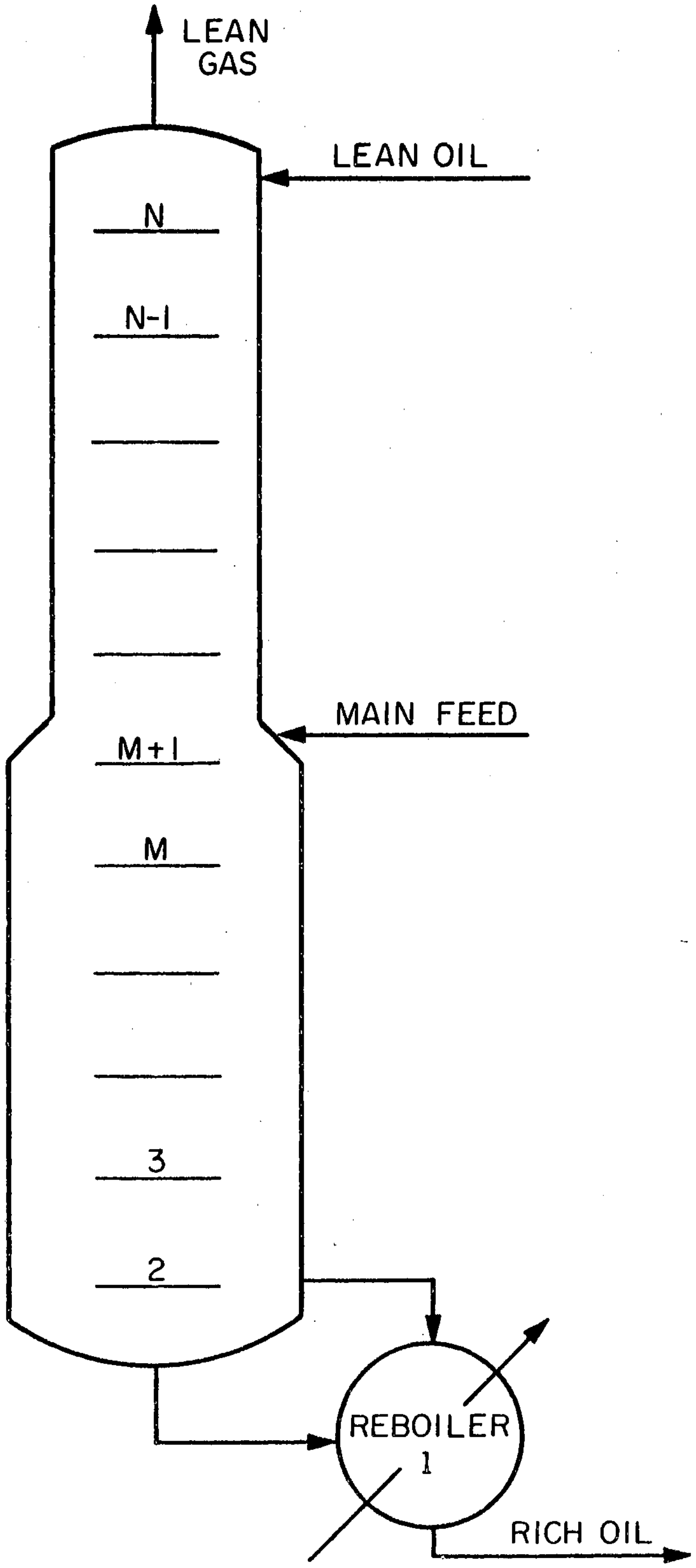

Figure 2. A "Simple" N Tray Reboiled Absorber

vapor stream returning from the reboiler, rises through the lower portion of the column and serves to preferentially strip the more volatile components from the absorption oil, thereby affording a sharper separation.

The degrees of freedom associated with a process unit can be ascertained by summing the restricting relationships and the number of intensive and extensive variables for each element. The analysis of the entire unit is complete when the results of all the diverse elements are combined.

The simple absorption column with a single wet gas feed and N trays, where each tray is considered a simple equilibrium stage, is defined by a total number of variables, N_V, equal to

$$N_V = 1 + N(2C + 6). \qquad (1)$$

Each simple equilibrium stage is described by (2C + 6) variables while the specification of the number of plates is in itself a variable.

However, some of these variables are not independent and need to be subtracted to obtain the degrees of freedom for the column. The new restrictions are the stream identities which exist in each interstream between two elements. Thus, C + 2 new restricting relationships associated with each interstream must be subtracted. There are 2(N - 1) interstreams in the simple absorption column and, therefore, the number of independent restrictions is:

$$N_i = 1 + N(2C + 6) - 2(N - 1)(C + 2) = 2C + 2N + 5. \qquad (2)$$

For the more complex reboiled absorber, the number of variables for the entire unit is the sum of the four elements listed below:

$N - (M + 1)$ simple equilibrium stages	$2C + 2(N - M - 1)$	$+ 5$
Feed stage	$3C$	$+ 8$
$M - 1$ simple equilibrium stages	$2C + 2(M - 1)$	$+ 5$
Partial reboiler	C	$+ 4$
Total	$8C + 2N + 18$	

Six interstreams are created by the combination of the elements and, thus, $6(C + 2)$ variables must be subtracted to give $2C + 2N + 6$ degrees of freedom available to the designer.

Both types of columns can be modified with a number of complex features. Any tray in the column can have an intercooler, vapor, and liquid side streams or an additional feed.

As seen above the addition of a feed tray to a simple tray increases the number of independent variables from $2C + 6$ to $3C + 8$. Since the location of the feed plate is an additional independent variable there are $C + 3$ additional independent variables associated with each feed tray.

The addition of a side stream to a simple tray increases the number of independent variables by one. Since the location of this tray and the side stream rate must be specified; two additional independent variables are associated with each side stream tray. For an n tray complex column having f feed streams and s liquid and v vapor side streams a general set of specifications for the degrees of freedom is:

Heat leak on each stage	n
Pressure for each stage	n
Feed streams and locations	f(C + 3)
Liquid side streams and locations	2s
Vapor side streams and locations	2v
Number of stages	1
Total	2(n + s + v) + f(C + 3) + 1

B) Calculation Method

Owing to the importance of absorbers and reboiled absorbers, intensive research for solutions of absorber problems having various complex configurations has been carried out. Two basic approaches have been used to describe the absorber type of columns - one being that developed from mass transfer theories leading to the concepts of transfer units and the height equivalent of a packed column to a theoretical plate. However, stagewise process type calculations employing the assumption of equilibrium stages are in wider usage. An equilibrium stage is defined as one from which the vapor rising from a tray is in equilibrium with the liquid overflowing to the plate below.

Prior to the advent of high speed digital calculating machines, the stagewise computations were too tedious for hand calculations. The large number of calculations made these methods impractical. Consequently, labor-saving methods that gave rapid answers were developed and used extensively as bases for design.

A short-cut graphical solution can be obtained for simple absorbers by constructing an equilibrium curve similar to the McCabe-Thiele (2) diagram. Operating lines are assumed and the required number of stages is determined by the McCabe-Thiele approach. This method lends iteself adequately to simple systems such as binary and ternary separation problems. However, multi-component systems require trial and error searching techniques.

An empirical absorption factor was developed by Cox and Arthur (4). However, these authors failed to consider the number of equilibrium plates as well as the composition of the lean oil. Kremser (4) developed an absorption factor based on Raoult's law. Raoult's law is a relation used for determining the partial pressure of a constituent in a liquid solution. The partial pressure of component C, is defined as the product of the mole fraction of C in the liquid and the vapor pressure of C, at the temperature of the system. The assumption of Raoult's law in effect assumes an ideal liquid phase. Using partial pressures, Kremser defined an absorption factor for each component on any equilibrium tray as

$$A = \frac{Gq}{100}. \qquad (3)$$

In Kremser's analysis a perfectly stripped lean oil was assumed.

An absorption factor, free from the errors of Raoult's law and ideal gaseous assumptions was developed by Brown and Souders (4). These authors employed an equilibrium constant which was a function of the temperature and pressure. Then, for any equilibrium plate, i,

$$K = \frac{y_i}{X_i}. \qquad (4)$$

Since the total moles of liquid and gas are constant, the moles absorbed in the liquid from any tray are equal to the moles removed from the gas,

$$L(X_i - X_{i-1}) = V(y_{i+1} - y_i). \qquad (5)$$

Substituting Equation (4) into (5) yields the definition of the Souder absorption factor:

$$A = \frac{L}{KV} = \frac{y_{i+1} - y_i}{y_i - y_{i-1}}. \qquad (6)$$

A general equation describing the composition of the gas from the top plate, n, of the absorber was developed by applying Equation (5) to each tray. The equation is

$$y_n = \frac{y_{n+1}(A^n - 1) + A^n(A - 1)y_0}{A^{n+1} - 1} \qquad (7)$$

Edmister (8) introduced more convenient relationships employing absorption and stripping (S = KV/L) factor functions. General functions for the A and S factors were developed and arranged for application in distillation operations in the chemical industry.

A component material balance about the top of the absorber to include plates 1 through i, and noting that

$$\ell_{i+1} = \frac{L_{i+1}}{K_{i+1} \ V_{i+1}} v_{i+1} = A_{i+1} \ v_{i+1} \tag{8}$$

gives upon rearrangement

$$\ell_{i+1} = (\ell_i - \ell_0 + v_i) A_{i+1} . \tag{9}$$

For multi-stage absorption a general relationship is obtained by combining Equation (9) for each plate, yielding:

$$\begin{aligned} \ell_n = {} & v_1 (A_1 A_2 A_3 \ \ldots \ A_n + A_2 A_3 \ \ldots \ A_n + A_3 \ \ldots \ A_n \\ & + \ldots + A_n) - \ell_0 (A_2 A_3 \ \ldots \ A_n + A_3 \ \ldots \ A_n \\ & + \ldots + A_n) \end{aligned} \tag{10}$$

In a similar manner a material balance about a stripping section yields the following relationship:

$$\begin{aligned} v_m = {} & \ell_1 (S_1 S_2 S_3 \ \ldots \ S_m + S_2 S_3 \ \ldots \ S_m + S_3 \ \ldots \ S_m \\ & + \ldots + S_m) - v_0 (S_2 S_3 \ \ldots \ S_m + S_3 \ \ldots \ S_m \\ & + \ldots + S_m) \end{aligned} \tag{11}$$

By defining a fraction of a component not recovered by absorption as

$$\varphi_A = \frac{1}{A_1 A_2 A_3 \ldots A_n + A_2 A_3 \ldots A_n + A_3 \ldots A_n + \ldots + A_n + 1} \qquad (12)$$

and a similar fraction for stripping,

$$\varphi_S = \frac{1}{S_1 S_2 S_3 \ldots S_n + S_2 S_3 \ldots S_n + S_3 \ldots S_n + \ldots + S_n + 1} \qquad (13)$$

one can rearrange Equation (10) and (11) to

$$\ell_n = \varphi_S \ell_o + (1 - \varphi_A) v_{n+1} \qquad (10a)$$

and

$$v_m = \varphi_A v_1 + (1 + \varphi_S) \ell_{m+1} . \qquad (11a)$$

These equations can then be coupled with the appropriate material balance equations to give relationships which can be used to predict the performance of any stagewise processing unit. By this method the equation used to describe a reboiled absorber is

$$\frac{d}{b} = \frac{\varphi_{AA} \left(\frac{S_o \varphi_{AX} + 1}{\varphi_{SX}} \right) + \left(1 - \varphi_{SA} - \varphi_{AA} \right) \frac{\ell_o}{b}}{(1 - \varphi_{AA})} . \qquad (14)$$

Equation (14) cannot be solved directly even if all the recovery fractions are known since b appears on both sides of the equation.

For ease of calculations, effective absorber and stripping factor relationships were developed, thereby eliminating the calculation of the respective factors for each plate.

Lewis and Matheson (15) developed a rigorous procedure analogous to the graphical Ponchin-Savarit (2) method. Heat and mass balances are solved simultaneously using assumed light and heavy key product rates. Calculations are started from the terminal positions of the tower and carried to the feed plate. The composition of the calculated overflow stream from the feed stage is compared with the calculated liquid stream entering the stripping section of the column. If a significant mismatch occurs, new product compositions are assumed until the mesh at the feed zone is converged. In this manner the number of equilibrium stages and the product distributions may be determined.

Bonner (3) used a simplified version of the Lewis-Matheson procedure. He specified the number of stages above and below the feed. Temperatures and the liquid and vapor profiles are assumed and end product compositions are then determined in a similar manner, with the feed plate mesh technique. The product compositions are adjusted after each succeeding pass.

Thiele and Geddes (24) developed a rigorous multicomponent distillation method in which the trial calculations can be performed after assuming a temperature profile as well as the liquid and vapor profiles. The products are calculated by Equation (15). This relationship is of the form,

$$\frac{\ell_{i+1}}{d} = A_{i+1}\left(\frac{\ell_i}{d} + 1\right). \qquad (15)$$

This equation was derived from a combined equilibrium and material balance relationship. The temperature and liquid vapor profiles are corrected by calculations similar to that of the Lewis-Matheson procedure. When the feed plate is reached, the terminal compositions are adjusted and the calculations are repeated until there are no changes in the distillate composition.

For machine solution, special techniques devised by Lyster and Holland (14, 16), such as the Q and constant composition methods, must be applied to obtain converged solutions. The Q method employs side heaters on each stage to force a satisfactory energy balance. The constant composition method is used to avoid round-off errors in the enthalpy balance computations. Neither of these methods are practical and the latter method cannot be utilized conveniently when using Chao-Seader correlations.

Both of the preceding methods (the Bonner/Lewis-Matheson approach and the Thiele/Geddes procedure) experience several problems when applied to digital computers. The most serious problem arises from the accumulated errors generated by roundoff and truncation errors in the solution. Additionally, both methods require that all components be distributed. In many cases the concentration of non-ideal components goes to zero in various portions of the column. In general, there is no assurance that either of these methods will converge at all.

Napthali and Sandholm (17) approached the solution of stagewise separation calculations by grouping the equations of conservation of mass and energy and the equilibrium relationships by stages. After linearization, the resulting set of equations are solved simultaneously by a modified Newton-Raphson procedure. The matrix of the partial derivatives employed in the Newton-Raphson technique is assembled into a form such that inversion can be easily accomplished by Gaussian elimination. As the final solution values are approached, the procedure accelerates convergence. However, problems are encountered in this solution technique due to the instability of the Newton-Raphson method if the initial profiles are far from the final solution values.

More recent developments in predicting fractionator performances have branched out into two distinct but similarly constructed computational methods. These methods are designated as the Sum Rates Method and the Bubble Point Relaxation Technique. In the first approach, the Sum Rates Method, a material balance about any non-feed plate yields the following relationship:

$$\ell_i + v_i = \ell_{i+1} + v_{i-1} . \tag{16}$$

The equilibrium relation between the component vapor and liquid streams leaving any tray, i, is given by,

$$v_i = \frac{K_i V_i}{L_i} \ell_i = S_i \ \ell_i . \tag{17}$$

The material balance relationship can then be written in the following form:

$$-\ell_{i+1} + (1 + S_i)\ell_i - S_{i-1} \ \ell_{i-1} = 0. \tag{18}$$

For any feed plate, this relationship is modified by setting the left-hand side of Equation (18) equal to the component feed rate to that plate. The material balance can be further modified by writing Equation (18) in the following form:

$$-A'_{i-1} \ell_{i-1} + B'_i \ell_i - C'_{i+1} \ell_{i+1} = D'_i \tag{19}$$

where the coefficients of Equation (19) are defined as,

$$A'_{i-1} = S_{i-1} \tag{19a}$$

$$B'_i = (1 + S_i) \tag{19b}$$

$$C'_{i+1} = 1 \tag{19c}$$

$$D'_i = f_n \tag{19d}$$

For any given component, N+2 equations are written. If one designates the reboiler as plate zero and the condenser as n=N+1, then the equations for any one component assume the following form:

$$\begin{array}{ll}
\text{reboiler} & B_0'\ell_0 - C_1'\ell_1 = D_0' \\
\text{plate 1} & -A_0'\ell_0 + B_1'\ell_1 - C_2'\ell_2 = D_1' \\
\text{plate 2} & -A_1'\ell_1 + B_2'\ell_2 - C_3'\ell_3 = D_2' \\
 & \vdots \\
\text{top plate} & -A_{N-1}'\ell_{N-1} + B_N'\ell_N - C_{N+1}'\ell_{N+1} = D_N' \\
\text{condenser} & -A_N'\ell_N + B_{N+1}'\ell_{N+1} = D_{N+1}'
\end{array} \tag{19e}$$

The equations can be solved by a procedure suggested by Grabbe (13), detailed below:

$$h_0 = C_1'/B_0' \tag{20}$$

$$g_0 = D_0'/B_0' \tag{21}$$

for the reboiler and,

$$h_k = C_{k+1}'/(B_k' - A_{k-1}'h_{k-1}) \tag{22}$$

$$g_k = (D_k' - A_{k-1}'g_{k-1})/(B_k' - A_{k-1}'h_{k-1}) \tag{23}$$

for each tray and condenser where $K = 1, 2, 3, \ldots, N+1$.

The liquid flow rate of any component in the condenser is defined as

$$\ell_{N+1} = g_{N+1} \tag{24}$$

and on each tray and reboiler as

$$\ell_k = g_k - h_k\ell_{k+1} \tag{25}$$

where $k = N, N-1, N-2, \ldots, 0$.

Sujata (22) used the foregoing development to satisfactorily predict absorber performance. When the tridiagonal matrix has been solved for each of the components, the component liquid rates leaving each tray are known. If the sum of the computed component rates differs significantly from the assumed total rates, the initial rate assumptions are corrected and the material balance calculations repeated. When the component rates agree with the assumed total interstage flow, the computational scheme progresses to an energy balance of the system. Heat balances are used to determine a temperature profile which satisfies all the stage energy and mass balances. These steps are repeated until the converged values are attained.

Friday and Smith (12) outlined priorities in formulating suitable computational techniques for obtaining converged solutions. They recommended a procedure similar to the above for handling absorbers with intermediate and wide boiling range feeds.

The alternate Bubble Point Relaxation technique may be used to describe separation processes. The material balance Equation (16) for any non-feed stage may be modified by incorporating the following relationships:

$$v_1 = V_1 y_1 \tag{26}$$

and

$$\ell_1 = L_1 X_1 . \tag{27}$$

The material balance equation can then be written in terms of the component liquid compositions,

$$-V_{i-1}\ K_{i-1}\ X_{i-1} + (L_i + K_i V_i)X_i - L_{i+1}\ X_{i+1} = 0. \qquad (28)$$

For a feed tray, the left-hand side of Equation (28) is equated to the molar feed rate to that plate. For a complete description of any one component throughout the column, a tri-diagonal matrix is evolved. The coefficients of the matrix are defined by the following relationships:

$$A'_{i-1} = V_{i-1}\ K_{i-1} \qquad (29a)$$

$$B'_i = L_i + K_i V_i \qquad (29b)$$

$$C'_{i+1} = L_{i+1} \qquad (29c)$$

$$D'_i = F_i X_f \qquad (29d)$$

When the set of equations for any one component is written, the matrix assumes the following form:

$$\begin{array}{lll}
\text{reboiler} & B'_0\ X_0 - C'_0\ X_1 & = D'_0 \\
\text{plate 1} & -A'_0\ X_0 + B'_1\ X'_1 - C'_2\ X_2 & = D'_1 \\
\text{Plate 2} & -A'_1\ X_1 + B'_2\ X_2 - C'_3\ X_3 & = D'_2 \\
 & \vdots & \qquad (29e) \\
\text{top plate} & -A_{N-1}\ X_{N-1} + B'_N\ X_N - C'_{N+1}\ X_{N+1} & = D'_N \\
\text{condenser} & -A'_N\ X_N + B'_{N+1}\ X_{N+1} & = D'_{N+1}
\end{array}$$

When the matrix has been solved for each component, the liquid compositions are known. The dependence of the composition on any one tray to the composition on all the trays is readily apparent. The liquid compositions found from this technique will not sum to one on each stage until convergence is achieved. Therefore, a normalized composition profile can be used for the next iteration.

Wang and Henke (26) solved the component material balance equations by this method. Where previous techniques utilized Newton-Raphson techniques to predict the temperatures, Wang employed Muller's (26) method to determine the bubble point temperatures at each stage. A claimed advantage in the use of the Muller's technique is its greater likelihood of success in achieving the converged temperature profile. The technique measures the deviations, S_j', in the bubble point relationship,

$$S_j' = \Sigma K_j X_j - 1.0, \qquad (30)$$

to correct the temperature profile. This procedure is similar in scope to the false position method.

The method reported by Burningham and Otto (6) employs the same tri-diagonal material balance relationships to predict the tray and product compositions. Bubble point calculations are used to obtain better estimates of the stage temperatures and energy balances are used to correct the liquid and vapor flow rates. Burningham employed forcing techniques to control extreme fluctuations in the bubble point temperatures. A temperature weighting factor of 0.25 was used in the following manner:

$$t_{i+1} = t_i + 0.25(t_{BP} - t_i). \tag{31}$$

Tomich (25) uses similar material and heat balances in the evaluation of equilibrium stage operations. The material balance equations are reduced to a tri-diagonal matrix form. A vapor and temperature profile is assumed. From an over-all material balance the liquid profile is calculated. Compositions for each component on each plate are computed and the vapor compositions are calculated by vapor-liquid equilibria ratios. A new vapor and temperature profile is calculated by application of Broyden's (25) technique, an improved Newton-Raphson iteration method. This method employs the errors in tray material and heat summations for the i^{th} iteration in a Taylor series expansion to evaluate the changes in the vapor and temperature, where

$$V_j^{i+1} = V_j^i + t_i \, \Delta V_j \tag{32}$$

$$T_j^{i+1} = T_j^i + t_i \, \Delta T_j . \tag{33}$$

A search is made for t_i, whose values range between -1 and 1. No mention is made for the method of searching for this convergence accelerator but Tomich implies that each iteration will have its own unique value. The t_i's are chosen so that errors in the summations decrease with each succeeding iteration.

Tomich's method guarantees numerical stability in the use of the Broyden technique and emphasizes reduced computer time since only one matrix inversion per problem solution is encountered.

Rose (19, 20) described the transient behavior of a plate in a column by writing the following equation:

$$-R\frac{dX_n}{d\theta} = -L_{n+1}\ X_{n+1} - V_{n-1}\ y_{n-1} + L_n\ X_n + V_n\ y_n + P_n\ X_n - F_n\ X_f. \qquad (34)$$

If negligible vapor holdup and constant liquid holdup is assumed to exist, then Equation (34) describes the change in composition of a given component on plate n over a given time interval, $\Delta\theta$.

Once all the flow rates and compositions for a given time θ, are known, then the evaluation of all the concentration derivatives is possible. Using these derivative values, Rose (19) presented the following modification of Equation (34) to predict all of the column concentrations, after an interval of time, $\Delta\theta$:

$$X_n\big|_{\theta+\Delta\theta} = X_n\big|_{\theta} + \Delta\theta\left(\frac{dX_n}{d\theta}\Big|_{\theta}\right). \qquad (35)$$

Although the combination of the latter two equations gives reliable solutions for complicated problems, the equations in this form are inherently unsatisfactory, requiring extremely small values of the time increment $\Delta\theta$, yielding a large amount of machine time. In effort to facilitate a shorter convergence time, Ball (1) proposed a modification Equation (35),

$$X_n \big|_{\theta+\Delta\theta} = X_n \big|_{\theta} + \Delta\theta\left[\beta\left(\frac{dX_n}{d\theta}\Big|_{\theta+\Delta\theta}\right) + (1-\beta)\left(\frac{dX_n}{d\theta}\Big|_{\theta}\right)\right] \qquad (36)$$

where $0 \leq \beta \leq 1$.

The significance of β in Equation (36) may be discerned from inspection of Figure 3. If β is equated to zero, the slope of line A is used to predict the value of the tray composition at time $\theta + \Delta\theta$. For a value of $\beta =$ 1.0, a stabler but slower computational scheme is employed to describe the tray compositions for the next iteration. If $\beta > 1/2$, any value of $\Delta\theta$ may be used and the equations will remain stable. No significant variations are achieved for any of these values above $1/2$, so a $\beta = 1.0$ was used. This value of β does simplify the equations.

For $\beta = 1$, Equation (36) becomes

$$X_n \big|_{\theta+\Delta\theta} = X_n \big|_{\theta} + \Delta\,\theta\,\beta\left(\frac{dX_n}{d\theta}\Big|_{\theta+\Delta\theta}\right) \qquad (37)$$

and introducing this into Equation (34) yields the following convenient relationship,

$$-\frac{\Delta\theta}{R}\Big[-V_{n-1}y_{n-1} + V_n y_n + L_n X_n - L_{n+1}X_{n+1} + P_n X_n - F_n X_f\Big]_{\theta+\Delta\theta} + X_n\big|_{\theta} = X_n\big|_{\theta+\Delta\theta}. \qquad (38)$$

The assumption of negligible changes in the equilibrium constants, temperatures and liquid vapor profiles

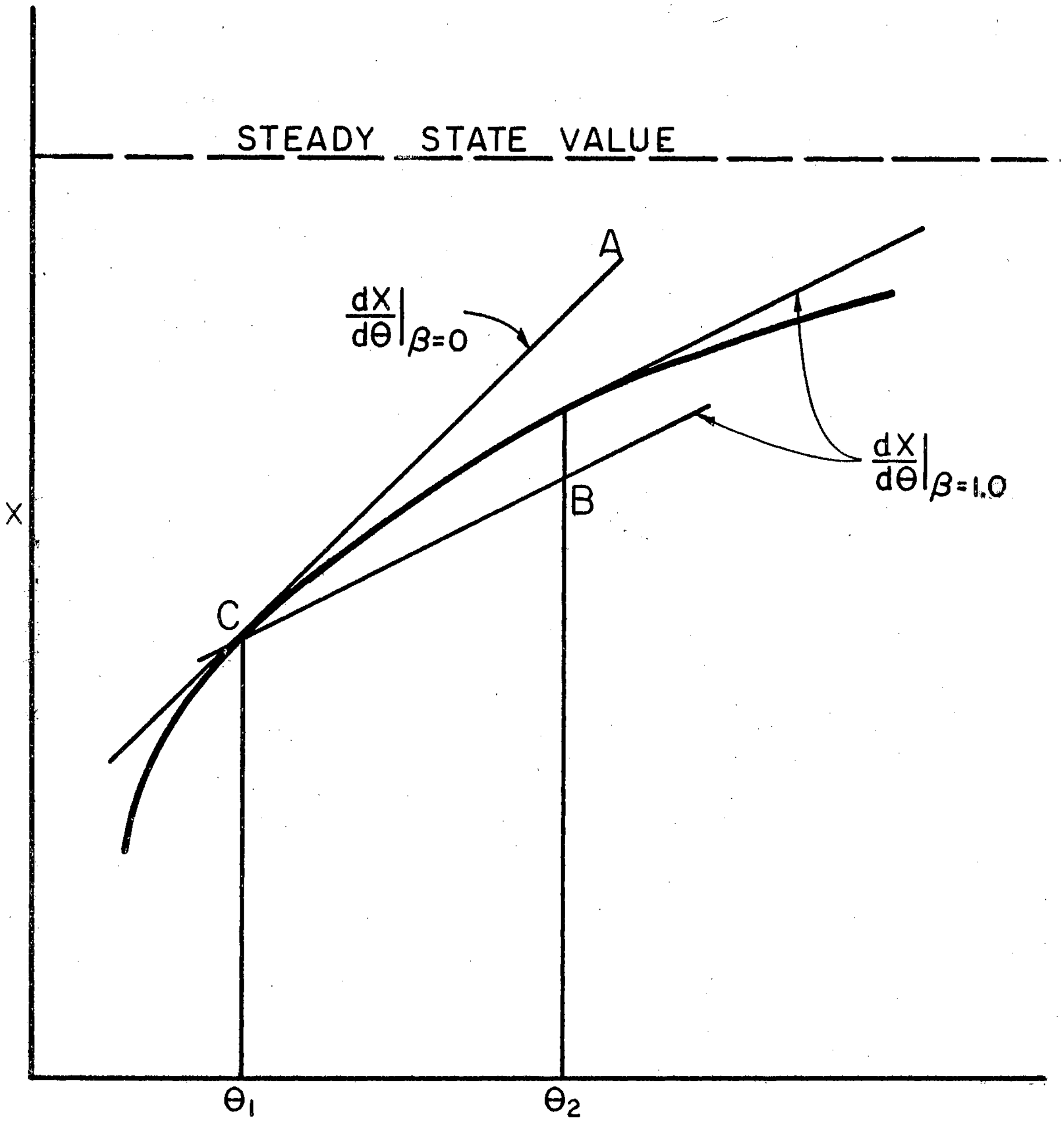

Figure 3. The Effect of β on the Slope Used in the Calculations

over the time interval, $\Delta\theta$, is made. This is a valid assumption after the first few iterations. When Equations (36) through (38) are assembled into a solution form, a tri-diagonal matrix results. This tri-diagonal matrix is nearly identical to matrix (29e). Different matrix coefficients are employed and these are presented in the succeeding chapter.

Heat balances are used to adjust the interstage traffics with the liquid rate on plate N+1 calculated directly from this over-all balance. The vapor rate from plate N is predicted by an over-all material balance.

The procedure with new interstage flows and compositions is repeated until the convergence criteria are met.

While sundry and diverse calculation methods have been formulated for separation operations, the procedures presented here are those most pertinent to this study. Procedures not wholly applicable to solving absorber and reboiled absorber problems were not discussed.

CHAPTER III

PROPOSED METHOD

The major factors involved in the formulation of a solution method include the selection of a rigorous set of equations, grouped together either by type or by stage, which is able to handle complex systems thereby including the possibility of solving columns with multi-feeds, side stream draws and side stream strippers. A system of equations which cannot handle complex column features has limited practical use.

The type of equations used in determining liquid compositions must be chosen with care, since computer solutions are susceptible to a wide variety of problems. Numerous ill-defined solution techniques experience round-off errors, instabilities in convergence techniques and, occasionally, extremely long computer solution times. In addition, an adequate method of predicting new stage temperatures, vapor and liquid interstage traffics must be incorporated in the computational scheme. Many other procedures exhibit grave deficiencies when trace component systems are being considered. These difficulties are not encountered when the proposed method is employed to describe separation process units.

The proposed method, the Ball-Rose algorithm is a satisfactory technique that is currently used to predict distillation performance and should be able to handle reboiled-absorbers. The method describes a column from start-up to steady-state. The procedure is initiated with assumed tray compositions, temperatures, and liquid vapor profiles. The tri-diagonal matrix is solved for new liquid compositions. Interstage temperatures are determined by bubble point calculations. Heat balances are made about each plate and the top of the column; these yield the revised vapor and liquid rates.

The assumptions inherent in the development of the method are few, indicating a wide range of applicability. Each tray is assumed to be an equilibrium tray, and vapor-liquid equilibria constants are assumed to be in the form $K = {}^{y}/X$. Constant column pressure is not required. Average column vapor and liquid rates and effective absorption factors are not assumed nor utilized in this method.

A) Material Balance

Using the equations presented earlier, the Ball-Rose material balance relationships may be further modified into a form applicable for machine computation. The use of the tri-diagonal matrix for predicting tray compositions and product rates is developed below. Upon suitable rearrangement, Equation (38) may be written for any component on any tray in the following form:

$$-A'_{i-1}X_{i-1} + B'_i X_i - C'_{i+1}X_{i+1} = D'_i \tag{39}$$

where,

$$A'_{i-1} = \frac{\Delta\theta}{R}(V_{i-1}\ K_{i-1}) \tag{39a}$$

$$B'_i = \frac{\Delta\theta}{R}(L_i + V_i\ K_i + P_i) + 1.0 \tag{39b}$$

$$C'_{i+1} = \frac{\Delta\theta}{R}(L_{i+1}) \tag{39c}$$

$$D'_i = X_i + \frac{\Delta\theta}{R}(F\ X_f). \tag{39d}$$

The ratio of the time interval to the tray holdup may be given any arbitrary value to achieve rapid convergence. For low values of the ratio, the predicted tray compositions depend strongly on the previously calculated composition profile. Larger values of the ratio tend to force the matrix into a conventional type of material balance relationship.

This algorithm allows compositions to go to zero and extensive coding is not required in any machine program to handle zero or negative compositions.

B) External Material Balance

During the course of the solution the calculated product compositions may not satisfy an over-all component material balance nor the predicted product rates. To keep the tower in external material balance and to decrease the number of iterations required to obtain a converged solution, a forcing procedure based on Holland's theta method

(14) and later modified by Burman (5) is employed in the computational scheme.

An over-all material balance about the entire column suggests

$$\sum_{j=1}^{np} P_j = \sum_{k=1}^{nf} F_k \tag{40}$$

$$\sum_{j=1}^{np} \sum_{i=1}^{ncp} p_{ij} = \sum_{k=1}^{nf} \sum_{n=1}^{ncp} f_{nk} \tag{41}$$

For a column with no sidestreams,

$$f_n = \Sigma p_i = b_i + d_i \, . \tag{42}$$

Equation (41) may be rearranged to an equivalent representation in terms of the individual product rate, p_i:

$$p_i = \frac{\Sigma f_k - (p_{i-1} + p_{i-2} + \ldots + p_1)}{1 + \frac{\Sigma p'_{i+1}}{p_i}} \tag{43}$$

where $\Sigma p'_{i+1}$ is the sum of the individual product rates indexed from the $(i+1)^{th}$ product to p_{ncp}.

The total product rate is the sum of the individual rates

$$P_j = \sum_{j=1}^{ncp} p_j \, . \tag{44}$$

If the total moles of each of the components are not equal to the calculated total moles of product; i.e., if $\Sigma\, p_j \neq P_{j\,(ca)}$, then an arbitrary multiplier θ_i, can be found such that

$$P_{i\,(ca)} = \sum \frac{\Sigma\, f_k - (p_{i-1} + p_{i-2} + \dots + p_1)}{1 + \left(\frac{\Sigma\, p_{i+1}}{p_i}\right)\theta_i}. \qquad (45)$$

This value of θ_i, can be determined by Newton's method. After θ_i is found, the p_i are known and the component material balance can be modified as follows:

$$p_{i+1} + p_{i+2} + \dots + p_n = \Sigma\, f_k - (p_i + p_{i-1} + \dots + p_1) \qquad (46)$$

permitting the evaluation of p_{i+1},

$$p_{i+1} = \frac{\Sigma\, f_k - (p_i + p_{i-1} + \dots + p_1}{1 + \theta_{i+1}\left(\frac{\Sigma\, p_{i+2}}{p_{i+1}}\right)} \qquad (47)$$

In columns with sidestream strippers, the material balance can be rearranged to include the vapor return stream from the stripper.

C) Temperature Adjustment

The temperature adjustment is made by bubble-point calculations on each plate. The equation describing the bubble-point equilibrium separation is

$$\varphi_T = \sum \frac{Z_f(1 - K_i)}{(1 - K_i) + K_i}. \qquad (48)$$

The temperature that reduces the above expression to zero is defined as the bubble-point temperature. A trial and error iterative calculation technique can be employed to converge to the desired temperature. The temperature for the $(i+1)^{th}$ iteration is calculated by a false-position technique,

$$T^{i+1} = T^{i} - \frac{(T^{i-1} - T^{i})}{(\varphi_T^{i-1} - \varphi_T^{i})} \varphi_T^{i}. \qquad (49)$$

As each plate temperature is found, the equilibrium relationship between the liquid and vapor compositions is calculated for each component.

D) Heat Balance

After the new temperature profile has been found, heat balance calculations are used to determine the inter-stage traffic on each plate. An over-all heat balance about the top of the column and any tray is

$$H_n^V V_n - H_{n+1}^L L_{n+1} = Q_C + \Sigma\, H^P P_j + Q_k + \Sigma\, H^F F_i . \qquad (50)$$

Where no feeds, intercoolers or products are found between the condenser and tray n, the right-hand side of Equation (50) remains constant. In any case, let $\overline{C}_1$ be denoted as follows:

$$H_n^V V_n - H_{n+1}^L L_{n+1} = \overline{C}_1 \qquad (51)$$

The liquid enthalpy is the sum of the product of the partial liquid enthalpies and the liquid composition,

$$H^L = \Sigma \bar{H}^L X \tag{52}$$

and

$$H^L_{s+1} L_{s+1} = L_{s+1} \Sigma \bar{H}^L_{s+1} X_{s+1} . \tag{53}$$

Similar relationships exist for the vapor enthalpies; however, they can be further modified, thus

$$H^V_s V_s = \Sigma \bar{H}^V_s v_n = \Sigma \bar{H}^V_s(\ell_{s+1} - \Sigma p_s + \Sigma f_s) . \tag{54}$$

Letting $\bar{C}_2 = (\Sigma p_s - \Sigma f_s)$, Equation (51) becomes upon the substitution of the vapor and liquid enthalpy terms,

$$\Sigma \bar{H}^V_n \ell_{s+1} - \Sigma \bar{H}^V_s \bar{C}_2 - L_{s+1} \Sigma \bar{H}^L_{s+1} X_{s+1} = \bar{C}_1 . \tag{55}$$

Noting that

$$\Sigma \bar{H}^V_n \ell_{s+1} = L_{s+1} \Sigma \bar{H}^V_s X_{s+1} \tag{56}$$

and substituting (56) into (55) permits the direct evaluation of the liquid flow, as follows:

$$L_{s+1} = \frac{(\bar{C}_1 + \Sigma \bar{H}^V_s \bar{C}_2)}{(\Sigma \bar{H}^V_s X_{s+1} - \Sigma \bar{H}^L_{s+1} X_{s+1})} \tag{57}$$

The vapor rate can then be predicted by an over-all material balance.

E) Description of the Program Operation

The specifications required in the computer program employed in this study are similar to that of those employed by most other programs predicting fractionator performance. They are:

1) Feed compositions, rates, conditions, and locations
2) Distillate rate and condition
3) Number of theoretical trays
4) Location and rates of all sidestreams
5) Location and rates of heat removal of all interstage coolers
6) Number of sidestream strippers and number of trays in each
7) Draw trays and vapor return trays and distillate rates in all sidestream strippers
8) Constants for equilibrium and enthalpy equations
9) Top tray vapor rate
10) Various tolerances employed in the course of the calculations.

The input and preliminary sections of the computer program performs the specified calculations of the feeds and prints the results as well as the input data.

The feed condition can be specified as a bubble or a dew point solution and provisions are also embodied in the program to compute feed flash calculations where either the temperature or the liquid to feed ratio are the unknown factors.

The array setup section makes the preliminary assumptions of the composition, liquid, vapor and temperature profiles, the product distributions and readies the program for the final solution phase. Constant molal overflow is assumed to calculate an initial liquid-vapor profile, using the specified top tray vapor rate, feed rates and all side draw rates if any appear in the column. The product distributions are calculated by assuming a perfect split of the components based on the specified product rates. An initial composition profile used to initiate the start of the formal computational phase of the program, is calculated by assuming a linear profile from the distillate to the feed or feeds and from the feeds to the bottoms. A bubble point calculation on the assumed liquid composition profile is employed to calculate the initial temperature profile.

The next phase of the program operation performs the tray-by-tray calculations consisting of material and heat balance calculations, terminal stream adjustments, and determination of new temperature profiles. The material balance calculations are repeated until the largest change in composition for any component falls within the tolerance specified by the design engineer. Heat balances are then performed to adjust the liquid and vapor rates. When the complete composition, temperature and vapor profiles have converged to within the limits of the tolerances, the problem is considered solved and all the calculated variables are printed.

The program's format leaves no flexibility in eliminating the reboiler and condenser calculations. It would be far simpler to write a newer, more general program than to incorporate such coding as to solve the simple absorber system.

CHAPTER IV

EVALUATION PROCEDURE

The primary objective of this thesis is an evaluation of the Ball-Rose calculational method as a tool for predicting the performance of absorption equipment. This investigation attempts to: (a) present a general computational procedure that is capable of fully describing a reboiled absorber, (b) determine any limitations in the method and report any failings in the procedure, and to (c) provide a guide to be used in choosing a suitable convergence accelerator.

Column Test Data

In the evaluation of the Ball-Rose calculation method, five columns were used as test data. A brief description of each of these columns appears below. The feed compositions and operating condition for each of these columns are tabulated in Tables VII through XI, respectively. The coefficients of the equilibrium and enthalpy equations are given in Appendix A.

Column A

This column is a simple absorber with nine components and five equilibrium stages. The data for the column were reported by Ravicz (18). The original data were from an industrial absorption column operated by the Phillips Petroleum Company. The column contained 20 bubble cap trays and was operated at 232 psia. The absorber oil was a mineral seal oil fraction having a molecular weight of 223.

Column B

This column is a low temperature de-methanizer, operated at 350 psia and strips methane from a gas feed. The feed consists of six components and is about 91% methane and ethane. Both the data and operating conditions for this sixteen equilibrium tray column were furnished by Erbar (11).

Column C

This column is a reboiled absorber with nine components and fourteen equilibrium stages. The data were supplied from a thirty-five tray industrial column designed by the Chevron Research Corporation. The column operates at a pressure of 234 psia. The absorber oil whose molecular weight is 135 appears in both feeds.

Column D

This column is a typical reboiled absorber containing sixteen equilibrium stages and fifteen components. The data source for this column was Burningham (6). The column pressure is 270 psia. The absorber oil is broken into five hypothetical components. These five fractions are characterized by molecular weights of 89.6, 103.6, 127, 145, and 166, respectively.

Column E

This column is a reboiled absorber with twelve equilibrium stages and fifteen components. The column pressure is 75 psia. The data and operating conditions for this problem are from Edmister (9). The absorber oil was broken into five hypothetical components. These fractions were assumed to have molecular weights of 170, 175, 180, 185, and 200.

CHAPTER V

RESULTS AND DISCUSSION OF RESULTS

The evaluation of the Ball-Rose method is based on how well the technique predicts the component product rates, the interstage flows and the temperature profile through the column. The crucial term determining the number of iterations required to achieve the finally converged solution is the ratio of the time interval to the tray holdup, $\frac{\Delta\theta}{R}$. To explicitly identify the role this factor plays in the computational scheme, a simple separation problem was assumed. Material balance calculations for one iteration with three different values of $\frac{\Delta\theta}{R}$ were performed by hand. Stage temperatures were determined by bubble point calculations. The assumed initial liquid tray compositions, interstage flows, stage temperatures, and equilibrium data are tabulated in Tables I, II, and III.

Tables IV and V illustrate the variation in the liquid tray compositions and stage temperatures calculated for each of the three values of $\frac{\Delta\theta}{R}$. As a general rule, the larger the values of the ratio of the time interval to the tray holdup the more pronounced are the fluctuations in the temperatures and tray compositions. For the

TABLE I

COMPOSITIONS OF FEED AND ASSUMED PRODUCT SPLITS FOR ILLUSTRATIVE PROBLEM

Component	Feed moles/hr	Distillate moles/hr	Bottoms moles/hr
1	10.0	10.0	0.0
2	40.0	30.0	10.0
3	50.0	15.0	35.0

Operating Conditions:

Number of stages including reboiler	5
Feed tray number	2
Feed condition	Vapor

TABLE II

EQUILIBRIUM VALUE DATA FOR ILLUSTRATIVE PROBLEM

$\ln K = C_1 + C_2/T + C_3/T^2$; T (°R)

Component	C_1	C_2	C_3
1	-38.1029	525.805	-1618.29
2	-2.4391	55.1486	-248.265
3	-3.0507	64.297	-309.317

TABLE III

INITIAL PROFILES FOR ILLUSTRATIVE PROBLEM

	X_1	X_2	X_3	L moles/hr	V moles/hr	T (°F)
Condenser	0.182	0.545	0.273	55.0	0	25.97
Plate 3	0.010	0.667	0.323	95.0	150.0	91.70
Plate 2	0.010	0.520	0.470	95.0	150.0	94.82
Plate 1	0.010	0.373	0.617	95.0	50.0	98.04
Reboiler	0.001	0.222	0.777	45.0	50.0	232.81

demonstration problem, both the smallest composition and temperature changes were calculated at a value of $\frac{\Delta\theta}{R}$ equal to 10^{-4}. At this lower value, the solution to the material balance relationships depended very heavily on the initial tray compsitions. At the larger values of the ratio, the equations settled into straight material balance equations, where the component liquid and vapor rates were the dominant terms in the coefficient matrix.

At the values of $\frac{\Delta\theta}{R} = 1.0$ and 10^{+4}, the tray compositions changed more rapidly. The variation in the temperature profile suggests that the drastic increments calculated from pass-to-pass would tend to hinder the attainment of a converged solution at an early stage.

For these latter two values of the time increment over the tray holdup, the system was apparently computed at a condition above some critical value of the ratio, $\frac{\Delta\theta}{R}$. The critical value may be defined as that terminal value of the ratio above which an excessive amount of machine time is required to converge to the correct solution. The critical value is a discrete value for each particular problem and is dependent on various factors; e.g., initial profiles, problem specifications and types of column configurations. At a value of $\frac{\Delta\theta}{R}$ just above the critical value, there is an abrupt change in the time required to obtain a solution.

Burman (5) reported a study of the effect of the $\frac{\Delta\theta}{R}$ term on a four component, thirty-eight tray distillation

TABLE IV

LIQUID COMPOSITIONS AFTER ONE ITERATION FOR ILLUSTRATIVE PROBLEM

Stages	Component Identification	Liquid Compositions for $\Delta\theta/R$ Equal to		
		10^{-4}	1	10^{4}
Condenser	X_1	0.18655	0.32491	0.23437
	X_2	0.54294	0.36058	0.40775
	X_3	0.27050	0.31450	0.35787
Plate 3	X_1	0.00904	0.00278	0.00271
	X_2	0.66309	0.30069	0.29491
	X_3	0.32786	0.69651	0.70237
Plate 2	X_1	0.00738	0.00111	0.00111
	X_2	0.51474	0.33232	0.31774
	X_3	0.47787	0.66655	0.68113
Plate 1	X_1	0.00783	0.00003	0.00001
	X_2	0.37114	0.32828	0.19059
	X_3	0.62102	0.67168	0.80939
Reboiler	X_1	0.00082	0.0000	0.00000
	X_2	0.22308	0.26744	0.15114
	X_3	0.77608	0.73225	0.84885

TABLE V

STAGE TEMPERATURES AFTER ONE ITERATION FOR ILLUSTRATIVE PROBLEM

Stages	Temperature Identification (°F)	Temperatures and Changes in Temperatures for $\Delta\theta/R$ Equal to		
		10^{-4}	1	10^{4}
Condenser	T	25.59	17.62	22.36
	ΔT	0.38	8.35	3.61
Plate 3	T	95.31	180.46	182.81
	ΔT	3.61	88.76	91.11
Plate 2	T	107.03	213.28	215.23
	ΔT	12.21	118.46	120.41
Plate 1	T	108.79	230.85	250.78
	ΔT	10.75	132.81	152.74
Reboiler	T	235.16	239.84	257.42
	ΔT	2.35	6.03	24.61

column. At values greater than 10 the same number of passes were required regardless of the size of the ratio. With respect to this study, the critical values for $\frac{\Delta\theta}{R}$ were found to be about unity for two different reboiled absorbers and one de-methanizer.

A guide to predetermining the critical value of the ratio prior to the start of the calculations is presented with respect to the cube root of the product of the ratios of the most and least volatile components in the distillate, feed and bottoms. A plot of the logarithm of $\frac{\Delta\theta}{R}$ as a function of the logarithm of the relative volatilities is presented in Figure 4. This plot defines the regions for which the ratio of time increment to the tray holdup are greater than the critical values. At values greater than these no solutions were obtained. However, the steady-state values could probably be determined for these values of $\frac{\Delta\theta}{R}$ provided unlimited computer time is available to the investigator.

A comparison of the results obtained by the Ball-Rose technique was made with results obtained from those with other procedures. The results of the machine calculations compared very favorably with the results obtained by these other methods. Five columns were studied and solutions to two reboiled absorbers and one de-methanizer were calculated. The results for all five problems are tabulated in Tables VII through XI. The equilibrium and enthalpy data coefficients are presented in Appendix A. Vapor and

TABLE VI

CRITICAL VALUES FOR $\frac{\Delta\theta}{R}$

Problem	$\Delta\theta/R$	$[\alpha_T\alpha_f\alpha_B]^{1/3}$
Burman (5)	10	2.06
Column B	1.0	2.0×10^4
Column C	3.0	8.5×10^3
Column D	3.0	3.7×10^5

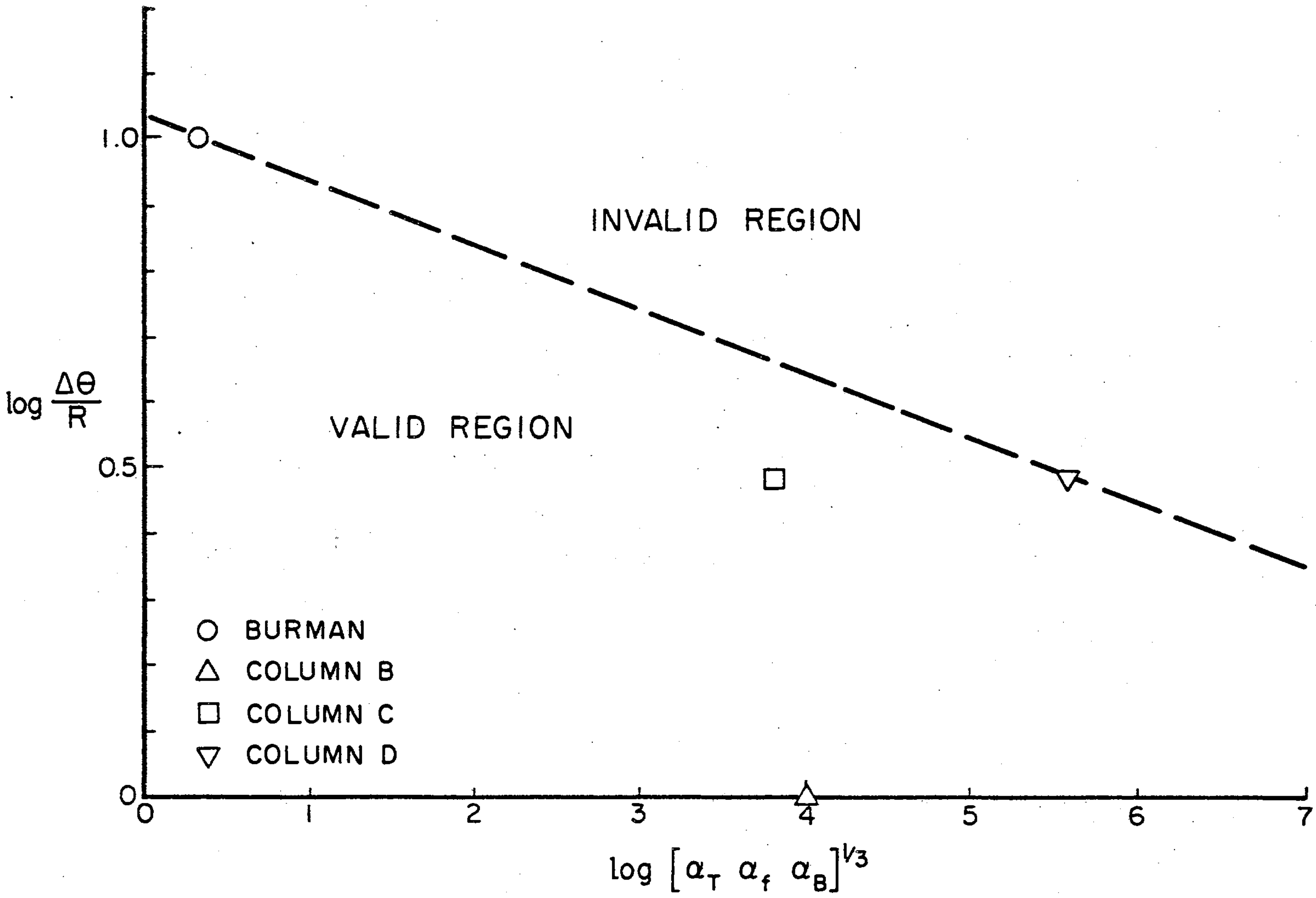

Figure 4. Critical Time Intervals Over the Tray Holdup

temperature profiles appear in Appendix B.

A solution for the simple absorber, Column A, was never strictly achieved. Limitations in the program's calculational procedure denied a reasonable solution. The reboiler and condenser calculations could not be conveniently eliminated from the computational sequence, consequently these two stages entered into the calculational procedure and both elements played a significant role in the heat balance calculations. The results from Table VII strongly indicate that with the elimination of the reboiler and condenser calculation in the computational scheme, the method would then be able to fully describe the simple absorber system.

The Ball-Rose relaxation method is also applicable in solving simple de-methanizer and de-ethanizer columns operating in the cryogenic regions. The program functions well with this type of tower.

Three reboiled absorbers were included as test cases, two of which converged to the desired solution. The solutions to Columns C and D compared extremely well with existing solutions derived from other computational methods. The trivial differences between the solutions computed by the Ball-Rose method and those obtained by other sources may be explained by differences in the form of the enthalpy and vapor liquid equilibria data equations.

Column E could not be solved. The highly vaporized gas feed condition coupled with stringent lean oil restrictions and a poorly specified distillate rate are believed to be the factors that denied a reasonably converged solution. This problem illustrates that the requirement of an accurate and well defined problem has to be met. If the specifications of the problem are not reasonable, then the predicted profiles will display abrupt discontinuities and a converged solution may never be approached.

Previously, Friday and Smith have reported that absorber calculations can only be satisfactorily solved by a Sum Rates type of procedure. Similarly, Burningham reports that for reboiled absorbers as large as the ones studied in this report, solutions can only be obtained by a bubble-point Thiele-Geddes approach. However, these conclusions are in conflict with the results obtained by this study. Neither Burningham nor Smith used a damping factor in the sense of the time increment over the tray holdup employed by the Ball-Rose technique. Hence, their conclusions are not necessarily valid.

TABLE VII

COMPARISON OF RESULTS FOR COLUMN A

Component	Feed I moles/hr	Feed II moles/hr	Distillate moles/hr. Ref. No. (23)	Relaxation
Nitrogen	0.000	210.456	209.729	210.193
Methane	0.000	985.455	972.510	969.294
Ethane	0.000	88.829	81.802	77.012
Propane	0.000	51.248	37.850	36.333
I-Butane	0.000	6.148	2.479	3.370
N-Butane	0.023	14.213	3.303	6.665
Pentane	0.513	6.423	0.091	2.608
Heptane	0.178	3.826	0.0	0.025
Lean Oil	203.687	0.000	0.0	0.0

Operating Conditions:

Number of stages including reboiler	7
Feed I tray number	5
Feed condition	Liquid
Feed II tray number	1
Feed condition	Vapor
Pressure	232 Psia
Distillate rate	1305.5

TABLE VIII

RESULTS FOR COLUMN B

Component	Feed moles/hr	Distillate moles/hr
Methane	720.280	711.507
Ethane	108.050	8.975
Propane	43.190	0.000
I-Butane	15.460	0.000
N-Butane	9.180	0.000
Hexane	15.800	0.000

Operating Conditions:

Number of stages including reboiler	17
Feed tray number	8
Feed condition	Vapor/Liquid
Pressure	350 Psia
Distillate rate	720.5 moles/hr
Reboiler duty	0.002 MMBTU

TABLE IX

COMPARISON OF RESULTS FOR COLUMN C

Components	Feed I moles/hr	Feed II moles/hr	Distillate moles/hr. Ref. No. (9)	Distillate moles/hr. Relaxation
Methane	0.000	46.200	46.1	46.196
Ethane	0.000	41.580	28.3	26.264
Propane	0.000	65.940	8.2	10.024
I-Butane	0.000	13.020	-	0.069
N-Butane	0.000	49.140	-	0.034
I-Pentane	0.000	10.920	-	0.000
N-Pentane	0.000	20.580	-	0.000
Hexane	0.000	24.360	-	0.000
Lean Oil	40.000	148.260	0.1	0.075

Operating Conditions:

Number of stages including reboiler	15
Feed I tray number	15
Feed condition	Sub-cooled liquid
Feed II tray number	7
Feed condition	Vapor/Liquid
Pressure	215-220 Psia
Distillate Rate	82.7 moles/hr
Reboiler Duty	3.132 MMBTU

TABLE X

COMPARISON OF RESULTS FOR COLUMN D

Components	Feed I moles/hr	Feed II moles/hr	Distillate moles/hr Ref. No. (6)	Distillate moles/hr Relaxation
Nitrogen	0.00	0.70	0.700	0.700
Carbondioxide	0.00	12.40	12.398	12.370
Methane	0.00	167.40	167.400	167.400
Ethane	0.00	474.50	452.263	439.219
Propane	0.00	440.20	43.815	56.292
I-Butane	0.00	64.30	0.229	0.416
N-Butane	0.00	128.80	0.095	0.185
I-Pentane	0.00	19.50	0.000	0.000
N-Pentane	0.00	19.40	0.000	0.000
N-Hexane	0.00	13.10	0.000	0.000
Hypth Cpnt 1	0.50	9.00	0.007	0.008
Hypth Cpnt 2	2.10	5.30	0.008	0.010
Hypth Cpnt 3	95.30	128.30	0.100	0.125
Hypth Cpnt 4	149.30	203.30	0.050	0.061
Hypth Cpnt 5	18.20	24.70	0.002	0.003

Operating Conditions:

Number of stages including reboiler	16
Feed I tray number	16
Feed condition	Vapor/Liquid
Feed II tray number	10
Feed condition	Sub-cooled liquid
Pressure	270.0 Psia
Distillate Rate	677 moles/hr.
Reboiler duty	11.27 MMBTU

TABLE XI

RESULTS OF COLUMN E AFTER 175 PASSES

Components	Feed I moles/hr	Feed II moles/hr	Distillate moles/hr Relaxation
Hydrogen	0.000	145.000	144.020
Methane	0.000	114.200	112.138
Ethylene	0.000	9.300	8.944
Ethane	0.000	31.700	30.159
Propylene	0.000	2.640	2.360
Propane	0.000	0.886	0.786
Butene-1 + I-Butene	0.000	30.200	16.973
Trans 2-Butene	0.000	5.140	1.912
Cis 2-Butene	0.000	1.7150	0.491
I-Butane	0.000	1.242	0.818
N-Butane	0.000	2.380	0.939
Hypth Cpnt 1	15.500	0.000	0.046
Hypth Cpnt 2	31.100	0.000	0.017
Hypth Cpnt 3	69.000	0.000	0.046
Hypth Cpnt 4	86.300	0.000	0.004
Hypth Cpnt 5	143.100	0.000	0.231

Operating Conditions:

Number of stages including reboiler	12
Feed I tray number	12
Feed Condition	Liquid
Feed II tray number	4
Feed condition	Vapor
Pressure	75 Psia
Assumed Distillate Rate	319.883
Reboiler Duty	6.597 MMBTU

CHAPTER VI

CONCLUSIONS

A critical evaluation of a rigorous relaxation procedure for tray and product compositions for absorber systems was made. A computer program written for the IBM 7040 was utilized to determine the versatility of the Ball-Rose relaxation technique.

Several problems were solved in order to determine the range of applicability of the method. Tray compositions, product distributions, liquid vapor interstage flows and bubble-point temperatures were the variable predicted by this method. The material balance data were used as a basis for determining the reliability of the Ball-Rose technique.

Significant effects are produced in the material balance calculations by varying the time increment to the tray holdup. In this procedure, the $\frac{\Delta\theta}{R}$ ratio serves as a damping function to control excessive temperature variations from pass-to-pass. The implementation of such a variable in the computational scheme eliminates arbitrary temperature forcing procedures such as the one proposed by Burningham.

The results indicate that the Ball-Rose technique is applicable in determining the solution to various absorber columns including the simple absorber system. In order to fully describe a simple absorber, the present program requires modifications in the calculation procedure to eliminate the reboiler and condenser calculations. For these systems, extremely low values of the time increment over the tray holdup (on the order of 10^{-5}) are needed to approach the converged solution. The Ball-Rose relaxation technique is ideally suited to solving the reboiled absorber system. To achieve a rapidly converged solution, a suitably chosen $\frac{\Delta\theta}{R}$ slightly less than the critical value is required.

The method as it stands is extremely valuable. Further investigations of absorber performance predictions with a Ball-Rose type of computer program is highly recommended. A great degree of flexibility could be attained if a newer and more general computer program is written. The greatest flexibility could be achieved if provisions are made to vary the liquid vapor and temperature profiles and to eliminate the reboiler and condenser calculations when necessary.

NOMENCLATURE

A - absorption factor defined by $A = \frac{L}{KV}$

A' - constant in material balance equation

B' - constant in material balance equation

b - molar flow rate of any component in the bottoms

C - component designation

C_1, C_2, C_3 - constants in equilibria and enthalpy equations

$\bar{C}_1$ - constant in heat balance equation

$\bar{C}_2$ - constant in heat balance equation

C' - constant in material balance equation

D' - constant in material balance equation

d - molar flow rate of any component in distillate

f - molar flow rate of any component in feed

G - molal oil to gas ratio

g - variable used in solving tri-diagonal matrix

H - enthalpy per mole

$\bar{H}$ - partial enthalpy

h - variable used in solving tri-diagonal matrix

K - vapor liquid equilibrium constant defined by $K = y/X$

L - total molar liquid rate

ℓ - molar liquid rate for any component

M - number of trays in stripping section

N - total number of trays excluding reboiler and condenser

N_1 - degrees of freedom

N_V - total number of variables

n - total number of trays including reboiler and condenser

ncp - number of components

nf - number of feeds

np - number of product streams

P - total molar flow rate of side product

p - molar flow rate of any component in side stream

Q_C - condenser duty

Q_k - intercooler duty

q - vapor liquid equilibrium in terms of partial pressure

R - liquid holdup

S - stripping factor defined by $S = KV/L$

S′ - deviations in bubble point Equation (30)

T - temperature

t_1 - weighting factor

V - total molar vapor rate

v - molar flow rate of any component in a vapor stream

X - mole fraction in liquid

y - mole fraction in vapor

Z_f - fraction of component in feed

Greek Symbols

α - relative volatility

β - coefficient in Ball's Equation (36)

θ - time

θ_i - forcing function used in convergence procedure

$\Sigma\ p'_{i+1}$ - sum of individual product rates from $(i+1)^{th}$ product to p_{ncp}.

φ_A - fraction of entering gas stream not recovered in absorbing section

φ_S - fraction of entering liquid stream not recovered in stripping section

φ_T - variable used in Equation (48)

Subscripts

A - absorber section

B - bottoms

BP - bubble point

ca - calculated variable

f - feed

i, j, k, n - dummy variables

ncp - number of components

S - stripping section

T - distillate

X - exhausting section

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APPENDIX A

EQUILIBRIUM AND ENTHALPY COEFFICIENTS

EQUILIBRIUM AND ENTHALPY COEFFICIENTS

The coefficients for the equilibrium constant equations and for the vapor and liquid state enthalpy equations are tabulated in this section for the five columns studied in this report.

The equilibrium constant equation in the program is of the form

$$\ell n\ K = C_1 + {}^{C_2}/T + {}^{C_3}/T^2.$$

The vapor enthalpy equation is of the form

$$HV = C_1 + C_2 T + C_3 T^2 .$$

The liquid enthalpy equation is of the form

$$HL = C_1 + C_2 T + C_3 T^2 .$$

TABLE XII

COLUMN A: EQUILIBRIUM COEFFICIENTS

Component	C_1	C_2	C_3
Nitrogen	5.738	-9.724	1.371
Methane	1.263	29.221	-154.120
Ethane	2.327	17.823	-197.610
Propane	2.045	19.098	-233.090
I-Butane	1.899	20.856	-271.070
N-Butane	2.315	15.494	-265.440
Pentane	2.396	11.011	-258.860
Heptane	5.028	-26.236	-204.820
Lean Oil	3.803	-21.370	-406.880

TABLE XIII

COLUMN A: ENTHALPY COEFFICIENTS

Component	Liquid			Vapor		
	C_1	C_2	C_3	C_1	C_2	C_3
Nitrogen	5765.170	-1245.600	123.482	3581.830	695.915	68.678
Methane	4977.570	-1600.700	198.055	1321.480	610.440	26.724
Ethane	5765.170	-1245.600	123.482	3581.820	695.915	68.678
Propane	6753.190	-1561.600	219.267	4432.690	1203.550	65.999
I-Butane	8458.710	-2049.300	284.476	7581.410	848.454	137.985
N-Butane	8458.710	-2049.300	284.476	7581.410	848.454	137.985
Pentane	11980.600	-3083.100	414.618	9558.970	1002.160	164.953
Heptane	-11215.000	3508.650	176.880	11955.500	1563.360	206.030
Lean Oil	-18711.000	4457.470	640.320	34528.800	-444.000	765.520

TABLE XIV

COLUMN B: EQUILIBRIUM COEFFICIENTS

Component	C_1	C_2	C_3
Methane	2.946	-2.982	-17.227
Ethane	5.438	-29.568	12.004
Propane	7.918	-54.582	45.547
I-Butane	10.035	-76.200	80.427
N-Butane	10.762	-83.162	88.484
Hexane	14.315	-123.325	149.297

TABLE XV

COLUMN B: ENTHALPY COEFFICIENTS

Component	Liquid C_1	Liquid C_2	Liquid C_3	Vapor C_1	Vapor C_2	Vapor C_3
Methane	-2.933	0.552	0.077	-1.510	1.159	-0.009
Ethane	-8.087	1.428	0.021	-12.423	5.742	-0.484
Propane	-7.988	0.265	0.209	-20.554	9.194	-0.827
I-Butane	-7.994	-0.396	0.333	-27.480	12.073	-1.094
N-Butane	-8.550	-0.183	0.313	-29.124	13.004	-1.191
Hexane	-7.533	-1.580	0.538	-43.450	19.432	-1.809

TABLE XVI

COLUMN C: EQUILIBRIUM COEFFICIENTS*

Component	C_1	C_2	C_3
Methane	-1916.000	13.410	-0.004
Ethane	-4083.000	16.770	-0.005
Propane	-3924.000	13.740	-0.002
I-Butane	-4640.000	14.260	-0.003
N-Butane	-4937.000	14.470	-0.003
I-Pentane	-5416.000	14.260	-0.002
N-Pentane	-5736.000	14.630	-0.002
Hexane	-7036.000	14.240	-0.001
Lean Oil	-7956.000	12.670	0.001

*Note: $\ell n\ KP = \frac{C_1}{T} + C_2 + C_3 T$

TABLE XVII

COLUMN C: ENTHALPY COEFFICIENTS

Component	Liquid C_1	C_2	C_3	Vapor C_1	C_2	C_3
Methane	-891.000	14.080	0.017	1112.000	8.606	0.001
Ethane	-1446.000	22.520	0.014	3437.000	12.460	0.005
Propane	-1810.000	29.470	0.011	5621.000	17.210	0.008
I-Butane	-2147.000	34.860	0.014	6539.000	22.530	0.011
N-Butane	-2041.000	32.990	0.016	7284.000	22.840	0.010
I-Pentane	-2219.000	35.220	0.028	8511.000	27.540	0.014
N-Pentane	-2410.000	38.910	0.020	8975.000	28.200	0.012
Hexane	-3125.000	50.130	0.030	12530.000	38.470	0.018
Lean Oil	-4028.000	64.590	0.042	16430.000	52.250	0.024

TABLE XVIII

COLUMN D: EQUILIBRIUM COEFFICIENTS

Component	C_1	C_2	C_3
Nitrogen	-18.103	254.665	-743.360
Carbondioxide	-0.154	42.168	-186.970
Methane	-8.679	142.265	-444.930
Ethane	-6.230	113.685	-406.790
Propane	-5.940	105.441	-404.370
I-Butane	-4.046	79.855	-346.370
N-Butane	-3.372	71.943	-332.220
I-Pentane	-0.120	29.380	-222.020
N-Pentane	0.291	25.094	-218.210
N-Hexane	4.389	-26.748	-90.167
Hypth Cpnt 1	15.298	-162.350	297.302
Hypth Cpnt 2	20.769	-232.360	478.813
Hypth Cpnt 3	20.800	-236.750	464.801
Hypth Cpnt 4	23.598	-275.290	557.492
Hypth Cpnt 5	16.660	-193.350	289.401

TABLE XIX

COLUMN D: ENTHALPY COEFFICIENTS

Component	Liquid C_1	 C_3	 C_3	Vapor C_1	 C_2	 C_3
Nitrogen	-19477.000	-6839.730	-438.810	1627.330	46.613	68.894
Carbondioxide	7661.330	-5101.500	631.892	-424.320	514.203	48.036
Methane	-12191.000	3646.150	-169.700	1586.110	44.170	84.739
Ethane	-18686.000	5117.560	-292.970	-378.140	458.494	89.316
Propane	-17403.000	3551.500	-72.217	-1798.300	772.284	109.123
I-Butane	-16610.000	2702.350	56.358	-3463.000	1195.200	125.356
N-Butane	-16631.000	2713.150	55.632	-3627.800	1446.380	105.347
I-Pentane	-14843.000	1666.960	184.782	-4959.400	1737.430	127.753
N-Pentane	-14476.000	1515.960	199.922	-4994.900	1917.260	115.037
N-Hexane	-11473.000	87.599	357.950	-5988.200	2286.360	132.225
Hypth Cpnt 1	-734.180	-3204.800	609.609	-5194.000	2589.070	102.204
Hypth Cpnt 2	2483.940	-4747.100	770.020	-6994.900	3124.890	105.299
Hypth Cpnt 3	473.471	-4408.300	812.209	-8660.000	3737.690	135.573
Hypth Cpnt 4	1815.730	-5100.200	912.544	-9839.100	4190.990	152.556
Hypth Cpnt 5	-557.270	-4553.400	932.882	-11400.000	4729.120	180.605

TABLE XX

COLUMN E: EQUILIBRIUM COEFFICIENTS

Component	C_1	C_2	C_3
Hydrogen	1.403	39.516	-108.480
Methane	0.596	47.437	-173.100
Ethylene	3.693	6.458	-79.003
Ethane	4.191	-0.305	-68.393
Propylene	4.095	-0.855	-94.905
Propane	6.890	-36.256	12.305
Butene-1 + I-Butene	9.287	-67.905	83.112
Trans 2-Butene	6.218	-29.871	-40.196
Cis 2-Butene	5.876	-26.844	-48.706
I-Butane	8.375	-57.694	59.574
N-Butane	7.688	-49.311	24.002
Hypth Cpnt 1	-54.825	677.631	-2318.000
Hypth Cpnt 2	-59.975	736.603	-2520.000
Hypth Cpnt 3	-57.127	713.483	-2509.400
Hypth Cpnt 4	-64.938	798.107	-2775.900
Hypth Cpnt 5	9.396	-150.250	174.088

TABLE XXI

COLUMN E: ENTHALPY COEFFICIENTS

Component	Liquid			Vapor		
	C_1	C_2	C_3	C_1	C_2	C_3
Hydrogen	-3537.400	1870.480	-100.040	-1124.300	1052.480	-30.121
Methane	4792.340	-2505.600	320.139	-13825.000	4641.990	-319.830
Ethylene	68.727	-284.500	120.041	1221.490	183.771	80.019
Ethane	-7349.900	2198.820	-59.740	10.880	688.357	64.233
Propylene	126947.000	-45439.000	4119.590	-9136.900	4199.660	-199.970
Propane	39853.900	-15667.000	1580.080	-685.580	1264.310	59.482
Butene-1 + I-Butene	-11540.000	1588.300	150.548	-3444.000	2712.500	-40.369
Trans 2-Butene	-8604.900	794.385	200.459	13454.100	-2676.700	399.736
Cis 2-Butene	-8604.900	794.385	200.459	13454.100	-2676.700	399.736
I-Butane	359.547	-2381.500	480.451	-5062.300	2911.930	-40.322
N-Butane	11031.600	-5856.600	760.379	22081.300	-5986.400	699.713
Hypth Cpnt 1	-103400.000	28775.200	-1678.300	-1275800.000	399642.000	-29884.000
Hypth Cpnt 2	-85173.000	22580.200	-1147.900	-1275800.000	399642.000	-29884.000
Hypth Cpnt 3	-63559.000	15227.600	-518.660	-1275800.000	399642.000	-29884.000
Hypth Cpnt 4	-48750.000	10206.300	-88.634	-1275800.000	399642.000	-29884.000
Hypth Cpnt 5	-31611.000	4379.130	411.134	-1275800.000	399642.000	-29884.000

APPENDIX B

LIQUID AND TEMPERATURE PROFILES

TABLE XXII

VAPOR AND TEMPERATURE PROFILES FOR COLUMN A

Tray Number	Temperature (°R)	Vapor Rate (mole/hr)
5	455.3	1306.39
4	466.0	1306.39
3	479.4	1460.58
2	500.8	1403.38
1	574.2	1339.52

TABLE XXIII

VAPOR AND TEMPERATURE PROFILES
COLUMN B

Tray Number	Temperature (°R)	Vapor Rate (moles/hr)
Condenser	311.9	720.448
17	336.7	866.362
16	348.5	824.307
15	351.2	816.497
14	351.8	815.118
13	351.9	814.849
12	352.0	814.663
11	352.3	813.845
10	354.0	809.037
9	362.9	135.377
8	362.9	134.980
7	363.1	134.925
6	363.9	134.679
5	366.8	133.781
4	377.0	130.769
3	406.0	123.689
2	460.0	120.768
Reboiler	519.3	139.160

TABLE XXIV

VAPOR AND TEMPERATURE PROFILES
FOR COLUMN C

Tray Number	Temperature (°F)	Vapor Rate (moles/hr)
15	101.65	82.667
14	106.06	99.229
13	109.35	102.716
12	112.71	104.292
11	116.86	105.190
10	122.12	105.882
9	127.47	106.635
8	129.63	107.785
7	143.67	43.413
6	146.04	65.303
5	142.406	82.124
4	137.084	96.265
3	140.772	107.014
2	162.058	113.336
Reboiler	250.738	149.132

TABLE XXV

VAPOR AND TEMPERATURE PROFILES FOR COLUMN D

Tray Number	Temperature (°R)	Vapor Rate (moles/hr)
16	541.9	676.789
15	548.8	855.298
14	551.7	865.173
13	552.4	869.984
12	548.6	879.042
11	532.5	718.661
10	537.0	824.267
9	538.3	871.444
8	539.1	884.267
7	540.2	888.330
6	542.6	891.210
5	547.3	896.395
4	555.7	909.352
3	568.8	939.885
2	590.4	987.673
Reboiler	678.5	899.429

TABLE XXVI

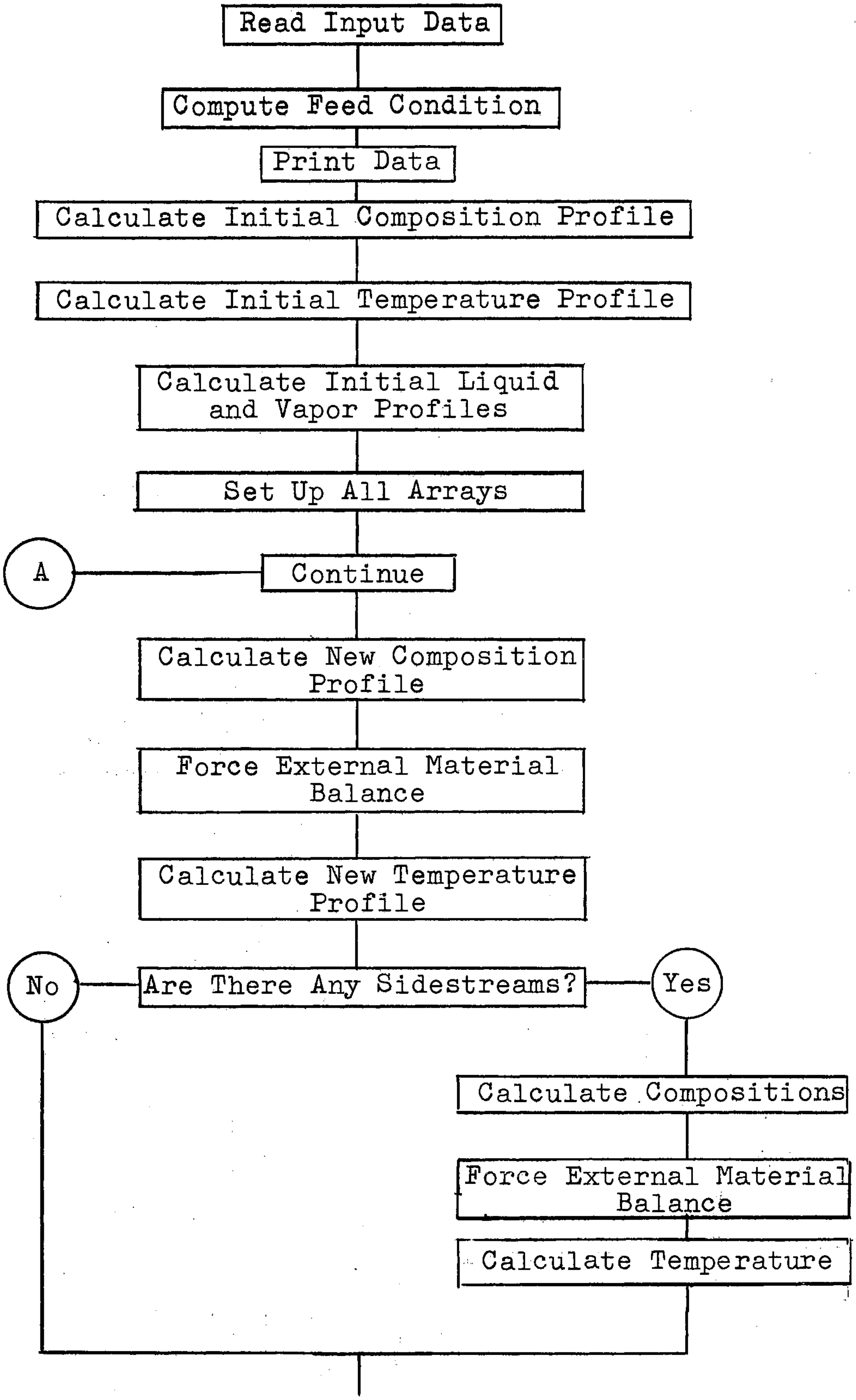
VAPOR AND TEMPERATURE PROFILES FOR COLUMN E

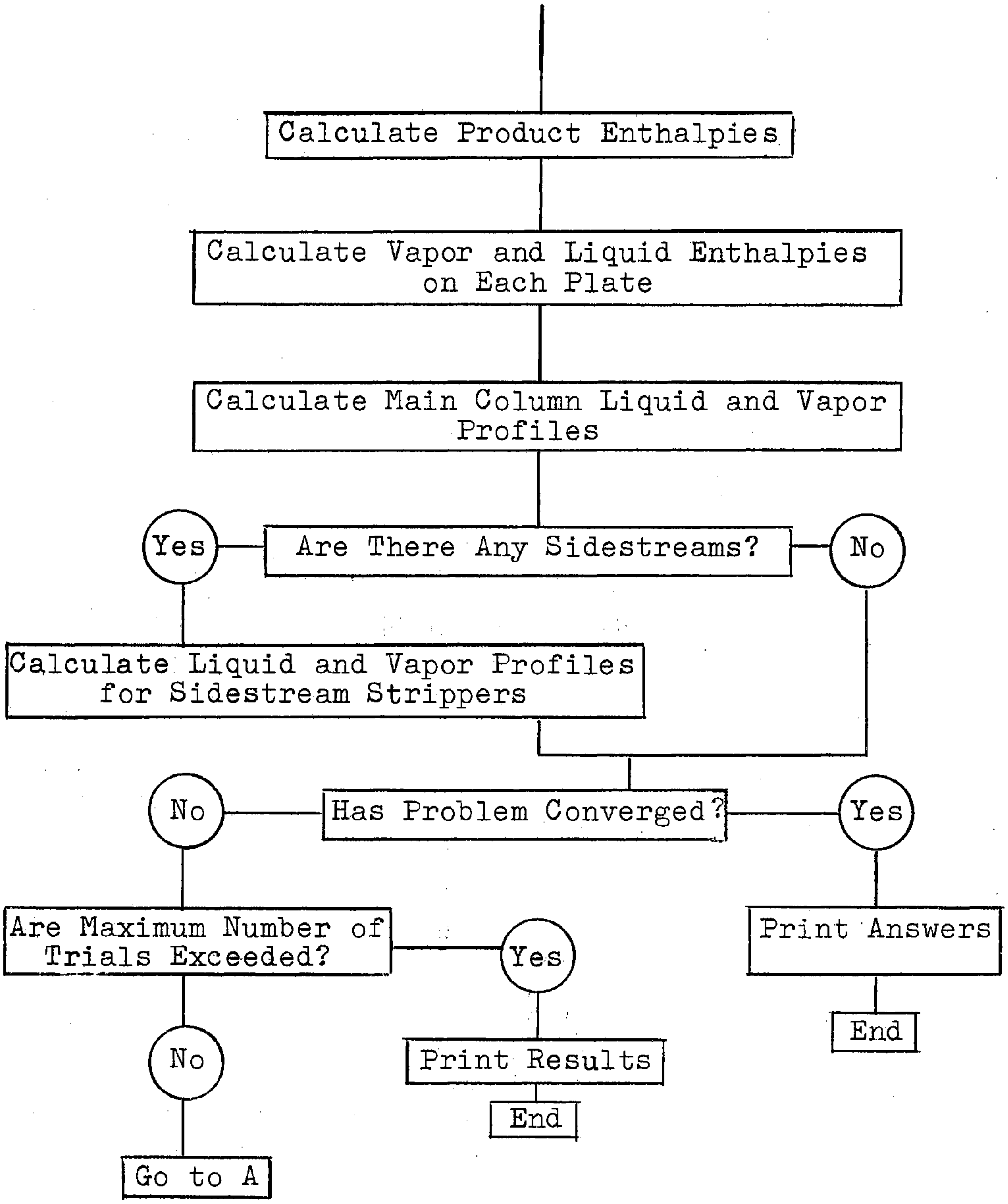
Tray Number	Temperature (°R)	Vapor Rate (moles/hr)
13	569.7	319.890
12	578.1	360.317
11	584.9	389.663
10	589.8	414.052
9	593.0	431.799
8	596.3	443.166
7	610.8	447.297
6	749.3	427.013
5	781.5	0.642
4	781.3	0.003
3	781.0	0.002
2	776.9	0.009
Reboiler	772.9	0.106

APPENDIX C

BLOCK DIAGRAMS

Main Diagram

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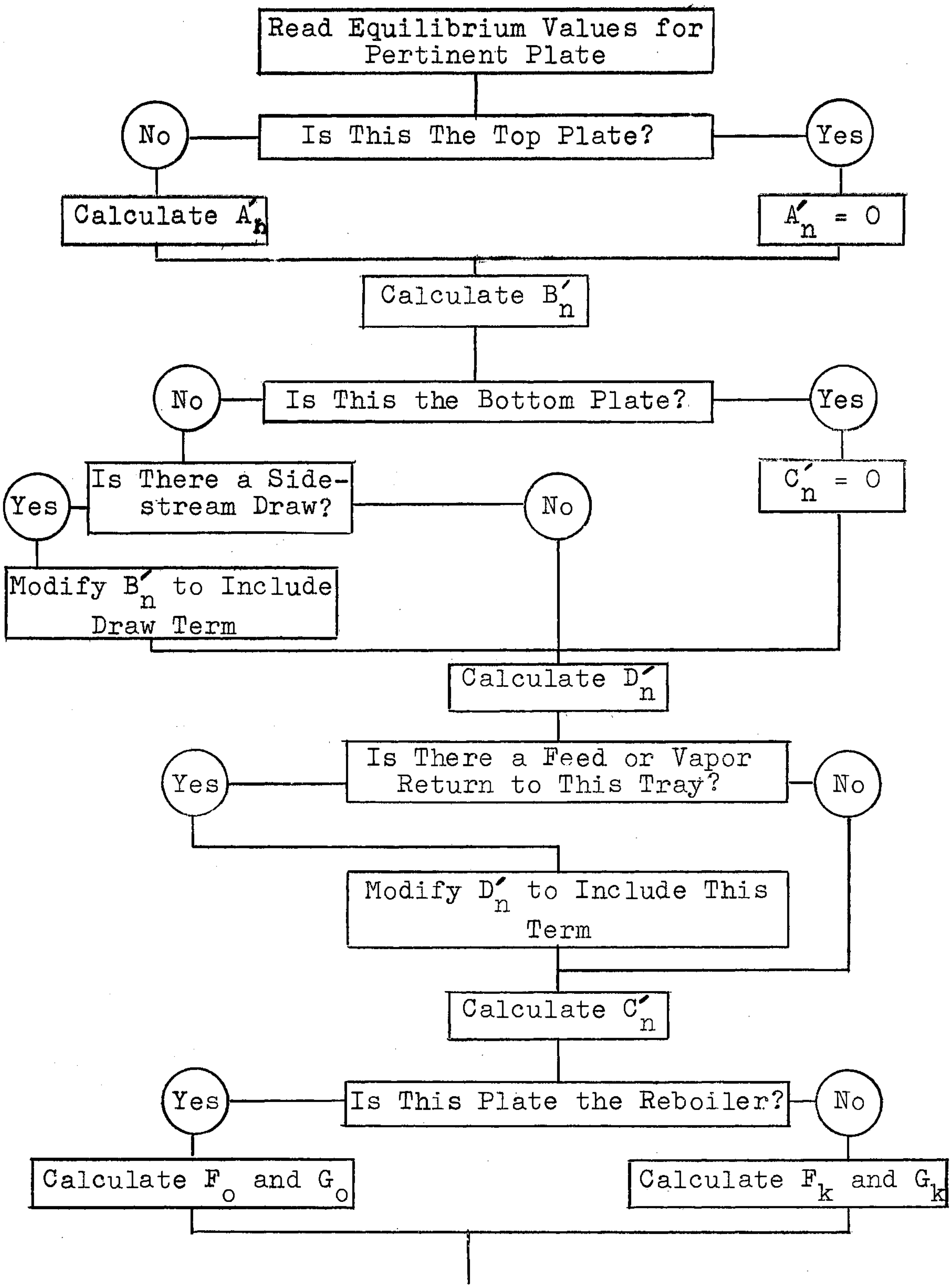
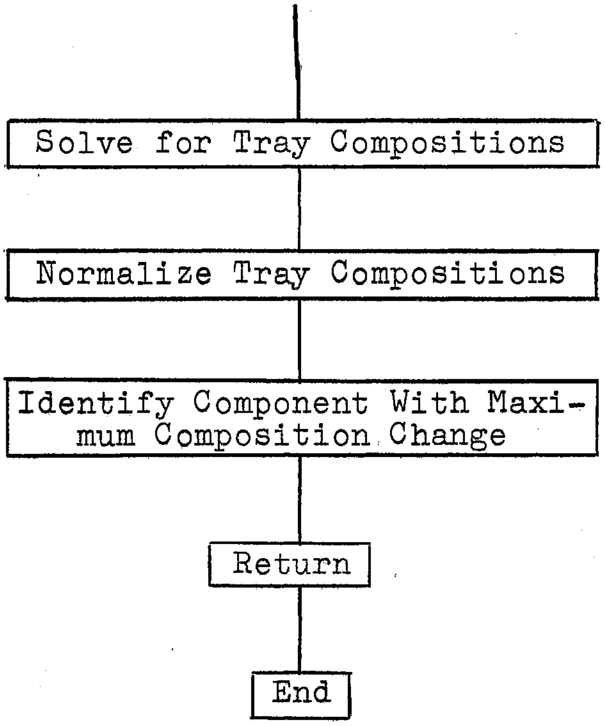
Calculate Vapor and Liquid Enthalpies on Each Plate
Calculate Main Column Liquid and Vapor Profiles
Yes
Are There Any Sidestreams?
No
Calculate Liquid and Vapor Profiles for Sidestream Strippers
No
Has Problem Converged?
Yes
Are Maximum Number of Trials Exceeded?
Yes
Print Answers
End
No
Print Results
End
Go to A

Relaxation Technique

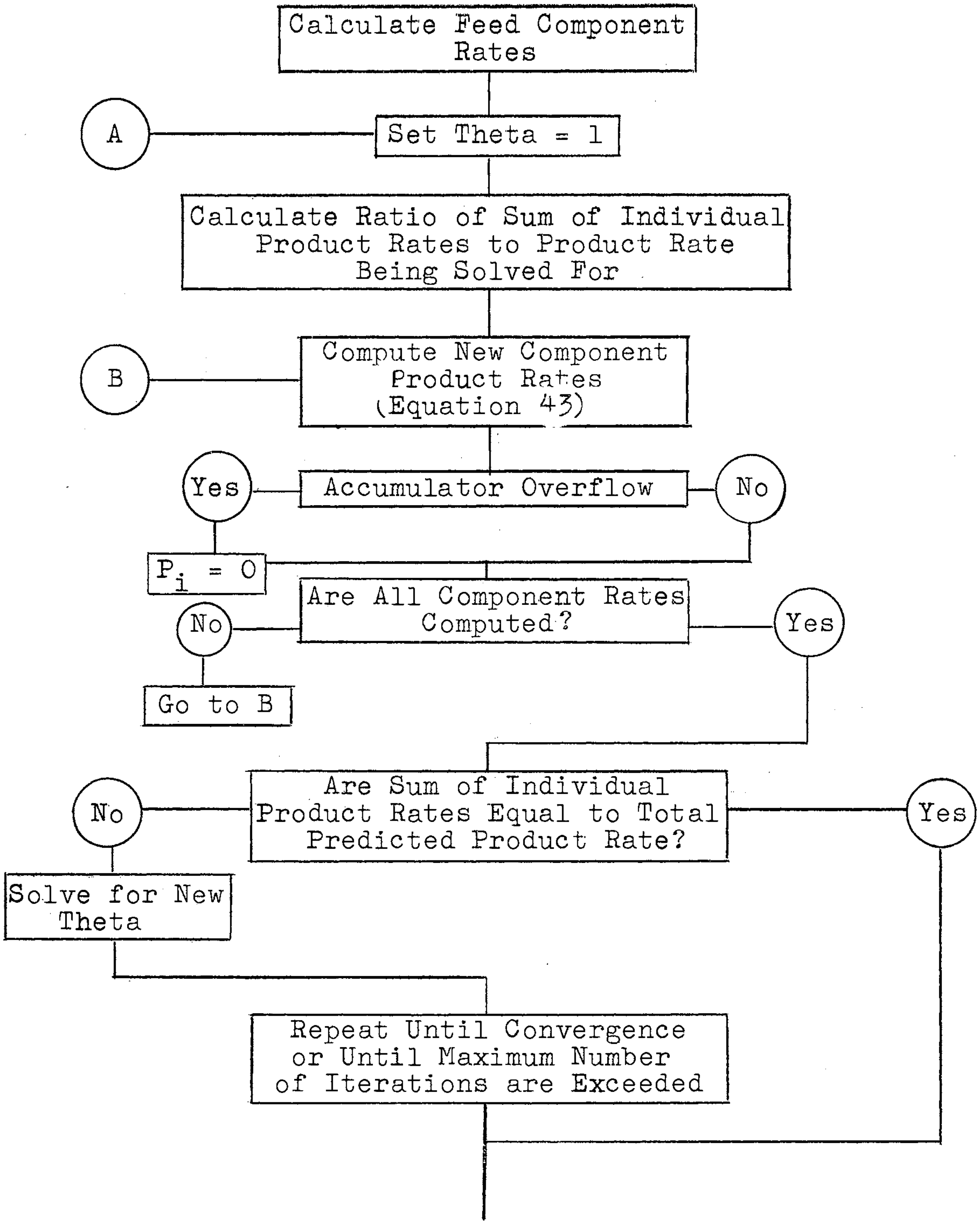
Subroutine XCALC

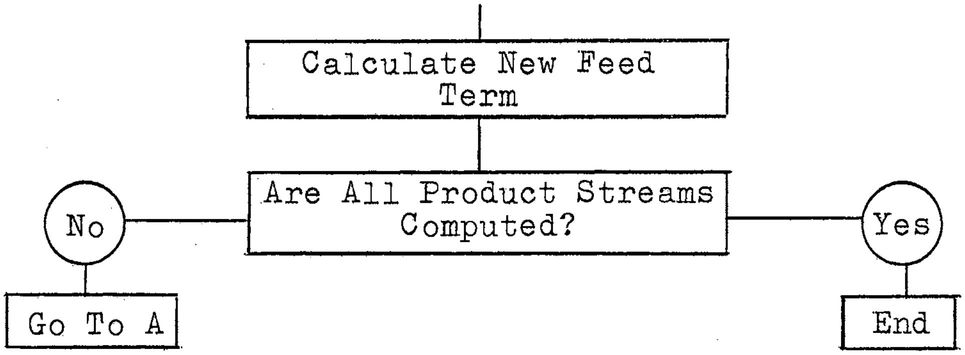



Solve for Tray Compositions
Normalize Tray Compositions
Identify Component With Maximum Composition Change
Return
End

External Material Balance

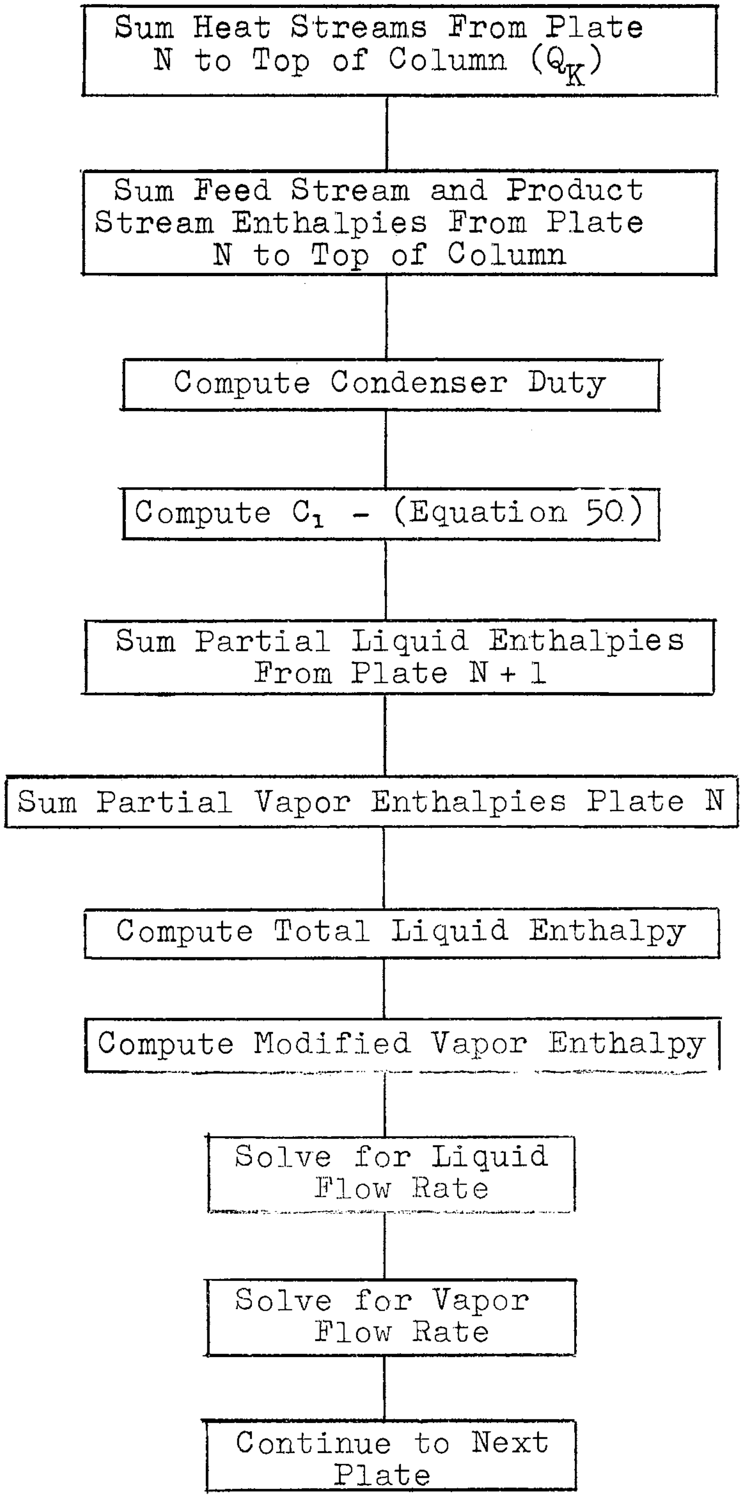
Subroutine Adjust




Calculate New Feed Term
Are All Product Streams Computed?
No
Go To A
Yes
End

Heat Balance

Subroutine HBAL



VITA

2

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