GENERAL-SOLUTION OF TAYLOR AND EDMISTER FOR MULTICOMPONENT, MULTISTAGE SEPARATIONS

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PREFACE

The "General-Solution" of Taylor and Edmister was applied to various distillation problems. The "General-Solution" can be applied easily with digital computers. In connection with K value and enthalpy expressions, new forms for K and H were incorporated in the computer program for "General-Solution".

Appreciation is expressed for the advice and direction of the members of the Masters Committee, Professors W. C. Edmister, J. H. Erbar, B. L. Crynes, and J. M. Jobe. The guidance of Professor W. C. Edmister, the author's thesis adviser, and Professor J. H. Erbar, has been especially helpful. The advice and guidance of Professor D. L. Taylor, from the University of Puerto-Rico, were very valuable.

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CHAPTER I

INTRODUCTION

Distillation is one of the most common and convenient methods for performing separation of a liquid mixture. Thus, design and evaluation of distillation columns is of paramount importance in the chemical process industry. The word "design" refers to either one or the other of the following:

1. Determination of number of theoretical stages for a given separation.
2. Determination of the operating reflux ratio for a given separation.

Thus, there are three primary variables in distillation calculations:

1. Number of theoretical stages.
2. Reflux and boil-up rates.
3. Product compositions and amounts.

The objective of rigorous stage-wise calculations is to find one, given the other two.

For rigorous calculation methods, the thermodynamic properties used are of great importance. The thermodynamic properties used in distillation calculations are K and H values. K is defined as equilibrium vapor/liquid distribution ratio, $K_i = y_i/x_i$. H, the enthalpy (heat content) for a mixture is defined as $H^L = \Sigma\, x_i \bar{H}_i^L$ and $H^V = \Sigma\, y_i \bar{H}_i^V$. H^L and H^V refer to enthalpies of vapor and liquid mixtures, respectively.

$\bar{H}_i^L$ and $\bar{H}_i^V$ are the partial molal enthalpies of the components of liquid mixtures and vapor mixtures, respectively. Thus, K_i, $\bar{H}_i^L$, and $\bar{H}_i^V$ are the component properties which are functions of temperature, pressure, and compositions of the coexisting equilibrium vapor and liquid phases. In this work, the K_i and $\bar{H}_i$ values have been obtained from NGPA-program (27) with the use of Chao-Seader (6) correlation. These values are then employed with "General Solution for distillation processes" developed by Taylor and Edmister (21, 22).

Since complex-hydrocarbon fractions are encountered frequently along with the "discrete" components (e.g., methane, ethane, etc.), it is also essential that a general calculation method have the capability of handling both types of mixtures simultaneously in distillation calculations. The use of Simpson's rule proposed by Taylor and Edmister for making distillation calculations for complex-fractions (i.e., petroleum mixtures that are defined by a laboratory batch distillation assay) has been extended to handle "hybrid-mixtures" in this study. Hybrid mixtures are the mixtures which contain both types of components, i.e., discrete and complex.

Chapter II reviews the previous stage-wise calculation methods and Chapter III presents the discussion of General Solution of Taylor and Edmister.

CHAPTER II

REVIEW OF PREVIOUS WORK

The objective of this chapter is to review briefly the background and present the current status of several multi-component stage-wise calculation procedures. In the presentation that follows, an effort has been made to arrange the discussion of developments in chronological order with an aim to show the gradual improvements in calculational procedures.

Direct Calculation Procedure

In 1932, Lewis and Matheson (16) proposed a direct equilibrium stage calculation procedure in which the objective was to find the number of theoretical stages for a desired separation and given reflux ratio. Equilibrium and material balance calculations were made from the top toward the feed plate and from the bottom toward the feed plate, starting with assumed distillate and bottom compositions. As the calculations proceed from the two terminals, the non-distributed components were introduced so that all the components would be present at the feed-plate mesh (8). The initial product assumptions and the introduction of the non-distributed components affect the convergence significantly. The Lewis-Matheson procedure is sometimes referred to as a "design" method, because of its objective, i.e., calculation of the number of equilibrium stages.

Indirect Calculation Procedure

In the "indirect" procedure, developed by Thiele-Geddes (24) in 1933, the objective is to find the product-compositions for a column with a given number of equilibrium stages and a known reflux ratio. Calculating the component distributions requires using assumed temperature and flow-rate profiles. With these as starting information, the method permits calculating the products and checking the primary assumptions.

Equilibrium and heat balance considerations are used to revise the temperature and flow-rate profiles. All the necessary equations have been presented (8). This method is sometimes referred to as an "analysis method" because of its objective, i.e., product compositions. Convergence is usually slow by this indirect method.

In a later work, Holland (12) claimed to improve the convergence of Thiele-Geddes method by combining it with a so-called "θ-method." Essentially θ is a multiplier that relates the calculated and converged product distribution. It may also be viewed as an arbitrary multiplier, introduced to force the calculations to give the desired total product distribution. θ is incorporated in the material balance equations which are then written in functional form. The solution of the function yields the value of θ, which is used in the revision of the temperature and flow-rate profiles. The proposed revision procedure is repeated until final calculated product rates match with the required rates within a specified tolerance. Detailed discussion appears in Holland (12).

Matrix Techniques

The Lewis-Matheson (16) and Thiele-Geddes (24) calculation procedures are inherently slow to converge. Because of these slow and awkward convergences, the computer techniques based on these methods were never very successful. In the Lewis-Matheson procedure, it was the "introduction of non-distributed components" that made this method slow. Thiele-Geddes procedure suffered from large round off errors. Besides, both these methods shared a common weak-point; i.e., they required that all components appear in both products and that none can be zero. To overcome some troubles, the use of matrices has been proposed.

Amundsen's Technique

Amundsen et al. (1) were the first to propose the use of matrices in distillation calculations. The usual over-all material balances, component-material balances, and heat balances were written around each stage. Combination of component-material balances and equilibrium relationships yields a matrix with x_{ji}'s, the liquid compositions on j^{th} stage, as unknowns. With an assumed set of temperature and vapor-flow profiles, the matrix is solved for the compositions. Equilibrium functions Φ_j ($\Phi_j = \Sigma K_{ji} x_{ji}$), were used to revise the temperatures on each stage. The heat balance equations are used at the revised temperatures to update the vapor-flow rate profile. The procedure is repeated until the equilibrium functions are satisfied on all of the stages.

Wang and Henke Method

Wang and Henke (26) used the Muller's (17) method to revise the stage temperatures by the solution of summation functions ($s_j = \Sigma x_{ji} - 1$).

Muller's (17) method is, in a sense, generalization of the method of false position. The vapor-flow profile is corrected in a way similar to that of Amundsen.

Tomich's Method

The method developed by Tomich (25) uses Broyden's (4) technique to solve the heat balances and summation functions, $S_j = \sum_{i=1}^{c} y_{ji} - \sum_{i=1}^{c} x_{ji}$. The over-all material balances, component-material balances, and heat balances are written for a loop enclosing the top and any stage, j. The component material balances are combined with equilibrium-relationships, $y_{ji} = K_{ji}\, x_{ji}$, to form a tridiagonal matrix with liquid compositions as unknown vectors.

With this method, the solution is also started by assuming temperature and vapor-flow profiles. Substituting the temperatures and vapor-flow rates in the over-all material balance equations gives the liquid flow rates, L_j. Knowledge of T_j, V_j, and L_j enables one to solve a tridiagonal matrix to obtain x_{ji}'s, the liquid compositions on j^{th} stage. Vapor compositions on j^{th} stage can be calculated with $y_{ji} = K_{ji}\, x_{ji}$. Knowing x, y, L, V, and T, one can solve the summation and heat balance functions. Broyden's (4) technique is used to solve these functions to get ΔT_j and ΔV_j which are used to revise the temperature and vapor-flow profiles. Broyden's technique is a "modified Newton-Raphson technique." The method is claimed to be numerically stable and fast in converging.

Burman's Method

Burman (4) started with the developments of Rose et al. (19) and Ball (2) and obtained a set of equations for each component in a

fractionator in which the plates are numbered from the bottom toward the top. The unique feature of the method is that the equations are written for unsteady-state. Introduction of a multiplier, β, is said to yield a faster convergence. The β is related to transient-composition changes on a general stage n, in the following way.

$$x_{n,1}\Big|_{\varphi+\Delta\varphi} = x_{n,1}\Big|_{\varphi} + \Delta\varphi\left[\beta\left(\frac{dx_{n,1}}{d\varphi}\right)\Big|_{\varphi+\Delta\varphi} + (1-\beta)\left(\frac{dx_{n,1}}{d\varphi}\right)\Big|_{\varphi}\right] \qquad (2.1)$$

where

$$0 \leq \beta \leq 1.0 \ .$$

In Equation (2.1), φ indicates the time. Thus, it could be realized that β performs the function of averaging the slope of "composition versus time curve" in the interval φ and $(\varphi+\Delta\varphi)$. Burman (4) concluded that β should be set equal to unity until steady-state has been reached. It has been claimed by that author that this method is superior to some other methods which require all the components to be present in both the products (4). All the Lewis-Matheson type procedures and the Thiele-Geddes procedure used by Holland et al. (12) require the assumptions that all the components are present in both the products.

General Solution of Taylor and Edmister

Recently Taylor and Edmister (21, 22) have developed a rigorous, general method for the solution of distillation processes.

Over-all material balances, component material balances, equilibrium relationships, and heat balances are written for a general stage, j. The stages are numbered from the top toward the bottom. The component material balances are arranged in a tridiagonal matrix form

which is solved for ℓ_{ji} and v_{ji} values, the component flow rates in liquid and vapor streams respectively on the stage j. The equilibrium relationships and the heat balances are cast in the functional form. The ℓ_{ji} and v_{ji} values obtained previously are used in evaluation of these functions. The Newton-Raphson technique is used for these functions to get ΔT_j and ΔL_j, required to revise temperature and flow rates, respectively. Gauss elimination was employed for simultaneous solution of the set of equations.

For a fixed number of stages, the "General Solution" strives to find product distributions at a given reflux ratio. Alternatively a reflux ratio for a desired key component distribution may be found.

The method has been successfully applied to multi-feed and multi-side draw distillation columns. An integral technique for applying this method to petroleum fractions has also been developed by the same authors (22). Convergence on all types of problems solved by this method is rapid and reliable. Mathematical details of the technique appear in Chapter III.

CHAPTER III

GENERAL SOLUTION OF TAYLOR AND EDMISTER

Since this study is based on "General-Solution of Taylor and Edmister", it is essential to have a full understanding of the derivation and application of the equations of this method. The following presentation follows that of Taylor and Edmister (21).

Component Material Balances

Making a component-material balance on the general stage (j^{th} stage) is shown in Figure 1, at steady-state,

$$\ell_{j-1,i} - w^{L}_{j-1,i} + f^{L}_{ji} + v_{j+1,i} - w^{V}_{j+1,i} + f^{V}_{ji} = v_{ji} + \ell_{ji} \quad . \tag{3.1}$$

Equilibrium relationship on j^{th} stage is,

$$y_{ji} = K_{ji}\, x_{ji} \tag{3.2}$$

$$\ell_{ji} = A_{ji}\, v_{ji} \quad . \tag{3.3}$$

For liquid and vapor side streams,

$$w^{L}_{j-1,i} = (W^{L}_{j-1}/L_{j-1})\,\ell_{j-1,i} \tag{3.4}$$

$$w^{V}_{j-1,i} = (W^{V}_{j+1}/V_{j+1})\,v_{j+1,i} \quad . \tag{3.5}$$

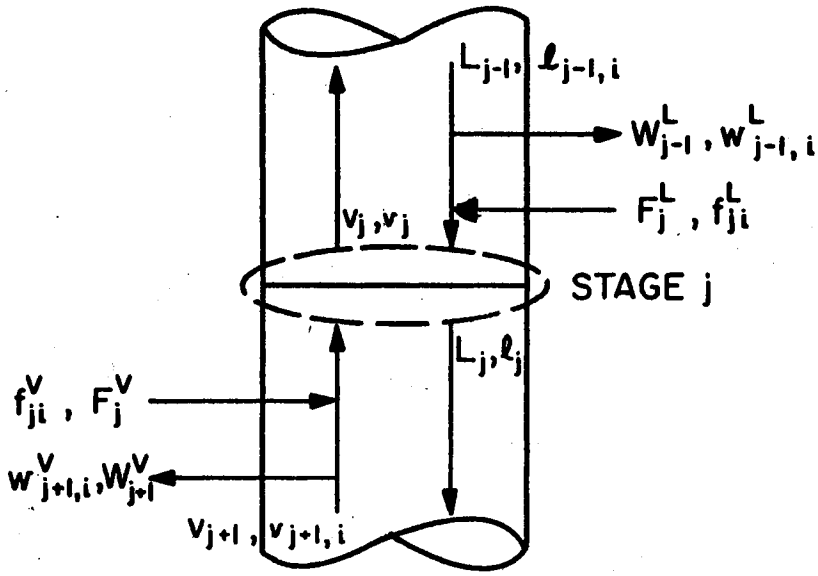

Figure 1. A General-Equilibrium Stage for a Distillation Process

Substituting Equations (3.3) through (3.5) into (3.1),

$$-(1-\frac{W^L_{j-1}}{L_{j-1}})A_{j-1,1}\ v_{j-1,1} + (1+A_{j1})v_{j1} - (1-\frac{W^V_{j+1}}{V_{j+1}})v_{j+1} = f^L_{j1} + f^V_{j1}\ . \quad (3.6)$$

Now define

$$B_j = 1 - W^V_j/V_j \qquad 2 \leq j \leq N \quad (3.7)$$

$$b_j = 1 - W^L_j/L_j \qquad 1 \leq j \leq N-1 \quad (3.8)$$

It should be noted that both B_j and b_j can have values from 0 to 1. Very small values of B_j or b_j indicate large amounts of withdrawal: one cannot withdraw such that the other passing streams would have negative flow rates.

Let

$$\Phi^L_{j1} = f_{j1} + f^V_{j1} \quad (3.9)$$

$$= \text{total component-feed rate on } j^{th} \text{ stage.}$$

Substitution of Equations (3.7), (3.8), and (3.9) into Equation (3.6) yields,

$$-b_{j-1}\ A_{j-1,1}\ v_{j-1,1} + (1 + A_{j1})v_{j1} - B_{j+1},\ v_{j+1,1} = \Phi_{j1}\ . \quad (3.10)$$

Note that there is no (j-1) stream when stage j is the condenser. Likewise, there is no (j+1) stream when j is the reboiler.

Tridiagonal-Matrix Formulation

Extending Equation (3.10) for the whole column,

$$\left.\begin{array}{llllll}
(1+A_{1i})v_{1i} & -B_2v_{2i} & & & & = \Phi_{1i} \\
-b_1A_{1i}v_{1i} & +(1+A_{2i})v_{2i} & -B_3v_{3i} & & & = \Phi_{2i} \\
 & -b_2A_{2i}v_{2i} & +(1+A_{3i})v_{3i} & -B_4v_{4i} & & = \Phi_{3i} \\
 & & -b_{j-1}A_{j-1,i}v_{j-1} & +(1+A_{ji})v_{ji} & -B_{j+1}v_{j+1,i} & = \Phi_{ji} \\
 & & & -b_{N-1}A_{N-1,i}v_{N-1,i} & +(1+S_{Ni})\ell_{Ni} & = \Phi_{Ni}
\end{array}\right\} . \tag{3.11}$$

The equation set (3.11) can be written in matrix notation as

$$A \cdot v = \Phi \tag{3.11a}$$

where A is the matrix that involves absorption factors, b_j and B_j values; v is the matrix for vapor-component flow rates; and Φ is the matrix for the entries on the right hand side of Equation (3.11). Equation set (3.11) can also be written in terms of ℓ_{ji} by the use of an expression to relate v_{ji} in terms of ℓ_{ji}, i.e.,

$$v_{ji} = S_{ji}\,\ell_{ji} \quad . \tag{3.12}$$

Substituting (3.12) in (3.11) set, to eliminate v_{ji} terms,

$$\left.\begin{array}{llllll}
(1+S_{1i}) & -B_2S_{2i}\ell_{2i} & & & & = \Phi_{1i} \\
-b_1\ell_{1i} & +(1+S_{2i})\ell_{2i} & -B_3S_{3i}\ell_{3i} & & & = \Phi_{2i} \\
-b_2\ell_{2i} & +(a+S_{3i})\ell_{3i} & -B_4S_{4i}\ell_{4i} & & & = \Phi_{3i} \\
 & -b_{j-1}\ell_{j-1,i} & +(1+S_{ji})\ell_{ji} & -B_{j+1}S_{j+1,i}\ell_{j+1,i} & & = \Phi_{ji} \\
 & & -b_{N-1}\ell_{N-1,i} & +(1+S_{Ni})\ell_{Ni} & & = \Phi_{Ni}
\end{array}\right\} \quad (3.13)$$

Equation set (3.13) can also be cast in tridiagonal matrix form similar to Equation (3.11a).

Over-all Material Blances

For j^{th} stage,

$$L_{j-1} - W^L_{j-1} + F^L_j + V_{j+1} - W^V_{j+1} + F^V_j = L_j + V_j \qquad (3.14)$$

$$\left.\begin{array}{ll}
V_1 - V_2 & = F^L_1 + F^V_2 - L_1 - W^V_2 \\
V_2 - V_3 & = F^L_2 + F^V_2 - L_1 - W^L_1 - W^L_3 \\
V_j - V_{j+1} & = F_j + F^V_j + L_{j-1} - L_j - W_{j-1} - W^V_{j+1} \\
V_N & = F^L_N + F^V_N + L_{N-1} - L_N - W^L_{N-1}
\end{array}\right\} \qquad (3.15)$$

Heat Balances and Equilibrium Relationships

Heat balance on stage, j, is,

$$\sum_{i=1}^{c} \ell_{j-1} h_{j-1,i} - \sum_{i=1}^{c} w^{L}_{j-1,i} h_{j-1,i} + \sum_{i=1}^{c} f^{L}_{ji} h^{F}_{ji} + \sum_{i=1}^{c} v_{j+1} H_{j+1,i}$$

$$- \sum_{i=1}^{c} w^{V}_{j+1,i} H_{j+1,i} + \sum_{i=1}^{c} f^{V}_{ji} H^{F}_{ji} + Q_j = \sum_{i=1}^{c} \ell_{ji} h_{ji} + \sum_{i=1}^{c} v_{ji} H_{ji}$$

$$1 \leq j \leq N \qquad (3.16)$$

where Q_j is the amount of heat added to the jth plate from an external source. Generally Q_j is zero except for the condenser and the reboiler. The equilibrium on a stage is given as

$$\sum_{i=1}^{c} K_{ji} \ell_{ji} = L_j \qquad 1 \leq j \leq N. \qquad (3.17)$$

Equation (3.17) is the bubble point equation for the liquid leaving the jth tray. Its equivalent dew point form for the coexisting equilibrium vapor is

$$\sum_{i=1}^{c} \left({}^{v_{ji}}/_{K_{ji}} \right) = V_j \qquad 1 \leq j \leq N \qquad (3.18)$$

Equation (3.18) is obtained from (3.17) by writing

$$\ell_{ji} = A_{ji} v_{ji} \qquad (3.19)$$

Combination of Equations

Equation sets (3.16) and (3.17) contain a total of 2N equations, N from each set. The total number of unknowns in a general distillation process are 4N; however, i.e., $(T_1, T_2, \ldots T_N)$, $(L_1, L_2, \ldots L_N)$, $(W_1^L, W_2^L, \ldots W_{N-1}^L)$, $(W_2^V, W_3^V, \ldots W_N^V)$, Q_1 and Q_N. Q_1 and Q_N refer to condenser and reboiler duties, respectively. Since the number of equations is 2N, and the number of unknowns, 4N, 2N quantities, i.e., (4N - 2N), must be specified. For a conventional distillation column, no side streams are present and, therefore, 2N - 2 values of W_j^L and W_j^V are all zero. The two remaining quantities might be reflux rate, L_1, and the bottom product rate, L_N. Other types of specifications can also be made.

Heat Balance and Equilibrium Functions

For the application of Newton-Raphson procedure, equation sets (3.16) and (3.17) are written in functional form. For a column with a partial condenser and a reboiler.

$$G_r = \frac{b_{j-1}\sum_{i=1}^{C} h_{j-1,i}\,\ell_{j-1,i} + B_{j+1}\sum_{i=1}^{C} S_{j+1,i}H_{j+1,i}\,\ell_{j+1,i} + \sum_{i=1}^{C} f_{ji}^{V}H_{ji}^{F} + \sum_{i=1}^{C} f_{ji}^{L}h_{ji}^{F}}{\sum_{i=1}^{C} h_{ji}\ell_{ji} + \sum_{i=1}^{C} S_{ji}H_{ji}\ell_{ji}} - 1$$

$$2 \leq j \leq N; \quad 1 \leq r \leq N-2 \qquad (3.20)$$

$$G_r = \frac{\sum_{i=1}^{C} \ell_{ji}\,K_{ji}}{L_j} - 1 \qquad 1 \leq j \leq N \text{ and } N-1 \leq r \leq 2N-2 \qquad (3.21)$$

Equation sets (3.20) and (3.21) contain b, B, h, H, ℓ, and K as variables: b and B are functions of L and V, respectively. V in turn can be expressed as a function of L from over-all material balance equations, i.e., Equation (3.15), h, H, and K can be expressed as functions of temperature only. ℓ is again a function of L. Thus, in Equation (3.20) and (3.21), L and T are implicit variables.

Newton-Raphson Technique

The chain rule is applied for this technique,

$$\left.\begin{aligned} \Delta G_1 &= \frac{\partial G_1}{\partial T_1}\Delta T_1 + \cdots + \frac{\partial G_1}{\partial T_N}\Delta T_N + \frac{\partial G_1}{\partial L_2}\Delta L_2 \cdots + \frac{\partial G_1}{\partial L_{N-1}}\Delta L_{N-1} \\ &\vdots \\ \Delta G_{2N-2} &= \frac{\partial G_{2N-2}}{\partial T_1}\Delta T_1 + \cdots + \frac{\partial G_{2N-2}}{\partial T_N}\Delta T_N + \frac{\partial G_{2N-2}}{\partial L_2}\Delta L_2 \cdots + \frac{\partial G_{2N-2}}{\partial L_{N-1}}\Delta L_{N-1} \end{aligned}\right\} \quad (3.22)$$

Equation (3.22) is the mathematical expression for multi-dimensional Newton-Raphson technique. Simultaneous solutions of Equation (3.22) will yield the values ($\Delta T_1 \cdots \Delta T_N$) and ($\Delta L_2 \cdots \Delta L_{N-1}$). The ΔT and ΔL values are used to revise temperature and flow profiles, respectively. The various derivatives $\frac{\partial G_1}{\partial T_1}$, $\frac{\partial G_r}{\partial T_r}$, etc., are needed before the solutions are possible. In the program, they are evaluated numerically. The program employs "Gauss-elimination and back substitution" for the simultaneous solution of Equation (3.22). This elimination method eliminates all but one variable from a set of equations. The back substitution starts with the retained variable. The Gauss-elimination is a powerful technique when the number of equations in a set is not too great, i.e., not greater than 50 (5). For frequently

encountered distillation operations, the method gives quick and reliable answers.

The method resembles with Tomich's tridiagonal matrix which uses modified Newton-Raphson technique for solution. The difference arises in the way the heat balance and equilibrium functions are set. Tomich's method uses the mixture enthalpies and deducts right-hand side from left-hand side of heat balances and equilibrium relationships to set them in functional form. The "General-Solution" makes use of partial molal enthalpies for heat balances (21). The arrangement in functional form is shown in Equations (3.20) and (3.21).

Round-Off Errors

As stated previously, Equations (3.11) or (3.13) can be used to get v_{ji} or ℓ_{ji} values, respectively. For the light components, ℓ_{1i} may be quite high compared to ℓ_{Ni}. Stripping factors are large for light components. As a result, if equation set (3.13) is used for light components, the first few equations will have very large numbers compared to those of the bottom-equations in the same set. The simultaneous solution would thus result in a considerable loss of accuracy. Similar reasoning holds for heavy components if Equation (3.11) is applied for them. To keep round-off errors to a minimum, it is recommended to use Equation (3.11) for light components and Equation (3.13) for the heavy components. A component is defined as "light" if $\prod_{j=1}^{N} A_{ji} \leq 1$, otherwise it is heavy. In the computer program, the sets (3.11) and (3.13) are arranged in different forms shown below. Before applying the Equations (3.24) and (3.25) presented below, it is essential to break up the mixture into light and heavy groups.

For the heavy group,

$$\left.\begin{aligned}
&\sigma_{0i} = 1 \\
&\sigma_{1i} = 1 + S_{1i} \\
&\sigma_{ji} = \sigma_{j-1,i}(1 + S_{ji}) - \sigma_{j-2,i}\, b_{j-1} B_j S_{ji} \qquad 2 \leq j \leq N \\
&\ell_{Ni} = \frac{\Phi_{Ni}\sigma_{N-1,i} + \sum_{q=1}^{N-1}\left[\left(\prod_{t=q}^{N-1} b_t\right)\Phi_{qi}\,\sigma_{q-1,i}\right]}{\sigma_{Ni}} \\
&\ell_{ji} = \frac{\Phi_{ji}\sigma_{j-1,i} + \sum_{q=1}^{j-1}\left[\left(\prod_{t=q}^{j-1} b_t\right)\Phi_{qi}\sigma_{q-1,i}\right] + \ell_{j+1,i} S_{j+1,i} B_{j+1}\sigma_{j-1,i}}{\sigma_{ji}} \\
&\qquad\qquad N-1 \geq j \geq 2 \\
&\ell_{1i} = \frac{\Phi_{1i} + \ell_{2i}\, S_{2i}\, B_2}{\sigma_{1i}}
\end{aligned}\right\} . \tag{3.24}$$

For the lighter group,

$$\left.\begin{aligned}
&\alpha_{N+1,i} = 1 \\
&\alpha_{Ni} = 1 + A_{Ni} \\
&\alpha_{ji} = \alpha_{j+1,i}(1 + A_{ji}) - B_{j+1} b_j A_{ji}\alpha_{j+2,i}, \quad N-1 \geq j \geq 1 \\
&v_{1i} = \frac{\Phi_{1i}\alpha_{2i} + \sum_{q=2}^{N}\left[\left(\prod_{t=2}^{q} B_t\right)\Phi_{qi}\alpha_{q+1,i}\right]}{\alpha_{1i}}
\end{aligned}\right\} \tag{3.25}$$

$$v_{ji} = \frac{\Phi_{ji}\alpha_{j+1,\,i} + \sum_{q=j+1}^{N} \left[\left(\prod_{t=j+1}^{q} B_t \right) \Phi_{qi}\alpha_{q+1,\,i} \right] + A_{j+1,\,i} b_{j-1} v_{j-1,\,i}\alpha_{j+1,\,i}}{\alpha_{ji}}$$

$$2 \leq j \leq N-1$$

$$v_{Ni} = \frac{\Phi_{Ni} + A_{N-1,\,i}\, b_{N-1}\, v_{N-1,\,i}}{\alpha_{Ni}} \quad .$$

The subroutine MATBAL employs these equations to calculate ℓ_{ji} and v_{ji}'s needed for use in heat balance and equilibrium functions.

CHAPTER IV

THERMODYNAMIC PROPERTIES

The thermodynamic properties K and H are needed for the components of the mixture in calculating component distribution and heat balances in equilibrium stage computations. K is defined as the vapor liquid equilibrium distribution ratio, i.e., y_i/x_i, whereas, H is the enthalpy (heat content) of a particular component. Both, K and H, are functions of temperature, pressure, and mixture composition and chemical nature of the component. For computer algorithms, these values should be represented by empirical equations expressing K and H as separate functions of temperature for the particular conditions of interest. The coefficients appearing in these equations depend on the type of component, type of mixture and pressure of the system. The forms of the empirical equations used by Taylor and Edmister (21, 22) were taken directly from Holland (12) and used in the demonstration of the "General-Solution" because of convenience.

Holland's (12) Equations

At constant pressure,

$$\sqrt[3]{\frac{K}{T}} = a_o + a_1 T + a_2 T^2 + a_3 T^3 \tag{4.1}$$

$$\sqrt{h_L} = b_o + b_1 T + b_2 T^2 \tag{4.2}$$

$$\sqrt{H_V} = c_o + c_1 T + c_2 T^2. \tag{4.3}$$

In Equations (4.1) through (4.3), T is the temperature in degrees Rankine and a_i's, b_i's, and c_i's are the coefficients for K, h_L, and H_V of a component, respectively. These coefficients are different for different components and depend also upon the pressure of the system. Holland (12) has presented these coefficients for frequently encountered hydrocarbons for a range of pressures; i.e., p = 50 psia, 120 psia, 264.7 psia, 300 psia, and 400 psia. For this work, the K and H equations were replaced with different forms of equations which appear in the next section. The objectives for this replacement are the following:

1. The operating pressures for distillation processes are not restricted to a particular set of values. They are generally fixed by the product requirements and the temperature of cooling water in the overhead condenser. Thus, it is desirable to have K and H equations that are flexible enough to handle at any pressure conditions.
2. The empirical equations presented by Holland (12) do not reflect the composition effects on the K and H values of a mixture component.
3. The NGPA - K & H computer program developed by Erbar-Persyn and Edmister (27) is well suited to generate K and H values of mixture components. These K and H values reflect the temperature, pressure, and composition effects. Once the K and H values have been generated by the program, they can be curve-fitted to yield the desired coefficients for empirical K and H equations.

Proposed New Forms of Equations

The new forms of the equations presented here have been successfully used and are recommended by Erbar (9):

$$\ln K_i = a_o' + a_1'/T + a_2'/T^2 \tag{4.4}$$

$$\bar{h}_L = b_o' + b_1'T + b_2'T^2 \tag{4.5}$$

$$\bar{H}_V = c_o' + c_1'T + c_2'T^2 \ . \tag{4.6}$$

Note that in Equation (4.4) T is the temperature in degrees Rankine divided by 100, i.e., $^{\circ}R/100$, while in Equations (4.5) and (4.6) T is the temperature in degrees Rankine. The new coefficients, a_i''s, b_i''s, and c_i''s are obtained by curve-fitting the K and H values obtained from NGPA K & H program (9, 27). By employing the scaling procedure on temperature (i.e., dividing it by 100) for Equation (4.4), a good curve-fit is obtained. The details of the curve-fit program appear in Appendix B.

Basis for New Forms of K & H Equations

The basis for the new form of K equation, Equation (4.4) is the Antoine vapor pressure expression (9); i.e.,

$$\ln p^{\circ} = A + B/(C+t) \ . \tag{4.7}$$

The value of C for most substances is 273 if t is in Centigrade units and 460 if t is in Fahrenheit units. Thus, the denominator of the second term on the right side of Equation (4.7) is the "absolute temperature scale." Now, for a mixture obeying Raoult's-Law,

$$K_i = p_i^o/p \tag{4.8}$$

or,

$$\ln K_i = \ln p_i^o - \ln p \quad . \tag{4.9}$$

Substituting for $\ln p_i^o$ from Equation (4.7)

$$\ln K_i = A + B/T - \ln p \quad . \tag{4.10}$$

At constant pressure, $\ln p$ is a constant and, hence, could be absorbed in A. Thus, Equation (4.10) is a straight line on $\ln K$ versus 1/T co-ordinates, and represents Raoults-Law-K values. To account for the deviations from Raoults Law, a third temperature dependent term, i.e., a_2'/T^2, has been included. Thus, the final equation is,

$$\ln K_i = a_o' + a_1'/T + a_2'/T^2 \quad . \tag{4.11}$$

The form of enthalpy-equation stems from empirical equations for C_p, the heat capacity. $\bar{H}_i = \int C_{p_i} dT$, the empirical C_p-expression could be integrated with respect to T analytically.

$$\bar{H}_i = \int(\alpha_i + \beta_i T)dT \tag{4.12}$$

$$= \alpha_i T + \beta_i \frac{T^2}{2} + C_o$$

$$= b_o' + b_1'T + b_2'T^2 \quad . \tag{4.13}$$

The purpose of modification of forms of K and H equations could now be made clear.

1. For the K-form, an excellent curve-fit is obtained since the order of magnitude of temperature (i.e., T/100) and K values is same. The reducing of temperature, i.e., T/100, is referred

to as "scaling." The previous form (Equation (4.1)) will, however, yield a poor fit because the vast difference in K values and temperatures will cause truncation errors.

2. The previous H-forms (Equations (4.2) and (4.3)) do not permit the negative enthalpy values. In practice, however, one encounters negative enthalpies for liquid, the ideal gas state being the reference state. The originally proposed forms (Equations (4.2) and (4.3)) do not permit negative enthalpies.

CHAPTER V

APPLICATION RESULTS

This chapter presents various problems solved with a modification of Taylor's (23) computer program for the Taylor-Edmister's calculation method. Incorporation of new K and H equations, i.e., Equations (4.4) through (4.6), is the main modification of the program. Wherever possible, the temperature and flow profiles found via previously used K and H equations (Holland's Equations (4.1) through (4.3)) are compared with those from the new equations. The K values from the new equations have also been compared with those used previously, i.e., Equation (4.1).

Finally, the application of integral technique with "General-Solution" has been demonstrated.

The new forms of K and H equations were tested on various problems selected from literature. The general procedure for the solution by "General-Solution" is as follows:

1. From the data on feed and column specifications, estimate the approximate compositions of the top and bottom results. As a quick estimate, "perfect-split" consideration was used for all the examples presented here. This is not absolutely necessary, however.
2. Calculate the K and H values of the mixture components at three points in the column, i.e., distillate temperature, feed

temperature, and bottom temperature, with the use of NGPA - K & H program (27).

3. Curve-fit the K and H values by using Erbar's linear-regression curve-fit. K values are curve-fitted by using Equation (4.4), while Equations (4.5) and (4.6) are used for the $\bar{h}^L$ and $\bar{H}^V$ curve-fits, respectively. This curve-fit procedure provides one with the coefficients in Equations (4.4), (4.5), and (4.6).
4. Prepare the INPUT DATA according to the instructions given on INPUT DATA preparation in Appendix E.
5. Tabulate the converged temperature and flow-rate profiles, composition of distillate, side-streams and bottoms.

All the examples were solved with the above procedure. In Example Number 5 (Feed - "hybrid-mixture"), the converged compositions of the products (i.e., the pseudo-compositions) had to be processed further to obtain the real-compositions. This has been explained in Example Number 5.

Application of Integral Technique to General-Solution

The Taylor-Edmister method has also been applied to processes treating complex, petroleum fractions (22). Simpson's rule has been used for numerical integration of equilibrium and heat-balance functions (22). An extension has been proposed for the composite-feeds, i.e., mixtures having plateaus and continuous curves in their TBP representation. The pseudo-feed compositions should be based on the continuous part of TBP curve only. This implies that if m_F' is the total mole fraction of all complex-fractions, then divide m_F' into some equal

sub-intervals, say 10. The pseudo-feed compositions will now be given as

Component No.	Pseudo-Feed Composition
1	$(1/30)\ m_F'$
2	$(4/30)\ m_F'$
3	$(2/30)\ m_F'$
4	$(4/30)\ m_F'$
⋮	⋮
11	$(1/30)\ m_F'$

The product-compositions obtained are in terms of pseudo-feed compositions, and have to be converted to real compositions (22).

The Use of Simpson's Rule

The developments leading to the use of Simpson's rule for "General-Solution" will now be presented. The equation is derived for equilibrium relationship and it holds similarly for heat balances.

At equilibrium on a general stage, j,

for discrete components,

$$\sum K_i x_i = 1.0 \tag{5.1}$$

for hypothetical components, however,

$$\int K_i \, dm_{Li} = 1.0 \tag{5.2}$$

dm_{Li} = mole fraction of 'i' present on any stage j. At this point, it is assumed that dm_{Li} can be expressed as a function of dm_{Fi}, mole fraction of the same component, i, in the feed to the column. This

follows from the expressions for compositions of "discrete" components on j^{th} stage. These expressions involve the feed-composition terms (Equations (3.24) and (3.25)).

Now suppose the functional relationship is

$$dm_{L1} = \varphi_1 \, dm_{F1} \tag{5.3}$$

where φ_1 is the function which accounts for temperature and flow profiles as well as withdrawal streams. Substituting (5.3) into (5.2),

$$\int K_1 \varphi_1 \, dm_{F1} = 1.0 \quad . \tag{5.4}$$

One has, usually, to resort to numerical integration of left-hand side of Equation (5.4), since no analytical expressions of K or φ in terms of dm_F are available. Equation (5.5) could be cast in summation form with the use of Simpson's rule. For 10 equal sub-intervals of feed, i.e., 11 components, one can write

$$\int K_1 \varphi_1 \, dm_{F1} = \sum K_1 \varphi_1 \cdot \left(\frac{1}{30}\right)\Big|_{t_1} + \sum K_1 \varphi_1 \left(\frac{4}{30}\right)\Big|_{t_2} + \sum K_1 \varphi_1 \left(\frac{2}{30}\right)\Big|_{t_3}$$

$$+ \sum K_1 \varphi_1 \left(\frac{4}{30}\right)\Big|_{t_4} \cdots + \sum K_1 \varphi_1 \left(\frac{1}{30}\right)\Big|_{t_{11}} \quad . \tag{5.5}$$

Equation (5.5) shows that $\frac{1}{30}$, $\frac{4}{30}$, $\frac{2}{30}$, ..., etc., could be replaced by x_F, the pseudo-feed compositions for the use of Simpson's rule. For the use of Simpson's rule, however, one uses the end-properties of the respective cuts (22).

The mixture had been divided into 18 components, i.e., 7 discrete-type and 11 complex-hydrocarbon fractions, for the Simpson's rule approach and 21 components (7 discrete + 14 hypothetical) for the "Hypothetical-Component" method for Example 5.

Example Number 1

The column for this example consists of 13 theoretical stages and has a pressure of 300 psia. Feed enters on the fifth stage and is a bubble point liquid at the column conditions. Product distributions and temperature and flow-rate profiles have been calculated.

Description of Feed and Column

Component	Feed Composition (mole fraction)
CH_4	0.02
C_2H_6	0.10
C_3H_6	0.06
C_3H_8	0.125
i-C_4	0.035
n-C_4	0.15
nC_5	0.152
nC_6	0.113
nC_7	0.09
nC_8	0.085
400°F nbp	0.07

Specifications

Column pressure ..... 300 psia

Number of stages including partial condenser and reboiler ... 13

Feed is a bubble point liquid at the column pressure, rate is 100 lb moles/hr

Feed temperature ..... 164.5°F

Feed entry ..... On the fifth stage (from top)

Overhead product is a dew point vapor.

Bottom-product rate ..... L_{13} = 68.4 lb moles/hr

Reflux rate ..... L_1 = 63.2 lb moles/hr

TABLE I

INITIAL AND FINAL TEMPERATURE AND FLOW-RATE PROFILES FOR EXAMPLE NUMBER 1

Stage No.	Assumed Initial Values		Final Solution					
			Via K and H equations (4.1), (4.2) and (4.3)			Via K and H equations (4.4), (4.5) and (4.6)		
	T_j (°F)	L_j	T_j (°F)	L_j	V_j	T_j (°F)	L_j	V_j
1	100.0	63.2	107.6	63.2	31.6	109.9	63.2	31.6
2	133.3	63.2	134.4	61.7	94.8	130.5	61.9	94.8
3	166.7	63.2	151.9	57.8	93.3	145.4	59.0	93.5
4	200.0	63.2	170.3	48.5	89.4	163.3	51.1	90.6
5	233.3	163.2	207.5	179.1	80.1	204.2	175.4	82.7
6	266.7	163.2	228.7	194.5	110.7	226.2	189.1	107.0
7	300.0	163.2	243.3	205.0	126.1	242.7	201.0	120.7
8	333.3	163.2	254.2	212.5	136.6	255.4	213.5	132.6
9	366.7	163.2	262.9	217.0	144.1	265.2	228.9	145.1
10	400.0	163.2	271.7	217.6	148.6	274.0	250.7	160.5
11	433.3	163.2	284.2	212.0	149.2	286.4	279.7	182.3
12	466.7	163.2	308.0	192.0	143.6	311.2	274.2	211.3
13	500.0	68.4	366.6	68.4	123.6	357.8	68.4	205.8
			$Q(C) = (0.397)10^6$ Btu/hr			$Q(C) = (0.390)10^6$ Btu/hr		
			$Q(R) = (0.141)10^7$ Btu/hr			$Q(R) = (0.133)10^7$ Btu/hr		
			No. of trials		5	No. of trials		5
			Processor time		39.312 secs	Processor time		38.088 secs
			on IBM 360/65			on IBM 360/65		

TABLE II

FINAL PRODUCT-DISTRIBUTIONS FOR EXAMPLE NUMBER 1

Component	Final Product Distribution			
	By K and H Equations (4.1), (4.2), and (4.3)		By K and H Equations (4.3), (4.4), and (4.5)	
	x_{d_f}	x_{b_f}	x_{d_f}	x_{b_f}
CH_4	$(0.632915)10^{-1}$	$(0.163650)10^{-10}$	$(0.632914)10^{-1}$	$(0.255143)10^{-9}$
C_2H_6	(0.316454)	$(0.170339)10^{-5}$	(0.316458)	$(0.753836)10^{-7}$
C_3H_6	(0.188999)	$(0.405185)10^{-3}$	(0.189160)	$(0.331839)10^{-3}$
C_3H_8	(0.390708)	$(0.224921)10^{-2}$	(0.391108)	$(0.206514)10^{-2}$
$i-C_4$	$(0.234765)10^{-1}$	$(0.403255)10^{-1}$	$(0.192860)10^{-1}$	$(0.422616)10^{-1}$
nC_4	$(0.169987)10^{-1}$	(0.211452)	$(0.204865)10^{-1}$	(0.209839)
nC_5	$(0.638544)10^{-4}$	(0.222197)	$(0.209763)10^{-3}$	(0.222131)
nC_6	$(0.297918)10^{-6}$	(0.165207)	$(0.239020)10^{-5}$	(0.165207)
nC_7	$(0.201018)10^{-8}$	(0.131581)	$(0.459735)10^{-7}$	(0.131581)
nC_8	$(0.140683)10^{-10}$	(0.124271)	$(0.822173)10^{-9}$	(0.124271)
400°Fnbp	$(0.206499)10^{-13}$	(0.102341)	$(0.766560)10^{-16}$	(0.102340)

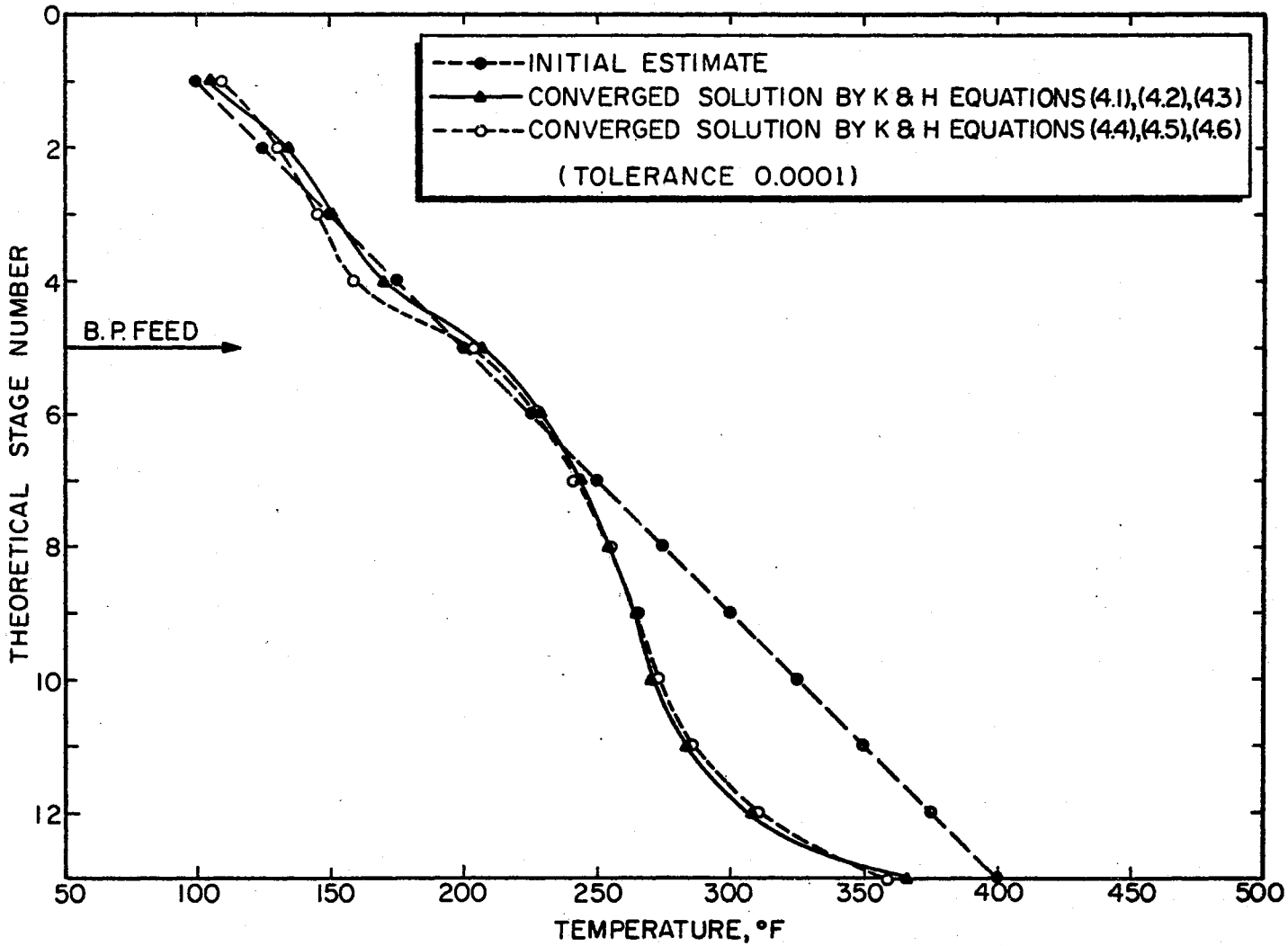

Figure 2. Comparison of Temperature Profile for Example No. 1

Example Number 2

This example illustrates the use of "General Solution" to a column with 16 equilibrium stages. The pressure of the column is 250 psia, feed enters on seventh stage and is at 225°F. Product compositions, temperature and flow-rate profiles have been calculated

Description of Feed and Column

Component	Feed Composition
C_2H_6	0.03
C_3H_8	0.20
C_4H_{10}	0.37
C_5H_{12}	0.35
C_6H_{14}	0.05

Specifications

Column pressure ..... 250 psia

Number of stages including partial condenser and reboiler ... 16

Feed is 16.4% vapor at column conditions.

Feed enters on seventh stage from top.

Feed rate ..... 100 lb moles/hr

Feed temperature ..... 225°F

Overhead product is a dew point vapor.

Bottom product rate ..... 77.4 lb moles/hr

Reflux ratio ..... $L_1/D = 5.0$

TABLE III

INITIAL AND FINAL TEMPERATURE AND FLOW-RATE PROFILES FOR EXAMPLE NUMBER 2

Stage No.	Assumed Initial Values for "General Solution"		Final Solution: Via K and H equations (4.4), (4.5) and (4.6) in "General Solution"		Final Solution: Solution obtained and presented by Amundsen et al. (1)		
	T_j (°F)	L_j	T_j (°F)	L_j	Initially Assumed T_j (°F)	Final T_j (°F)	Final Σx_{j1}
1	112.0	113.0	118.2	113.0	110.0	119.7	1.002
2	125.0	113.0	128.9	108.7	126.0	131.16	1.002
3	138.0	113.0	141.5	103.4	140.0	139.16	1.002
4	151.0	113.0	156.8	98.7	154.0	149.0	1.001
5	164.0	113.0	172.7	95.6	168.0	160.53	1.00
6	177.0	113.0	187.2	92.9	182.0	174.46	1.00
7	191.0	113.0	200.3	87.0	196.0	191.49	0.999
8	221.0	196.6	216.9	170.5	210.0	213.11	1.00
9	226.0	196.6	222.2	172.0	225.0	220.57	1.00
10	231.0	196.6	226.8	173.3	237.0	227.46	1.001
11	236.0	196.6	231.1	174.4	250.0	233.97	0.999
12	241.0	196.6	235.0	175.4	262.0	240.09	1.00
13	246.0	196.6	238.0	176.0	274.0	246.06	1.00
14	252.0	196.6	243.2	176.1	285.0	252.7	1.00
15	257.0	196.6	249.3	175.3	300.0	261.77	0.999
16	262.0	77.4	259.6	77.4	305.0	276.06	0.999
			$Q(C) = (0.713)10^6$ Btu/hr		Q(C) Not Reported		
			$Q(R) = (0.842)10^6$ Btu/hr		$Q(R) = (1.03)10^6$ Btu/hr		
			Tolerance 0.00001		No. of trials = 14		
			No. of trials = 5		Processor time on Univac 1103 50 secs for 5 iterations		
			Processor time on IBM 360/65 36.18 secs				

TABLE IV

FINAL PRODUCT DISTRIBUTIONS IN EXAMPLE NUMBER 2

Component	Final Distribution	
	Via K and H equations (4.4), (4.5) and (4.6) in "General Solution" (21)	
	x_{d_i}	x_{b_i}
C_2H_6	(0.132659)	$(0.250121)10^{-4}$
C_3H_8	(0.834246)	$(0.148106)10^{-1}$
nC_4H_{10}	$(0.330539)10^{-1}$	(0.4684)
nC_5H_{12}	$(0.404971)10^{-4}$	(0.452193)
C_6H_{14}	$(0.800586)10^{-8}$	$(0.646006)10^{-1}$

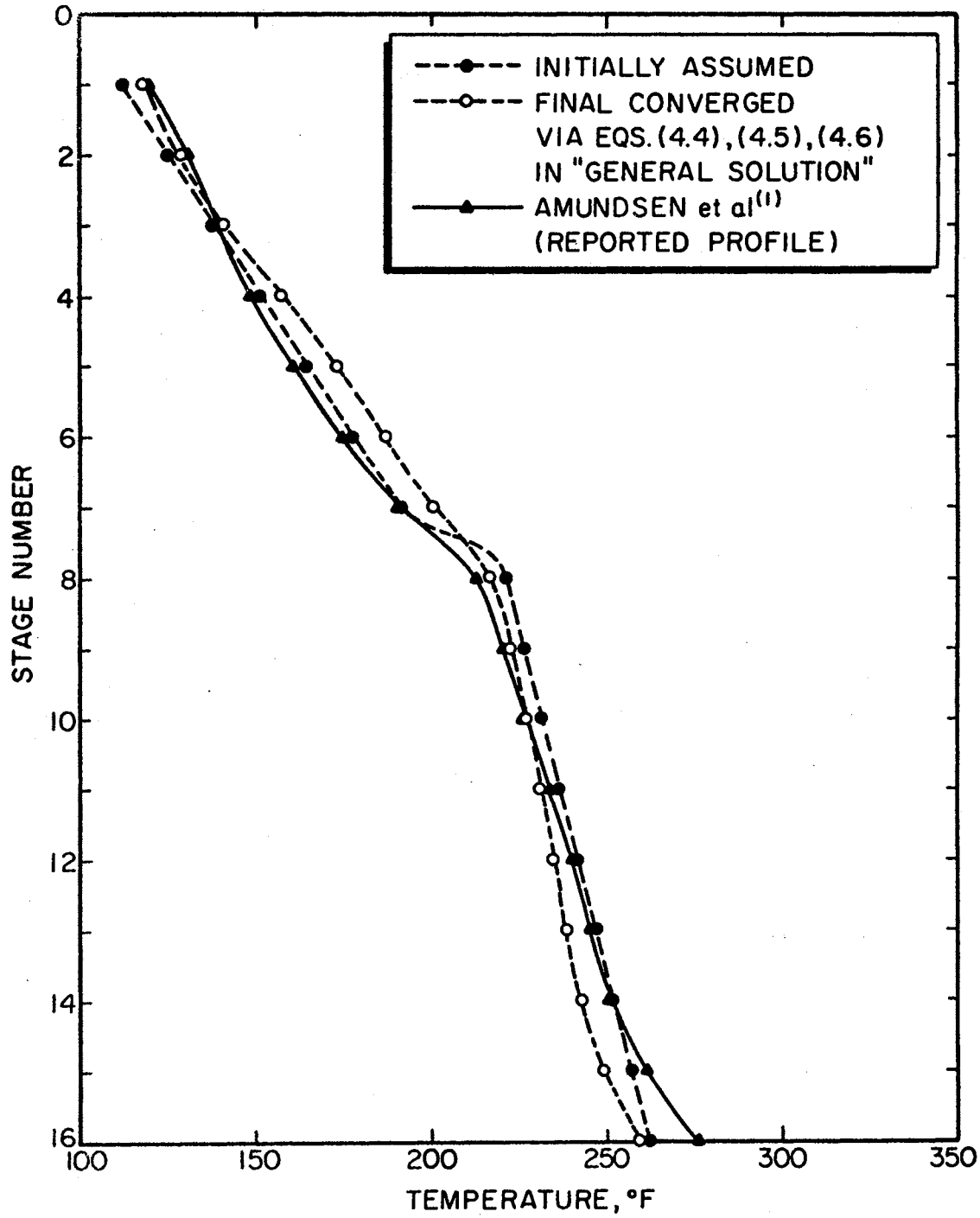

Figure 3. Comparison of Temperature Profile for Example No. 2

Example Number 3

The fractionator for this example consists of 30 equilibrium stages at 265 psia. Feed enters on sixteenth stage and is bubble point liquid at column conditions. Product distributions and temperature and flow-rate profiles have been presented.

Description of Feed and Column

Component	Feed Composition
CH_4	0.1260
C_2H_4	0.003
C_2H_6	0.0328
C_3H_6	0.0396
C_3H_8	0.1494
i-C_4	0.104
n-C_4	0.280
nC_5	0.2410
nC_6	0.091
350°F nbp	0.037

Specifications

Column pressure ..... 265 psia

Number of stages including partial condenser and reboiler 30

Feed is a bubble point liquid at column pressure.

Feed entry on sixteenth stage (from top).

Feed rate ..... 4.45 lb moles/min

Feed temperature ..... 187.07°F (Flash L/F = 1.0)

Distillate is a dew point vapor.

Distillate rate ..... 1.16 lb moles/min

Reflux rate ..... 3.68 lb moles/min

Find the product-compositions, temperature and flow-rate profiles.

TABLE V

INITIAL AND FINAL TEMPERATURE AND FLOW-RATE PROFILES FOR EXAMPLE NUMBER 3

Stage No.	Assumed Initial Values		Final Solution	
			Via K and H equations (4.4), (4.5) and (4.6)	
	T_j (°F)	L_j (lb moles/min)	T_j (°F)	L_j (lb moles/min)
1	107.0	3.7	116.7	3.7
2	112.0	3.7	134.3	3.6
3	117.0	3.7	146.5	3.5
4	122.0	3.7	156.8	3.5
5	127.0	3.7	165.0	3.4
6	132.0	3.7	171.0	3.4
7	137.0	3.7	175.3	3.4
8	142.0	3.7	178.4	3.4
9	147.0	3.7	180.6	3.4
10	152.0	3.7	182.4	3.4
11	157.0	3.7	184.0	3.3
12	162.0	3.7	185.8	3.3
13	167.0	3.7	188.0	3.3
14	172.0	3.7	191.2	3.2
15	180.0	3.7	196.8	3.0
16	187.0	3.7	209.9	8.0
17	192.0	8.1	218.3	8.2
18	197.0	8.1	223.9	8.3
19	202.0	8.1	228.2	8.3
20	207.0	8.1	231.6	8.4
21	212.0	8.1	234.4	8.4
22	217.0	8.1	236.6	8.5
23	222.0	8.1	238.4	8.5
24	227.0	8.1	239.9	8.5
25	232.0	8.1	241.2	8.5
26	237.0	8.1	242.6	8.6
27	242.0	8.1	244.3	8.5
28	247.0	8.1	247.0	8.5
29	253.0	8.1	252.3	8.3
30	260.0	3.3	267.2	8.3

$Q(C) = (0.239)10^5$ Btu/min

$Q(R) = (0.422)10^5$ Btu/min

Processing time on IBM 360/65 201.384 secs

Tolerance = .0001

TABLE VI

FINAL PRODUCT DISTRIBUTIONS IN EXAMPLE NUMBER 3

Component	Final Product Distribution	
	Via K and H equations (4.4), (4.5) and (4.6)	
	x_{d_i}	x_{b_i}
CH_4	$(0.483374)10^{-1}$	$(0.284104)10^{-14}$
C_2H_4	$(0.483371)10^{-1}$	$(0.557227)10^{-7}$
C_2H_6	(0.125830)	$(0.288460)10^{-6}$
C_3H_6	(0.151459)	$(0.161718)10^{-3}$
C_3H_8	(0.538547)	$(0.205302)10^{-2}$
i-C_4	$(0.755739)10^{-1}$	(0.114027)
nC_4	$(0.119214)10^{-1}$	(0.374537)
nC_5	$(0.358458)10^{-6}$	(0.325983)
nC_6	$(0.239771)10^{-13}$	(0.123088)
350°F nbp	$(0.647630)10^{-37}$	$(0.500468)10^{-1}$

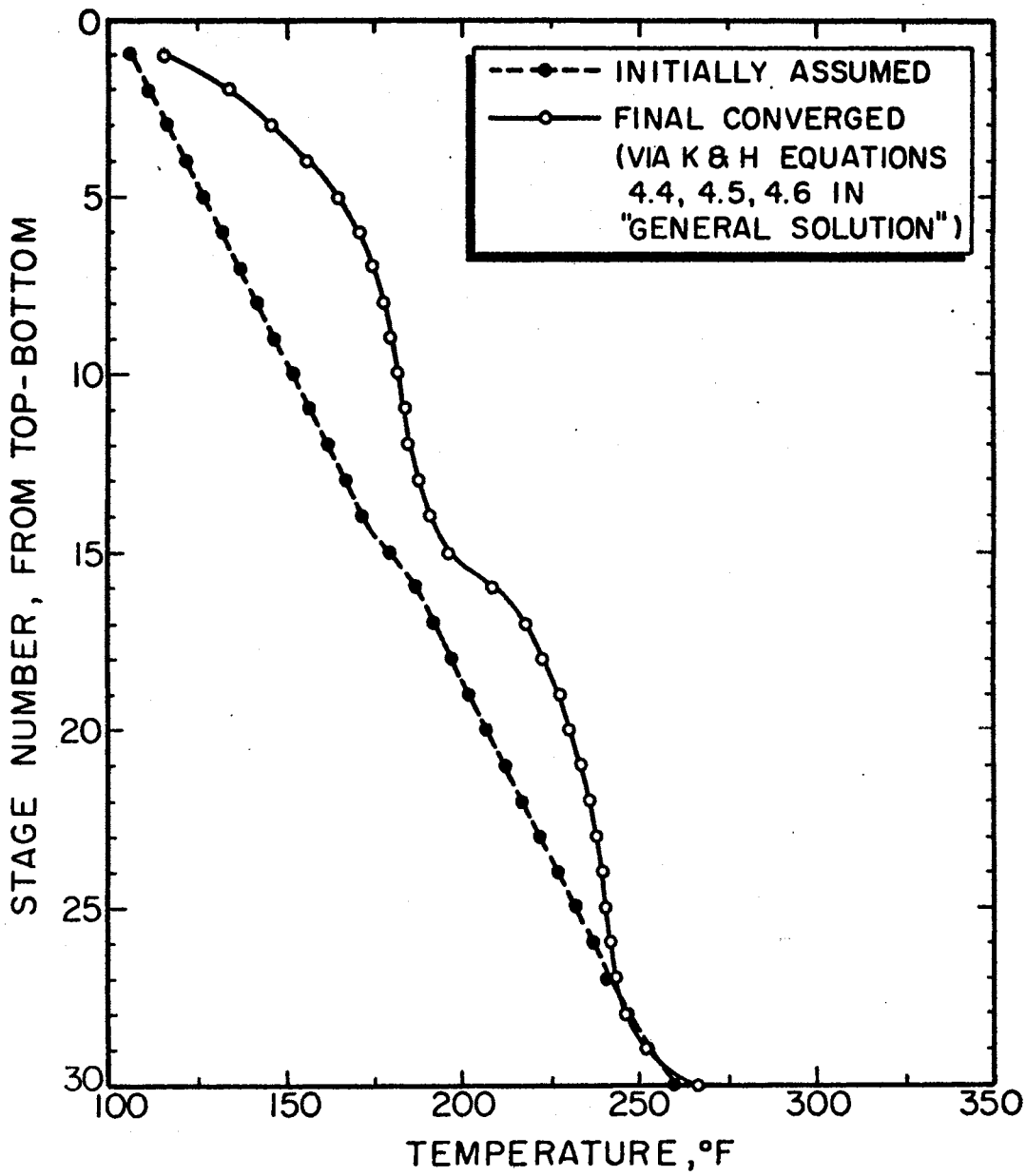

Figure 4. Temperature Profile for Example No. 3

Example Number 4

This example presents the application of "General Solution" to a column with two feeds and two side streams. The column pressure is 300 psia.

Description of Feed and Column

Component	Feed 1 (vapor)	Feed 2 (Liquid)
CH_4	0.04	0.0
C_2H_6	0.16	0.04
C_3H_6	0.08	0.04
C_3H_8	0.20	0.05
i-C_4	0.04	0.03
nC_4	0.180	0.12
nC_5	0.10	0.204
nC_6	0.10	0.126
nC_7	0.06	0.120
nC_8	0.04	0.13
400°F nbp	0.0	0.14

Specifications

Column pressure ..... 300 psia

Number of stages including partial condenser and reboiler ... 13

Feed Number 1 is vapor to stage 5.

Temperature of Feed 1 ..... 200°F

Feed 2 is liquid to stage 10.

Temperature of Feed 2 ..... 150°F

Feed 1 Rate = Feed 2 Rate = 50 lb moles/hr
liquid sidedraw from third stage 10 moles/hr
liquid sidedraw from eleventh stage 10 lb moles/hr

Overhead product dew point vapor.

Rate of distillate ..... 30 lb moles/hr

Reflux rate ..... 100 lb moles/hr

TABLE VII

INITIAL AND FINAL TEMPERATURE AND FLOW-RATE PROFILES FOR EXAMPLE NUMBER 4

Stage No.	Assumed Initial Values		Final Solution			
			Via K and H equations (4.1), (4.2) and (4.3)		Via K and H equations (4.4), (4.5) and (4.6)	
	T_j (°F)	L_j	T_j (°F)	L_j	T_j (°F)	L_j
1	100.0	100.0	120.7	100.0	118.1	100.0
2	125.0	100.0	161.1	101.2	150.0	132.9
3	150.0	100.0	184.2	99.3	178.4	737.4
4	175.0	90.0	202.4	82.4	209.4	653.6
5	200.0	90.0	225.8	82.8	223.0	73.5
6	225.0	90.0	240.4	87.0	206.1	389.0
7	250.0	90.0	248.5	87.8	227.8	303.8
8	275.0	90.0	256.0	87.1	230.7	303.8
9	300.0	90.0	265.8	82.7	253.5	179.4
10	325.0	140.0	287.5	186.8	293.5	267.4
11	350.0	140.0	313.8	186.2	327.0	184.9
12	375.0	130.0	352.5	162.2	363.5	96.2
13	400.0	50.0	426.2	50.0	420.2	50.0
			$Q(C) = (0.686)10^6$ Btu/hr		$Q(C) = (0.6087345)10^6$ Btu/hr	
			$Q(R) = (0.144)10^6$ Btu/hr		$Q(R) = (0.1994564)10^7$ Btu/hr	
			No. of trials = 9		No. of trials = 9	
			Processor time on IBM 360/65 43.776 secs		Processor time on IBM 360/65 57.204 secs	

TABLE VIII

FINAL PRODUCT-DISTRIBUTION FOR EXAMPLE NUMBER 4

Component	Final Solution			
	Via K and H Equations (4.1), (4.2), (4.3) ("General-Solution")			
	x_{d_i}	x_{w_3}	$x_{w_{11}}$	x_{b_i}
CH_4	$(0.66288)10^{-1}$	$(0.113669)10^{-2}$	$(0.263368)10^{-9}$	$(0.203858)10^{-11}$
C_2H_6	(0.322457)	$(0.306928)10^{-1}$	$(0.160700)10^{-2}$	$(0.674736)10^{-4}$
C_3H_6	(0.170508)	$(0.263368)10^{-9}$	$(0.667699)10^{-2}$	$(0.690827)10^{-3}$
C_3H_8	(0.340189)	$(0.160700)10^{-2}$	$(0.111715)10^{-1}$	$(0.134778)10^{-2}$
i-C_4	$(0.385205)10^{-1}$	$(0.667699)10^{-2}$	$(0.394070)10^{-1}$	$(0.956988)10^{-2}$
NC_4	$(0.618678)10^{-1}$	$(0.111715)10^{-1}$	(0.312988)	$(0.995654)10^{-1}$
NC_5	$(0.169122)10^{-3}$	$(0.394070)10^{-10}$	(0.316245)	(0.235919)
NC_6	$(0.130268)10^{-5}$	(0.312988)	(0.138488)	(0.197633)
NC_7	$(0.933515)10^{-8}$	(0.316245)	$(0.765980)10^{-1}$	(0.164604)
NC_8	$(0.652886)10^{-10}$	(0.138488)	$(0.577377)10^{-1}$	(0.15844)
400°Fnbp	$(0.355637)10^{-22}$	$(0.765980)10^{-1}$	$(0.390933)10^{-1}$	(0.132182)

TABLE IX

FINAL PRODUCT DISTRIBUTION FOR EXAMPLE NUMBER 4

Component	Final Solution			
	Via K and H Equations (4.4), (4.5) and (4.6) ("General-Solution")			
	x_{d_i}	x_{w_3}	$x_{w_{11}}$	x_{b_1}
CH_4	$(0.6635285)10^{-1}$	$(0.941443)10^{-3}$	$(0.323512)10^{-10}$	$(0.3395779)10^{-12}$
C_2H_6	(0.3234078)	$(0.291113)10^{-1}$	$(0.531061)10^{-3}$	$(0.2687850)10^{-4}$
C_3H_6	(0.1698592)	$(0.323512)10^{-10}$	$(0.226663)10^{-2}$	$(0.2786576)10^{-3}$
C_3H_8	(0.3352022)	$(0.531061)10^{-3}$	$(0.430893)10^{-2}$	$(0.5838136)10^{-3}$
iC_4	$(0.31242070)10^{-1}$	$(0.226663)10^{-2}$	$(0.452693)10^{-1}$	$(0.1222590)10^{-1}$
nC_4	$(0.3275597)10^{-1}$	$(0.430893)10^{-2}$	(0.391898)	(0.1331278)
nC_5	$(0.5709688)10^{-4}$	$(0.452693)10^{-1}$	(0.320430)	(0.2376529)
nC_6	$(0.5189140)10^{-6}$	(0.391898)	(0.146702)	(0.1962642)
nC_7	$(0.3899459)10^{-8}$	(0.320430)	$(0.823064)10^{-1}$	(0.1634869)
nC_8	$(0.2774415)10^{-10}$	(0.146702)	$(0.613920)10^{-1}$	(0.15771430)
400°Fnbp	$(0.3919305)10^{-23}$	$(0.823064)10^{-1}$	$(0.403689)10^{-1}$	(0.13192620)

TABLE X

A TYPICAL K-VALUE COMPARISON
(Temperature of system = 101.4272°F;
system pressure = 300 psia.)

Component	K by Eq. (4.1)[12]	K Predicted by NGPA-K and H Computer Program[27]	% Deviations* of Eq.(4.1), Chao-Seader
CH_4	13.160	7.2265	82.08643
C_2H_6	2.3493	1.8766	25.23529
C_3H_6	0.83178	0.80953	2.76614
C_3H_8	0.71869	0.71523	0.49936
iC_4	0.30580	0.36883	-17.07703
nC_4	0.22118	0.28217	-21.60361
nC_5	0.067759	0.12043	-43.72208
nC_6	0.021178	0.051549	-58.90146
nC_7	0.0067001	0.024251	-72.35963
nC_8	0.0020614	0.010666	-80.66223
400°nbp	0.00082049	0.00034035	141.32010

*These deviations have been graphically represented after this tabular comparison.

TABLE XI

K VALUE COMPARISON
(Temperature of system = 177.95°F;
system pressure = 300 psia)

Component	K by Eq. (4.1)[12]	K Predicted by NGPA K and H Computer Program[27]	% Deviations of Eq.(4.1) from NGPA
CH_4	14.187	10.134	40.0145
C_2H_6	3.580	3.5433	0.97837
C_3H_6	1.6060	1.5398	4.26963
C_3H_8	1.4148	1.3804	2.46669
iC_4	0.73010	0.73231	-0.32705
nC_4	0.56729	0.59534	-4.73707
nC_5	0.22948	0.27009	-15.07174
nC_6	0.092462	0.12298	-24.86394
nC_7	0.039250	0.059942	-34.57179
nC_8	0.016083	0.027903	-42.41550
400°Fnbp	0.0039829	0.0013377	197.2280

TABLE XII

K VALUE COMPARISON
(Temperature of system = 356°F;
system pressure = 300 psia)

Component	K by Eq. (4.1)	K Predicted by NGPA K and H Computer Program[27]	% Deviations of Eq. (3.1), Chao-Seader
CH_4	15.783	10.026	57.40648
C_2H_6	6.3747	12.445	-48.76491
C_3H_6	3.8185	4.1893	-8.84111
C_3H_8	3.5295	3.7298	-5.35945
iC_4	2.3141	2.1321	8.54508
nC_4	1.9699	1.8898	4.24471
nC_5	1.1062	1.1700	-5.44087
nC_6	0.62499	0.74646	-16.25551
nC_7	0.36513	0.4858	-24.81934
nC_8	0.20708	0.31092	-33.37605
400°Fnbp	0.046585	0.066487	-29.89444

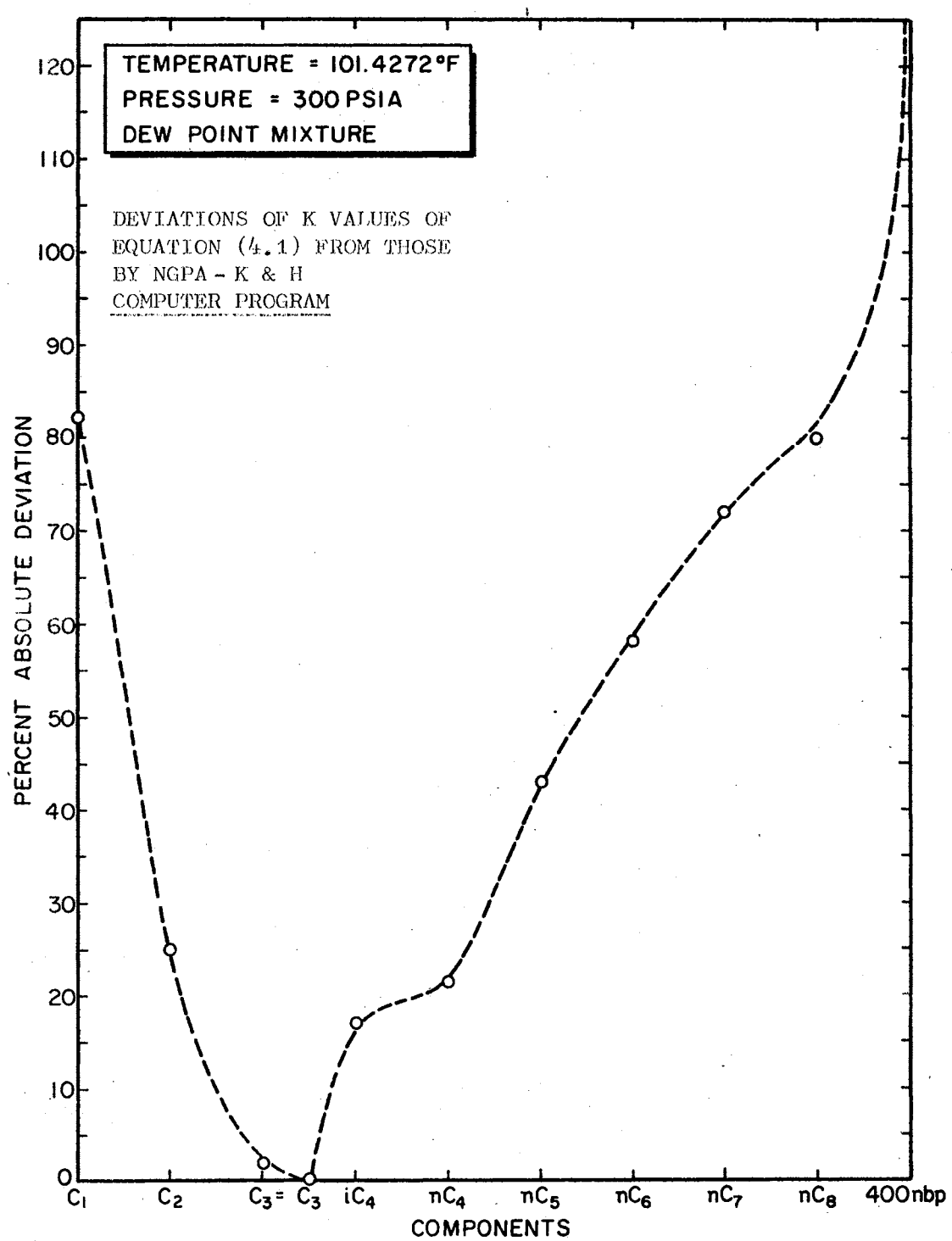

Figure 5. K Value Deviations

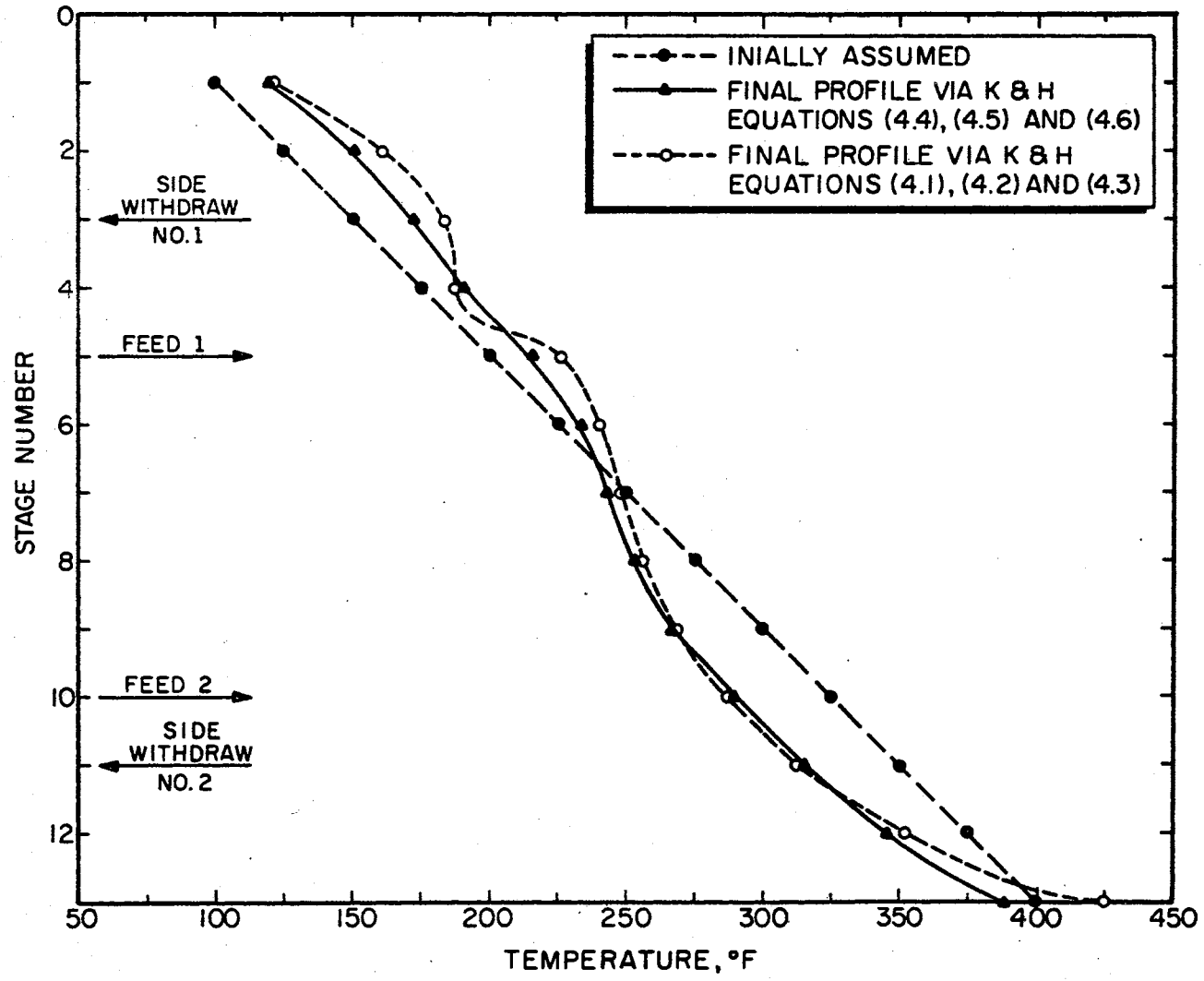

Figure 6. Temperature Profile Comparison for Example No. 4

Example Number 5

The feed to the column for this example is a hybrid-mixture containing both the discrete components and complex petroleum fractions. The example has been solved by two approaches:

1. Simpson's rule approach.
2. Hypothetical-component approach.

These two approaches differ in the way of handling the complex-fractions (i.e., C_7+). The Simpson's rule approach requires to break-up C_7+ into an odd-number of components and uses their pseudo-compositions for calculation purposes (22). For the application of hypothetical-component approach, one breaks the C_7+ fraction into an arbitrary number of narrow-boiling cuts. Average physical properties, i.e., critical temperature, critical pressure, accentric factor, $^{\circ}$API gravity, of these narrow-boiling cuts are used to predict their K and H values.

Description of Feed and Column

*Feed is a composite-mixture of discrete and complex-fractions.

Component	Mole fraction
C_2H_4	0.005
C_2H_6	0.005
C_3H_8	0.07
i-C_4	0.02
n-C_4	0.03
nC_5	0.12
nC_6	0.05
nC_7+	0.70

Molar TBP For C_{7+}

TBP	Mole fraction off
166°F	0.30
215	0.40
261	0.50
314	0.60
367	0.70
412	0.80
455	0.90
550	1.0

Specifications

Column pressure ..... 22 psia

Feed flash ..... L/F = 0.40

Saturated vapor part goes to stage number 6 and a co-existing liquid on the stage 7.

Top product ..... dew point vapor

Number of stages 10

Liquid side stream from stage number 3.

Rate of withdrawal ..... 110 lb moles/hr

Bottoms Rate ..... 156 lb moles/hr

Rate of Vapor feed ..... 483.86 lb moles/hr

Rate of liquid feed ..... 322.14 lb moles/hr

(Total Feed Rate ..... 806 lb moles/hr)

Feed temperature ..... 316.5°F

Reflux rate ..... 240 lb moles/hr

Feed Composition for Simpson's Rule Application (18 Components)

Component	Composition x_F
C_2H_4	0.005
C_2H_6	0.005
C_3H_8	0.07
i-C_4	0.03
nC_5	0.12
nC_6	0.05

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Pseudo-Compositions of C_7+ Fraction

166°F nbp	0.0233
204°F nbp	0.0935
232°F nbp	0.0467
266°F nbp	0.0935
303°F nbp	0.0467
340°F nbp	0.0935
377°F nbp	0.0467
407°F nbp	0.0935
435°F nbp	0.0467
475°F nbp	0.0935
550°F nbp	0.0233

First, the Simpson's rule solution has been presented and then the "Hypothetical-Component" method results have been tabulated. Finally, a comparison of temperature and flow profiles by two methods has been made. For this example, the two approaches yield essentially identical results.

TABLE XIII

TEMPERATURE AND FLOW-RATE PROFILE FOR EXAMPLE NUMBER 5
VIA THE APPLICATION OF SIMPSON'S RULE
FOR COMPLEX-FRACTIONS

Stage No.	Assumed Initial Values		Final Solution	
			Via K and H equations (4.4), (4.5) and (4.6), and Simpson's Rule	
	T_j °F	L_j	T_j °F	L_j
1	280.	240.	292.3	240.
2	288.	240.	332.8	230.2
3	297.	240.	347.3	215.5
4	305.	130.	356.6	97.0
5	313.	130.	360.9	91.3
6	322.	130.	363.6	91.3
7	330.	130.	414.3	501.6
8	386.	452.3	444.6	530.7
9	442.	452.3	463.1	532.9
10	498.	156.	481.7	156.0

Conversion of Pseudo-Compositions of Products Into Real Compositions

The compositions of the products reported in Table XIV, i.e., x_{d_i} x_{w_3}, and x_{b_i}, are the pseudo-compositions of the products. They have to be converted to real-compositions in order to get the TBP-assays of the products. A detailed treatment for this conversion has been presented by Taylor and Edmister (22).

For the "hybrid-mixtures," the compositions of the discrete components in the products, need not be processed further since Simpson's rule has been applied for the complex-fractions only. Thus, the following discussion applies for the complex-fractions (e.g., 166 nbp) only.

From the pseudo-compositions of the products in Table XIV, pseudo-feed compositions and product-rate specifications one gets (Dx_{d_i}/Fx_F), (Bx_{b_i}/Fx_F), and $(W_j x_{w_j}/Fx_F)$ for distillate, bottoms, and side-stream, respectively. For distillate product, the quantity Dx_{d_i}/Fx_F corresponds to (Ddm_D/Fdm_F) where dm_D is the real mole fraction of component "i" in distillate and dm_F is the real mole fraction of "i" in the feed. Therefore,

$$\frac{Dx_{d_i}}{Fx_F} = \frac{Ddm_D}{Fdm_F} \quad . \tag{5.1}$$

Thus, the ratio of pseudo-composition of a component "i" in distillate to its pseudo-composition in feed equals the ratio of real compositions of the same component in distillate and feed. Equation (5.1) can be used to construct TBP-assay of distillate. For this purpose, the quantitiy (x_{d_i}/x_F) should be plotted against m_F, and the area under the curve be computed between proper limits of m_F. For the present case,

m_F limits are 0.3 to 1.0. TBP-assay can now be constructed by following the procedure described by Edmister (7).

Areas can also be found with the computer. For this problem, area had been found with computer. The interval m_F = 0.3 to 1.0 was divided into 10 equal sub-intervals. The total area was found by summing up the areas of elementary sub-intervals. The areas of elementary sub-intervals can be approximated in several ways, e.g., Simpson's rule or chord-area method. Since the sub-intervals are sufficiently small, the chord-area approximation had been employed for calculating the areas of elementary sub-intervals. The TBP-assays are then constructed following the procedure of Edmister (7). The same procedure is repeated for side-stream and bottom assays. The feed and product TBP-assays are shown in Figure 7.

TABLE XIV

PRODUCT DISTRIBUTION FOR EXAMPLE NUMBER 5
VIA SIMPSON'S RULE APPLICATION

Component	x_{d_1}	x_{w_3}	x_{b_1}
Mole Fraction for Real Components			
C_2H_4	$(0.7428693)10^{-2}$	$(0.11590905)10^{-4}$	$(0.1153987)10^{-17}$
C_2H_6	$(0.7426397)10^{-2}$	$(0.228711)10^{-4}$	$(0.9760015)10^{-16}$
C_3H_8	(0.1041231)	$(0.132546)10^{-2}$	$(0.6178259)10^{-10}$
i-C_4	$(0.2968755)10^{-1}$	$(0.766705)10^{-3}$	$(0.8748876)10^{-9}$
n-C_4	$(0.4449108)10^{-1}$	$(0.134778)10^{-2}$	$(0.3123344)10^{-8}$
n-C_5	(0.176829)	$(0.105293)10^{-1}$	$(0.3278529)10^{-6}$
n-C_6	$(0.7285651)10^{-1}$	$(0.831464)10^{-2}$	$(0.2042785)10^{-5}$
Pseudo-Compositions for Complex-Fractions			
166°F nbp	$(0.3354315)10^{-1}$	$(0.396296)10^{-2}$	$(0.1000193)10^{-5}$
204°F nbp	(0.1340832)	$(0.268152)10^{-1}$	$(0.2791539)10^{-4}$
232°F nbp	$(0.6713565)10^{-1}$	$(0.120553)10^{-1}$	$(0.2156534)10^{-4}$
266°F nbp	(0.1266371)	$(0.626734)10^{-1}$	$(0.5406528)10^{-3}$
303°F nbp	$(0.5788539)10^{-1}$	$(0.553249)10^{-1}$	$(0.1558176)10^{-2}$
340°F nbp	$(0.9321749)10^{-1}$	(0.203673)	$(0.1689749)10^{-1}$
377°F nbp	$(0.2534067)10^{-1}$	(0.161292)	$(0.3948231)10^{-1}$
407°F nbp	$(0.1743383)10^{-1}$	(0.310502)	(0.2039064)
435°F nbp	$(0.1733877)10^{-2}$	$(0.94220)10^{-1}$	(0.1686631)
475°F nbp	$(0.1368148)10^{-3}$	$(0.469475)10^{-1}$	(0.4498429)
550°F nbp	$(0.1784474)10^{-7}$	$(0.213219)10^{-3}$	(0.1186458)

It is essential to make sure that convergence has been reached to the specified tolerance. This can be checked in many ways. One quick way to do this is by a component material balance around the whole column for typical components, as illustrated below.

$$Fx_{F_i} = Dx_{d_i} + Wx_{W_i} + Bx_B \ .$$

This will be demonstrated by an example, e.g., 204°F nbp component. (Refer to Table XIV.)

D	= 504 moles/hr	
B	= 156 moles/hr	
W	= 110 moles/hr	from the specifications
F	= 806 moles/hr	
x_{d_i}	= 0.1340832	
x_{b_i}	= 0.000027915	Table XIV
x_{w_i}	= 0.0268152	
x_{F_i}	= 0.0935	from specifications.

Thus, total output

$$Dx_{d_i} + Wx_{W_i} + Bx_{B_i} = (504)(0.1340832) + (110)(0.0268152) + (156)(0.000027915)$$

$$= 72.4 + 2.969 + .0004464$$

$$= 75.3694464 \ .$$

The moles of the same component in feed,

$$Fx_{F_i} = 806(0.0935)$$

$$= 75.39 \ .$$

These numbers are within the range of slide-rule accuracy and it has been concluded that convergence has been reached. Check can also be made with a computer. Similar balances hold for other components.

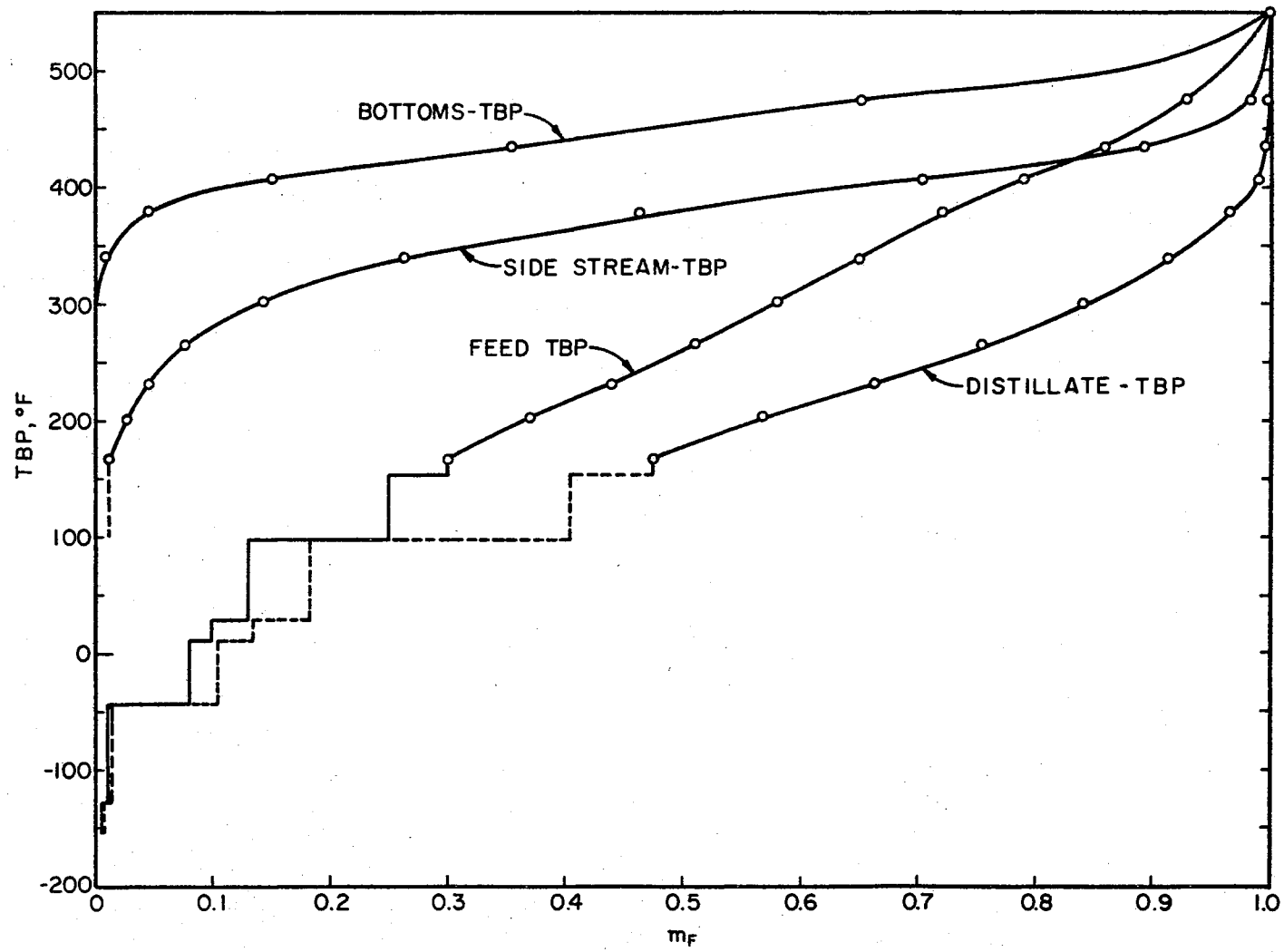

Figure 7. TBP Assays of Products (Via Simpson's Rule) for Example 5

Hypothetical Component Method

This method requires to break up C_7+ into a series of narrow-boiling cuts. The physical properties (P_c, T_c, °API, etc.) at their average boiling points are used to predict the K and H values of these components. For this example, C_7+ was broken up into 14 components, at interval of m_F = 0.05 on the TBP curve, i.e., the mole fraction of each narrow-boiling cut is 0.05. The average temperatures of all the narrow cuts are reported along with C_7+ break-up. The temperature and flow profiles obtained by this method agree closely with those obtained by Simpson's rule application.

Solution to Example Number 5

By Hypothetical-Component Method

Component	Mole fraction
C_2H_4	0.005
C_2H_6	0.005
C_3H_8	0.070
i-C_4	0.020
n-C_4	0.030
nC_5	0.120
nC_6	0.05
C_7+	0.70

C_7+ Break-Up

Mole fraction off	TBP °F	Average Temperature for K & H Values (°F)
0.3	166	
		180
0.35	194	
		200
0.4	215	
		225
0.45	240	
		247
0.50	261	
		274
0.55	289	
		297
0.60	314	
		325
0.65	342	
		352
0.70	367	
		380
0.75	392	
		402
0.80	412	
		425
0.85	432	
		442
0.90	455	
		475
0.95	480	
		518
1.0	550	

Feed flash (L/F = .4 P = 22 psia), Temperature 323.4°F

TABLE XV

TEMPERATURE AND FLOW-RATE PROFILE COMPARISON
FOR EXAMPLE NUMBER 5

Stage No.	Final Solution			
	Via Hypothetical-Component Method and K and H equations (4.4), (4.5) and (4.6)		Via Simpson's Rule and K and H equations (4.4), (4.5) and (4.6)	
	T_j °F	L_j	T_j °F	L_j
1	290.5	240.	292.3	240.0
2	330.5	230.8	332.8	230.2
3	344.8	215.3	347.3	215.5
4	354.2	96.4	356.6	97.0
5	358.7	90.3	360.9	91.3
6	361.6	88.7	363.5	91.3
7	412.1	496.	414.3	501.6
8	442.6	523.0	444.6	530.7
9	461.9	525.7	463.1	532.9
10	480.8	156.0	481.7	156.0
$Q(C) = (0.5698103)10^7$ Btu/hr			$Q(C) = (0.5725962)10^7$ Btu/hr	
$Q(R) = (0.8798178)10^7$ Btu/hr			$Q(R) = (0.8879458)10^7$ Btu/hr	
Iterations = 5			Iterations = 5	
Processor time 37.944 secs			Processor time 38.196 secs	
(IBM 360/65)			(IBM 360/65)	

TABLE XVI

PRODUCT COMPOSITIONS BY "HYPOTHETICAL-COMPONENT METHOD" FOR EXAMPLE NUMBER 5

	Component	x_{d_1}	x_{w_3} (side stream)	x_{b_1}
	C_2H_4	$(0.7428712)10^{-2}$	$(0.204835)10^{-4}$	$(0.1854383)10^{-16}$
	C_2H_6	$(0.7425425)10^{-2}$	$(0.366216)10^{-4}$	$(0.1002358)10^{-14}$
	C_3H_8	(0.1041015)	$(0.184985)10^{-2}$	$(0.2062781)10^{-9}$
	i-C_4	$(0.2963847)10^{-1}$	$(0.104313)10^{-2}$	$(0.2450487)10^{-8}$
	n-C_4	$(0.4440083)10^{-1}$	$(0.184393)10^{-2}$	$(0.8496599)10^{-8}$
	nC_5	(0.1761347)	$(0.153173)10^{-1}$	$(0.9372333)10^{-6}$
	nC_6	$(0.7194780)10^{-1}$	$(0.131458)10^{-1}$	$(0.6743780)10^{-5}$
- - - - -				
C_7 + Break-Up	180°F nbp	$(0.7132171)10^{-1}$	$(0.162091)10^{-1}$	$(0.1417689)10^{-4}$
	200°F nbp	$(0.6984902)10^{-1}$	$(0.233894)10^{-1}$	$(0.4937371)10^{-4}$
	225°F nbp	$(0.6751610)10^{-1}$	$(0.343409)10^{-1}$	$(0.1967322)10^{-3}$
	247°F nbp	$(0.6461798)10^{-1}$	$(0.485801)10^{-1}$	$(0.6024853)10^{-3}$
	274°F nbp	$(0.5937399)10^{-1}$	$(0.719007)10^{-1}$	$(0.2105794)10^{-2}$
	297°F nbp	$(0.5019132)10^{-1}$	(0.109144)	$(0.7839975)10^{-2}$
	325°F nbp	$(0.3539155)10^{-1}$	(0.149288)	$(0.3035468)10^{-1}$
	352°F nbp	$(0.1506110)10^{-1}$	(0.18083)	$(0.7870184)10^{-1}$
	380°F nbp	$(0.4212305)10^{-2}$	(0.112581)	(0.1645896)
	402°F nbp	$(0.8268706)10^{-3}$	$(0.52355)10^{-1}$	(0.2184665)
	425°F nbp	$(0.1129719)10^{-3}$	$(0.187726)10^{-1}$	(0.2447212)
	442°F nbp	$(0.1425552)10^{-4}$	$(0.627625)10^{-2}$	(0.2538744)
	475°F nbp	$(0.7310501)10^{-6}$	$(0.120452)10^{-2}$	(0.2573941)
	518°F nbp	$(0.6706184)10^{-8}$	$(0.882802)10^{-4}$	(0.2581837)

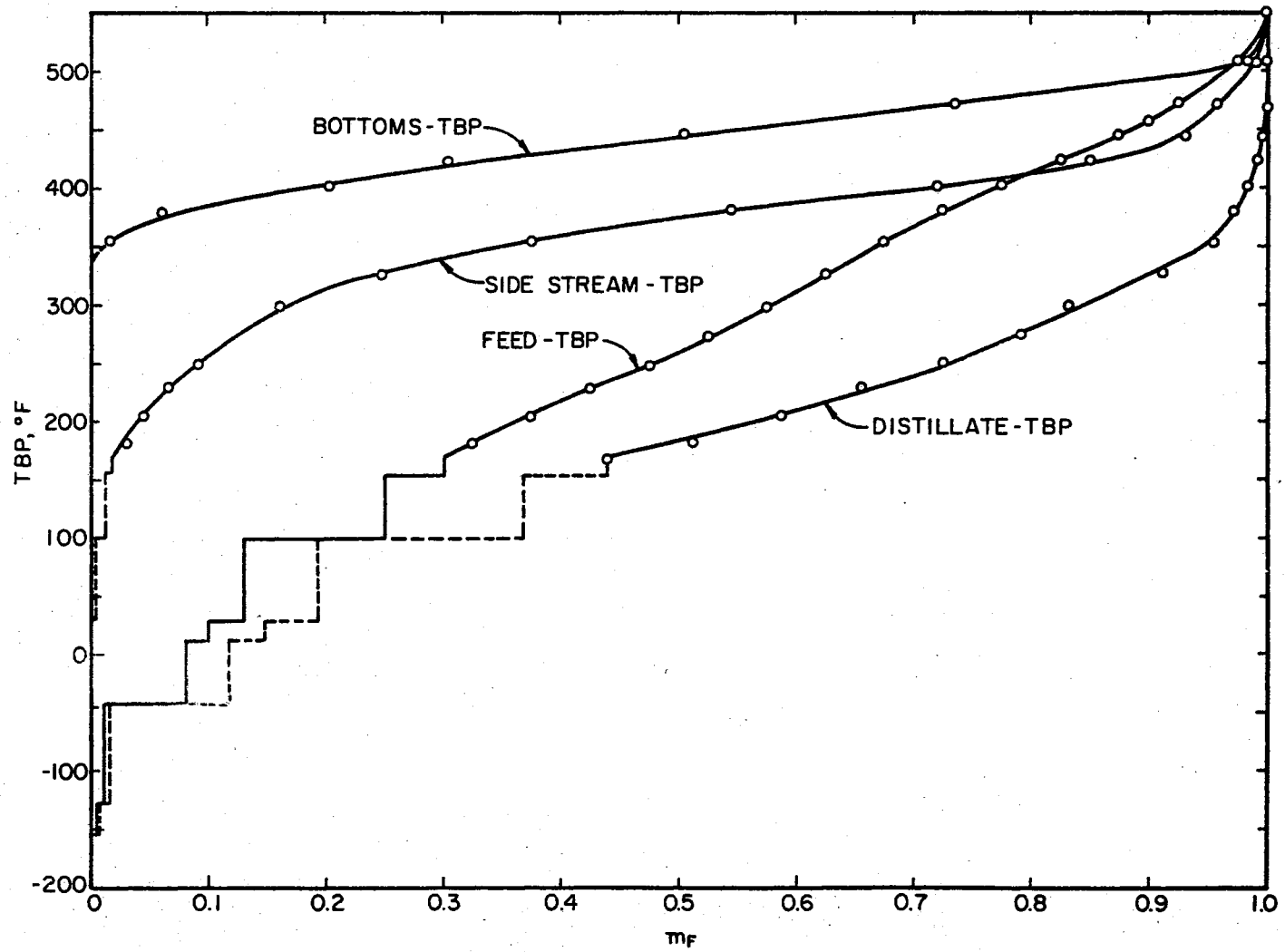

Figure 8. TBP Assays of Products (Via Hypothetical-Component Method) for Example 5

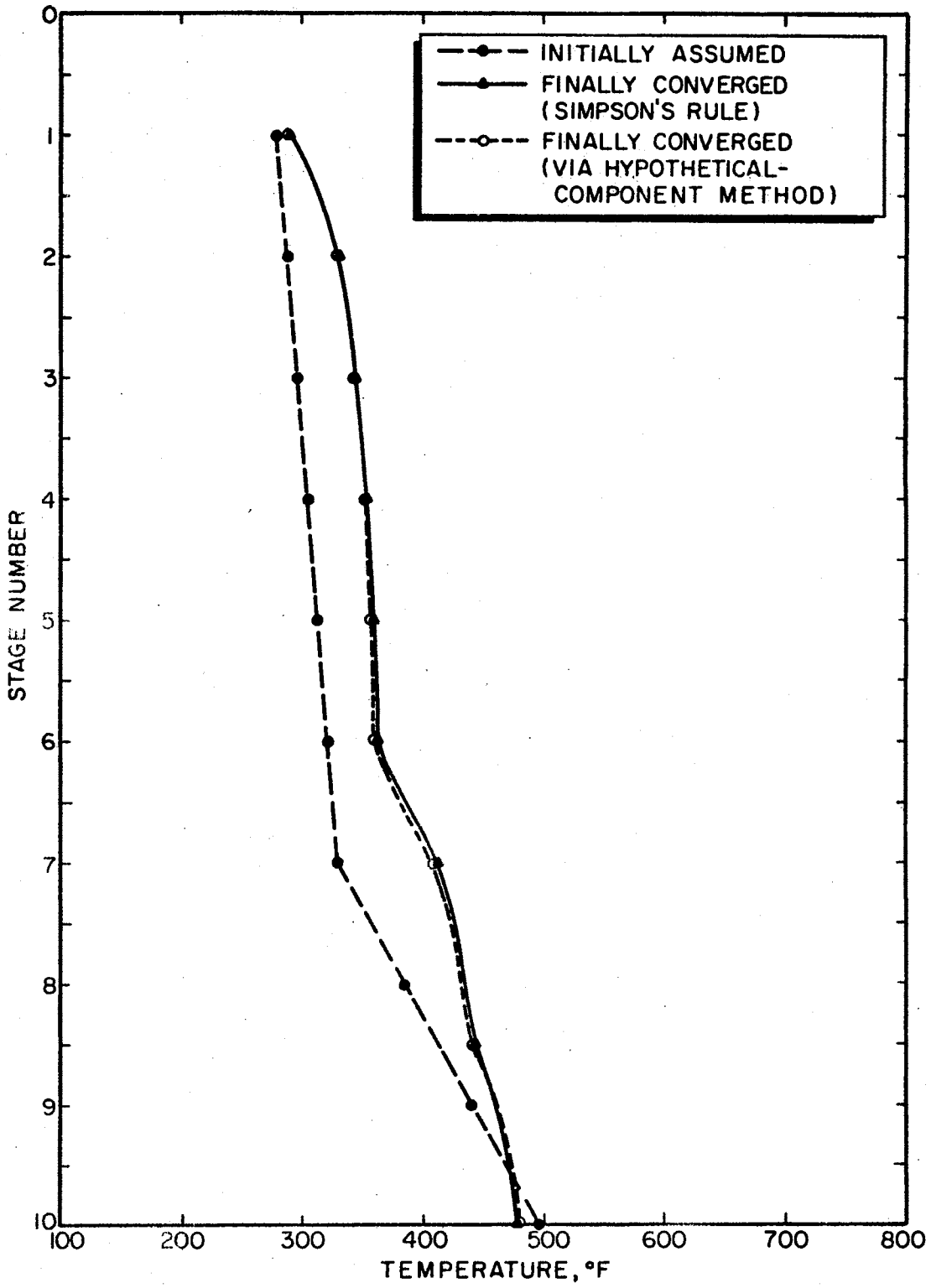

Figure 9. Temperature Profile Comparison (Example 5)

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

The primary objectives of this study were:

1. Adapt "Taylor's program" to the Oklahoma State University's IBM 360/65 computer.
2. Replace the Holland - K & H equations (12) that Taylor had used with the new forms of equations, i.e., Equations (4.4), (4.5), and (4.6). These new forms of K and H equations incorporate composition, temperature, and pressure effect on K and H values of components of a mixture.
3. Demonstrate the use of Simpson's rule for hybrid-mixtures. The use of Simpson's rule had been proposed by Taylor and Edmister (22) to handle complex-hydrocarbon treating columns.
4. Application of "Hypothetical-Component" method to hybrid-mixtures.
5. Prepare documentation and readable print-out format with explanation.

Conclusions

Based on the investigations conducted in this work, the following are concluded and recommended:

1. Adaptation of "Taylor's program" to IBM 360/65 installation at Oklahoma State University turned out to be fairly simple.

A few JOB CONTROL CARDS had to be changed.

2. The K values predicted by NGPA - K & H computer program differ appreciably from those obtained by Equation (4.1) (27). The deviations do not follow a specific trend with temperature; however, for methane, the NGPA - K & H computer program always predicts values lower than those by Equation (4.1) (27).
3. The temp. profile in enricher-section obtained by the use of new K & H equations, i.e., Equations (4.4), (4.5), and (4.6), is lower than that obtained by using Equations (4.1), (4.2), and (4.3).
4. The new-proposed K and H equations worked quite successfully for a variety of problems. Essentially, the convergence remains the same.
5. The hybrid-mixtures, i.e., mixtures containing discrete components and complex-fractions, can be solved with Edmister's Integral technique (4), via the use of Simpson's rule.
6. The present limit of the program to handle maximum of four feeds, four sidestreams, and fifty-two stages can easily be lifted by proper indexing.

Recommendations

1. During this investigation, it was observed that the limits listed in NGPA - K & H Program (27) for the reliable use of Chao-Seader correlation (6) had been exceeded frequently. The Lee-Edmister correlation (15) would cover a wider range of pressures and temperatures and would yield better K and H values.

2. A study should be made to include the ability to handle side-stream strippers.

3. Convergence characteristics of the method may be studied under special conditions, i.e., large number of stages and very small magnitudes of slopes, $\frac{\partial G}{\partial T}$. This may result in an improvement in the numerical stability of the method.

4. The computer-execution time may be reduced significantly by modifying the forms of equilibrium and heat balance functions. Taylor's program (23) uses the following forms for the functions:

$$G_r = \frac{b_{j-1} \sum_{i=1}^{c} h_{j-1,i} \ell_{j-1,i} + B_{j+1} \sum_{i=1}^{c} S_{j+1,i} H_{j+1,i} \ell_{j+1,i} + \sum_{i=1}^{c} f_{ji}^{v} H_{ji}^{v} + \sum_{i=1}^{c} f_{ji}^{l} h_{ji}^{v}}{\sum_{i=1}^{c} h_{ji} \ell_{ji} + \sum_{i=1}^{c} S_{ji} H_{ji} \ell_{ji}} - 1 \tag{3.20}$$

$$G_r = \frac{\sum_{i=1}^{c} \ell_{ji} K_{ji}}{L_j} - 1 \quad . \tag{3.21}$$

These functions have been obtained from heat balance and equilibrium relationships by dividing them throughout by their respective right-hand sides, and then deducting unity from both sides of the equations.

Thus, this formulation requires two instructions to computer, i.e., division and deduction.

Instead, if the right-hand side is deducted from left-hand side of an equation, functions similar to those in Equations (3.20) and (3.21) will be obtained; i.e.:

$$G_r' = \left(b_{j-1} \sum_{i=1}^{c} h_{j-1,i} \; \ell_{j-1,i} + B_{j+1} \sum_{i=1}^{c} S_{j+1,i} \; H_{j+1,i} \; \ell_{j+1,i} + \sum_{i=1}^{c} f_{ji}^{v} \; H_{ji}^{r} + \sum_{i=1}^{c} f_{ji}^{L} \; h_{ji}^{r} \right)$$

$$- \left(\sum_{i=1}^{c} h_{ji} \; \ell_{ji} + \sum_{i=1}^{c} S_{ji} \; H_{ji} \; \ell_{ji} \right) \qquad \text{Equation (3.20) Modified.}$$

$$G_r' = \sum_{i=1}^{c} \ell_{ji} \; K_{ji} - L_j \quad . \qquad \text{Equation (3.21) Modified.}$$

The formulation of G_r' requires only one operation, i.e., deduction. Since the functions are evaluated for each stage and in each iteration, a good amount of computer time may be saved by using Equations (3.20) and (3.21).

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APPENDIX A

THE NEWTON-RAPHSON ITERATION TECHNIQUE

The analytical solution of many equations encountered in chemical engineering is often extremely difficult, if not impossible. Under such circumstances, the iterative techniques offer valuable means for solution.

The Newton-Raphson technique is probably the most widely used technique for solution of algebraic or transcendental equations.

This section describes the Newton-Raphson technique, and illustrates its geometric-significance. The mathematical derivations follow.

Mathematical Derivations

Consider a function of one variable only. A Taylor's series expansion around $x^{(0)}$ leads to,

$$f(\overline{x}) = 0 = f(x^{(0)}) + (\overline{x} - x^{(0)})f'(x^{(0)}) + \frac{(\overline{x} - x^{(0)})^2}{2!} f''(x^{(0)}) + \cdots$$

$$= f(x^{(0)}) - \epsilon^{(0)} f'(x^{(0)}) + \frac{(\epsilon^{(0)})^2}{2!} f''(x^{(0)}) + \cdots \qquad (A.1)$$

where $\epsilon^{(0)} = x^{(0)} - \overline{x}$.

If the initial estimate of $x^{(0)}$ is a good one, i.e., $x^{(0)}$ lies in the neighborhood of $\overline{x}$, the desired value, then square of the error term may be neglected. So, one has,

$$f(x^{(0)}) - \epsilon^{(0)} f'(x^{(0)}) = 0. \tag{A.2}$$

or,

$$\epsilon^{(0)} = f(x^{(0)})/f'(x^{(0)}). \tag{A.3}$$

Consider the next improved estimate is made up as,

$$x^{(1)} = x^{(0)} - \epsilon^{(0)} \qquad \text{where } x^{(1)} \text{ denotes the next estimate}$$

$$= x^{(0)} - f(x^{(0)})/f'(x^{(0)}). \tag{A.4}$$

Repeating the process with $x^{(1)}$ and $\epsilon^{(1)}$ yields in the same way,

$$\epsilon^{(1)} = f(x^{(1)})/f'(x^{(1)}) \tag{A.5}$$

and

$$x^{(2)} = x^{(1)} - \epsilon^{(1)}. \tag{A.6}$$

Note that $x^{(2)}$ is the 2nd estimate of the independent variable.

Writing $\epsilon^{(1)}$ in functional form,

$$x^{(2)} = x^{(1)} - f(x^{(1)})/f'(x^{(1)}). \tag{A.7}$$

Substituting for $x^{(1)}$ from Equation (A-4),

$$x^{(2)} = x^{(0)} - \epsilon^{(0)} - \epsilon^{(1)}. \tag{A.8}$$

Thus, $x^{(2)}$ is a better estimate than $x^{(1)}$.

Now, by mathematical-induction, one can write,

$$x^{(r+1)} = x^{(r)} - \epsilon^{(r)} \tag{A.9}$$

$$\epsilon^{(r)} = f(x^{(r)})/f'(x^{(r)}). \tag{A.10}$$

Substitution of $\epsilon^{(r)}$ in Equation (A.9) yields,

$$x^{(r+1)} = x^{(r)} - f(x^{(r)})/f'(x^{(r)}) \ . \qquad (A.11)$$

Equation (A.11) is a "single-line" statement of Newton-Raphson method in one independent variable.

Equation (A.11) states that the function must be analytic in the region of estimates, and this often proves as a serious defect of this method, as will be seen later.

The geometric interpretation and certain cases where this method might not converge have been shown by Figures 10 and 11. Much depends on the initial estimate of x and shape of curve at or in the neighborhood of that point.

From Equation (A.11), one may say that the greater the slope of the function at a point, faster is the convergence. This, however, should not be extended further. In case of very steep slopes in neighborhood of selected points and when the value of the function is small compared to the slope at that point, the independent variable does not change at all and, in turn, the method does not converge. Algebraically, the convergence requirement may be completely stated as "$f'(x)$ and $f''(x)$ should not change in sign in the interval $(x^{(o)}, \bar{x})$ and $f'(x^{(o)})$ and $f''(x^{(o)})$ should have the same sign, in order to converge to $\bar{x}$ (11)." Geometrically, this implies that the curve should be smoothly convex to the x axis.

The discussion above applies to the functions of single independent variables.

The same method could be extended to the functions of more than one independent variable, by the use of "partial differential" type equations, as if $f_1(x_1, x_2) = 0$, $f_2(x_1, x_2) = 0$, then,

$$\frac{\partial f_1}{\partial x_1} \Delta x_1 + \frac{\partial f_1}{\partial x_2} \Delta x_2 = -f_1 \tag{A.12}$$

$$\frac{\partial f_2}{\partial x_1} \Delta x_1 + \frac{\partial f_2}{\partial x_2} \Delta x_2 = -f_2 \quad . \tag{A.13}$$

Simultaneous solution of (A.12) and (A.13) will give one Δx_1 and Δx_2; then,

$$(x_1)_{new} = (x_1)_{old} + \Delta x_1 \tag{A.14}$$

and

$$(x_2)_{new} = (x_2)_{old} + \Delta x_2 \ . \tag{A.15}$$

Equations (A.14) and (A.15) have been used for convergence of heat balance and equilibrium functions in the General-Solution of Taylor and Edmister.

Higher order methods may make convergence faster, however, the degree of complexity of the computations increase in the reverse order. The Newton-Raphson method is a good compromise between the speed of convergence and the complexity of calculations.

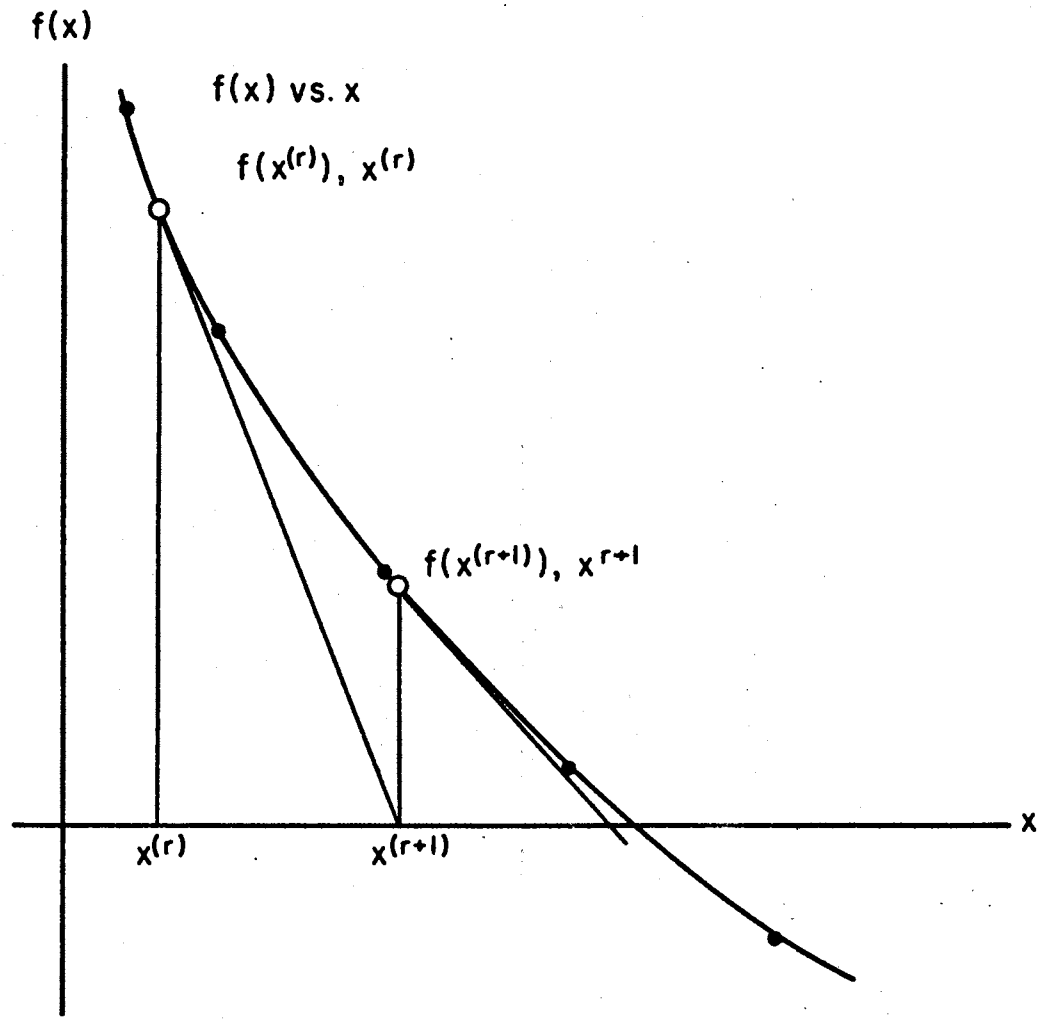
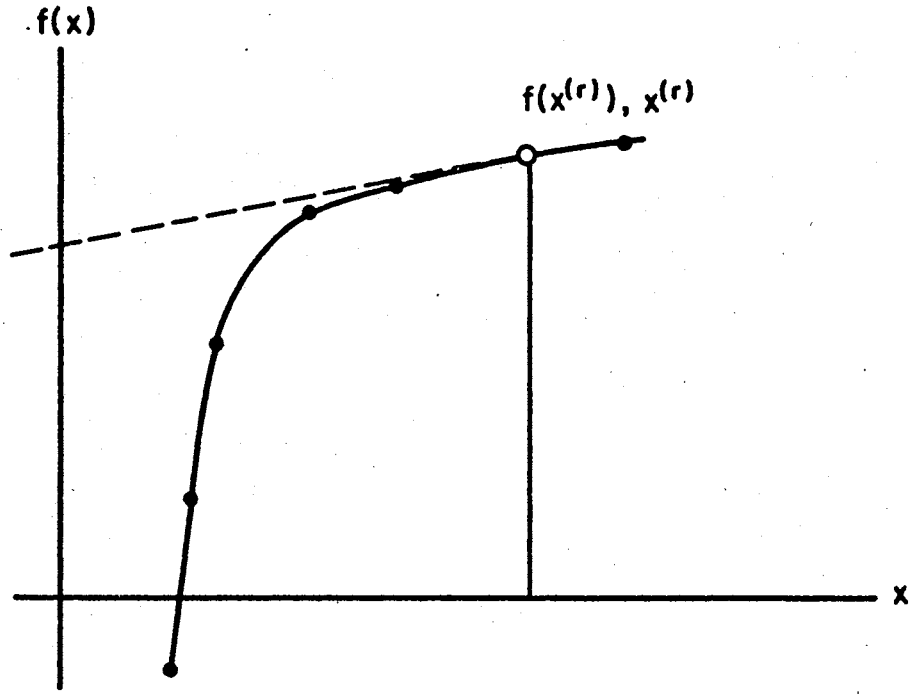


Figure 10. Geometric Interpretation of Newton-Raphson Method



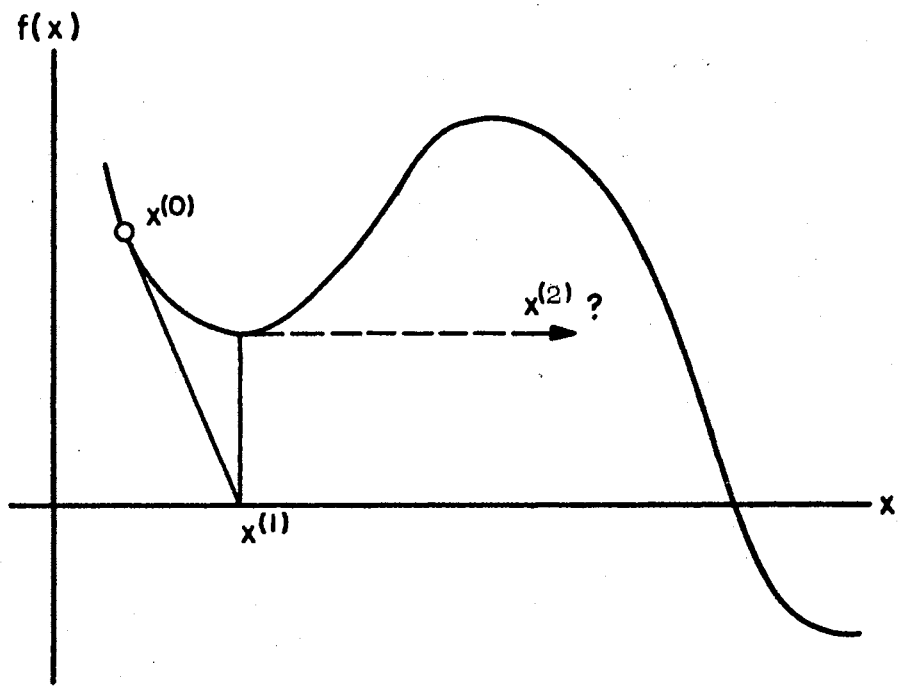


Figure 11. Typical Extreme Cases for Newton-Raphson Technique

APPENDIX B

ERBAR'S LINEAR REGRESSION CURVE-FIT

Regression is of utmost importance in relating a set of values of two different variables, e.g., in the field of chemical engineering, K or H's may be related to temperature or pressure by the use of regression on a set of data.

For the purpose of correlating K and H with temperature, Erbar's curve-fit (9) which employs the principle of linear regression, had been used. The first section of this appendix deals with the principle while the details of the curve-fit appear in the later section.

Linear Regression

By a linear regression model the author means an equation involving parameters and variables that is linear in parameters. The coefficients of x are known as parameters.

Consider that a curve of the form $\hat{y}_i = a_0 + a_1 x_i + a_2 x_i^2$ is to be fitted through a set of x-y points. It is believed that experimental errors in determination of x_i and y_i could be neglected.

The least-square criterion of curve-fitting seeks to fit the curve by minimizing the total sum of squares of deviations between calculated and given y_i values, i.e., values of dependent variable.

Mathematically this could be written as,

$$\sum (y_i - \hat{y}_i)^2 \longrightarrow \text{Minimum for a specific type of equation,} \qquad (B.1)$$

where

$$\hat{y}_i = a_0 + a_1 x_i + a_2 x_i^2 \ .$$

Substituting for $\hat{y}_i$ in Equation (B.1),

$$S = \sum (y_i - a_0 - a_1 x_i - a_2 x_i^2)^2 \qquad \text{minimum.} \qquad (B.2)$$

Note that in the Equation (B.2) y_i and x_i values are fixed and S, the sum of squares of deviations and the a_0, a_1, and a_2 are the variables. The type of equation that best fits a given x-y data could only be determined after trying various different forms of fit.

In order to minimize S, the derivatives of S with respect to all the variables should separately be zero.

Differenting Equation (B.2) with respect to a_0, a_1, and a_2 in turn, one obtains a set of equations as under,

$$\frac{\partial S}{\partial a_0} = (-1)(2) \sum (y_i - a_0 - a_1 x_i - a_2 x_i^2) = 0 \qquad (B.3)$$

$$\frac{\partial S}{\partial a_1} = (-2) \sum (y_i - a_0 - a_1 x_i - a_2 x_i^2)(x_i) = 0 \qquad (B.4)$$

$$\frac{\partial S}{\partial a_2} = (-2) \sum (y_i - a_0 - a_1 x_i - a_2 x_i^2)(x_i^2) = 0 \ . \qquad (B.5)$$

The equalities (B.3), (B.4), and (B.5) are generally referred to as Normal Equations. The number of equations required is determined by the

number of unknowns involved in the selected equation. The simultaneous solution of normal equations will give the required unknowns.

It is comparatively easier to solve these equations by a matrix-inversion technique. Expression the above equations in the matrix notation;

$$\begin{bmatrix} N & \Sigma x_i & \Sigma x_i^2 \\ \Sigma x_i & \Sigma x_i^2 & \Sigma x_i^3 \\ \Sigma x_i^2 & \Sigma x^3 & \Sigma x_i^4 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \Sigma y_i \\ \Sigma y_i x_i^2 \\ \Sigma y_i x_i \end{bmatrix} . \qquad (B.6)$$

To solve the matrix equation written above, one needs to have inverse of the first matrix on the left-hand side, then one has,

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} N & \Sigma x_i & \Sigma x_i^2 \\ \Sigma x_i & \Sigma x_i^2 & \Sigma x_i^3 \\ \Sigma x_i^2 & \Sigma x_i^3 & \Sigma x_i^4 \end{bmatrix}^{-1} \begin{bmatrix} \Sigma y_i \\ \Sigma y_i x_i \\ \Sigma y_i x_i^2 \end{bmatrix} . \qquad (B.7)$$

Note that the matrix whose inverse is required is a symmetric matrix.

Erbar's curve-fit program consists of a main program and an inversion subroutine. The main program could roughly be separated into three segments. The first segment performs reading the data and some of the writing activities. The second segment forms the entries of the matrix to be inverted, along with the entries on the right-hand side of matrix equation (B.6). These entries are supplied to the inversion subroutine, which performs the inversion task and subsequent solution of the matrix equation.

The third segment receives the values of constants from the inversion subroutine, and calculates $\hat{y}_i$'s with the use of the constants and the form of equation selected. This segment also performs the

activities of writing the values of constants, number of points, calculated values of y_i, the dependent variable and the observed values of y_i and x_i's.

As written, the program can handle 100 data points for a particular fit. The number could, however, be increased by increasing the dimension of x and y entries provided, which now is 100. In a similar way, the degree of polynomial fitted could also be increased. These two, however, are limited by round-off error. A series of problems could be solved only by one stacking since the program provides a statement to get out of DO LOOP when it encounters a zero value of the dependent variable; i.e., at the end of each problem, a card with a zero value of y_i or simply a blank card may be provided to switch over to the other problem. The program requires (the first READ statement) that each data set be preceded by an "identification card".

APPENDIX C

NGPA-K & H PROGRAM

In making stage-wise calculations, K_i and $\overline{H}_i$ values are essential. K and $\overline{H}$ are dependent on temperature, pressure, and composition. In Taylor's program for General-Solution, these values are fitted as functions of temperature at certain column-pressure, the composition effect being allowed by getting K-H values at feed-plate condenser and bottom.

In order to get K-H values, the computer program developed by Erbar, Persyn, and Edmister (27) has been used. Detailed description has been treated in NGPA manual; a summary has been presented here, however.

K_i is defined by,

$$K_i = \nu_i \gamma_i / \Phi_i \quad . \tag{C.1}$$

Φ_i is calculated by R-K equation of state, while calculation of γ_i employs the regular-solution theory of Scatchard and Hildebrand. ν_i values are obtained by curve-fits of Chao and Seader (6).

The calculation of $\overline{H}_i^V$ uses essentially the isothermal pressure-effect on enthalpy by R-K equation, while the liquid component, partial molal enthalpies are given by

$$\overline{H}_i^L = \overline{H}_i^0 - RTr_i^2 \; T_{c_i} \left[\left(\frac{\partial \ln \nu_i}{\partial T_{r_i}} \right)_{P_i} + \left(\frac{\partial \ln \gamma_i}{\partial T_{r_i}} \right)_{P, X} \right] . \tag{C.2}$$

The derivatives listed in bracket could be obtained for the corresponding functions for $\ln \nu_i$ and $\ln \gamma_i$. It should be noted that the second derivative in the bracket is the effect of composition on $\overline{H}_i^L$. The program also handles complex hydro carbon fractions by the use of modified Cavett's correlation which requires mean average boiling point, API gravity, and the molecular weight. These data, in turn, are used to calculate T_c, P_c, w, and V^L needed for further calculations.

The program makes available 11 different options to the user:

1.	B.P. temperature calculation,	P specified
2.	B.P. pressure calculation,	T specified
3.	D.P. temperature calculation	P specified
4.	D.P. pressure calculation	T specified
5.	$^L/F$ calculation	P, T specified
6.	$^L/F$ calculation over a range of T,	T, P, ΔT specified
7.	$^L/F$ calculation over a range of P,	T, P, ΔP specified
8.	Flash temperature calculation,	P, $^L/F$ specified
9.	Flash pressure calculation,	T, $^L/F$ specified
10.	T and $^L/F$ calculation,	$\underline{H}$, P specified
11.	P and $^L/F$ calculation,	$\underline{H}$, T specified

a. ν_i can be calculated both by Chao-Seader equations or Grayson-Streed equations, both of which are included in NGPA-K & H program as alternatives.

b. Hypothetical components could be handled by Cavett's method or by New-correlation. The latter needs fraction's specific-gravity and molecular weight. The method, however, has not been tested extensively.

Besides the required JCL, the cards mentioned below will be introduced as input. Here it has been assumed that the program has been stored in a particular computer-library.

1. Problem identification card with necessary codes to use the method desired.
2. If hypothetical component(s) is (are) present, its (their) physical properties. This card can be emitted if there is no such fraction present.
3. Type of calculation (one of 11 options) with necessary information.
4. Component-identification numbers. They are from 1 to 100 and in integer-type format.
5. Component-molal flow rates.

APPENDIX D

TAYLOR'S COMPUTER PROGRAM

The "General-Solution of Taylor and Edmister" has been programmed by Taylor (23). The program can handle multi-feeds, multi-draws and complex-hydrocarbon fractions treating columns. This compact program can handle as many as four feeds, four-side streams, and a maximum of 52 stages. The limit on the number of components that could be handled is 25. The indexing could be easily changed to increase the above mentioned limits.

First the program is fully described and then the block-diagrams are presented for a clearer explanation.

Description

The program consists essentially of a main program calling the subroutines INPUT, MATBAL, FCAL, DERCAL, and SIMQ. The functions of these subroutines will be described next.

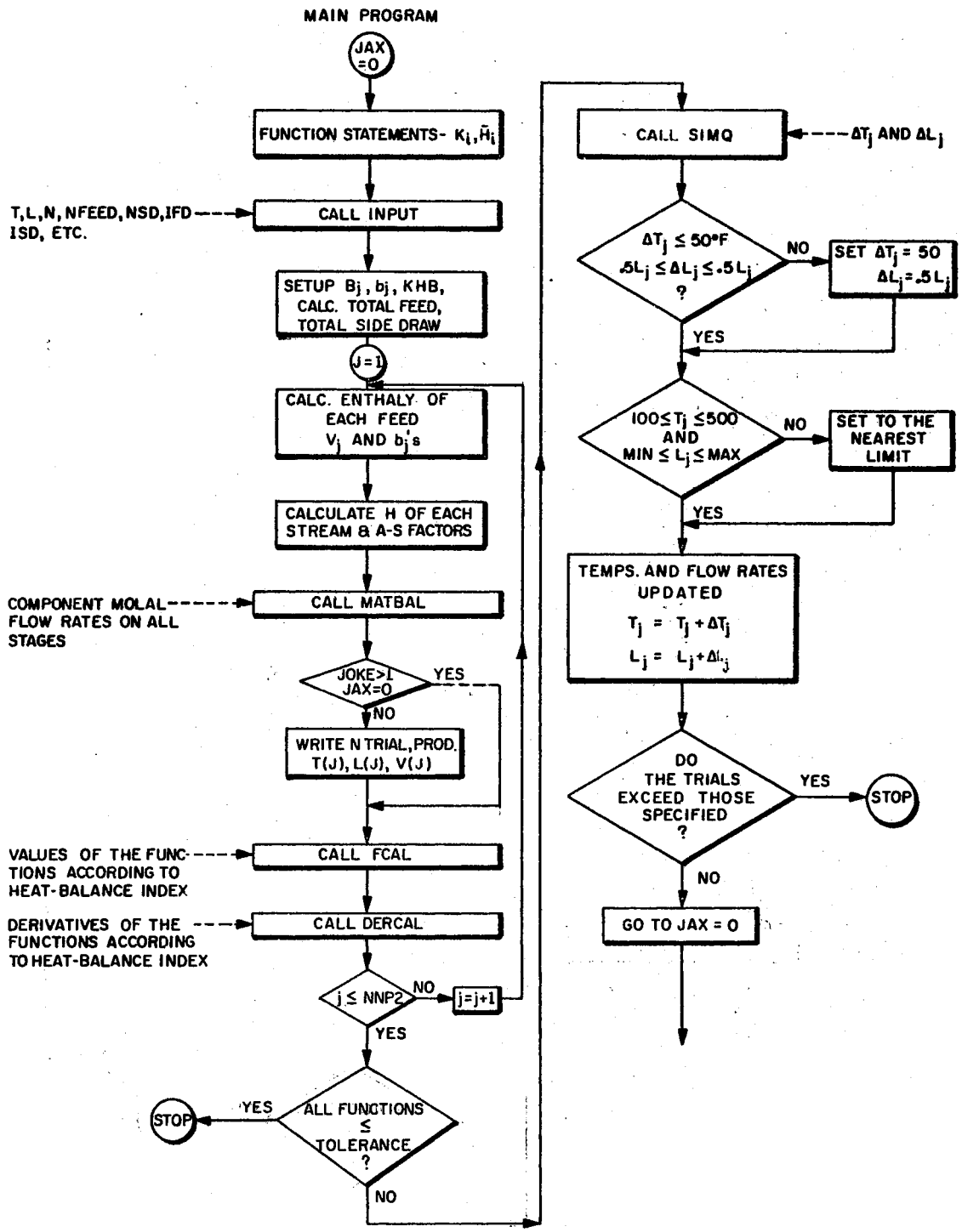
The subroutine INPUT reads the input data which includes maximum number of trials, number of components, number of stages, (including the condenser and the reboiler), type of problem (i.e., the unknown is to be determined from other specifications. 1 denotes that product compositions are to be determined at given reflux-rate while 2 shows the determination of reflux ratio at given key component distributions), number of feeds to the column, state of feed (i.e., vapor or

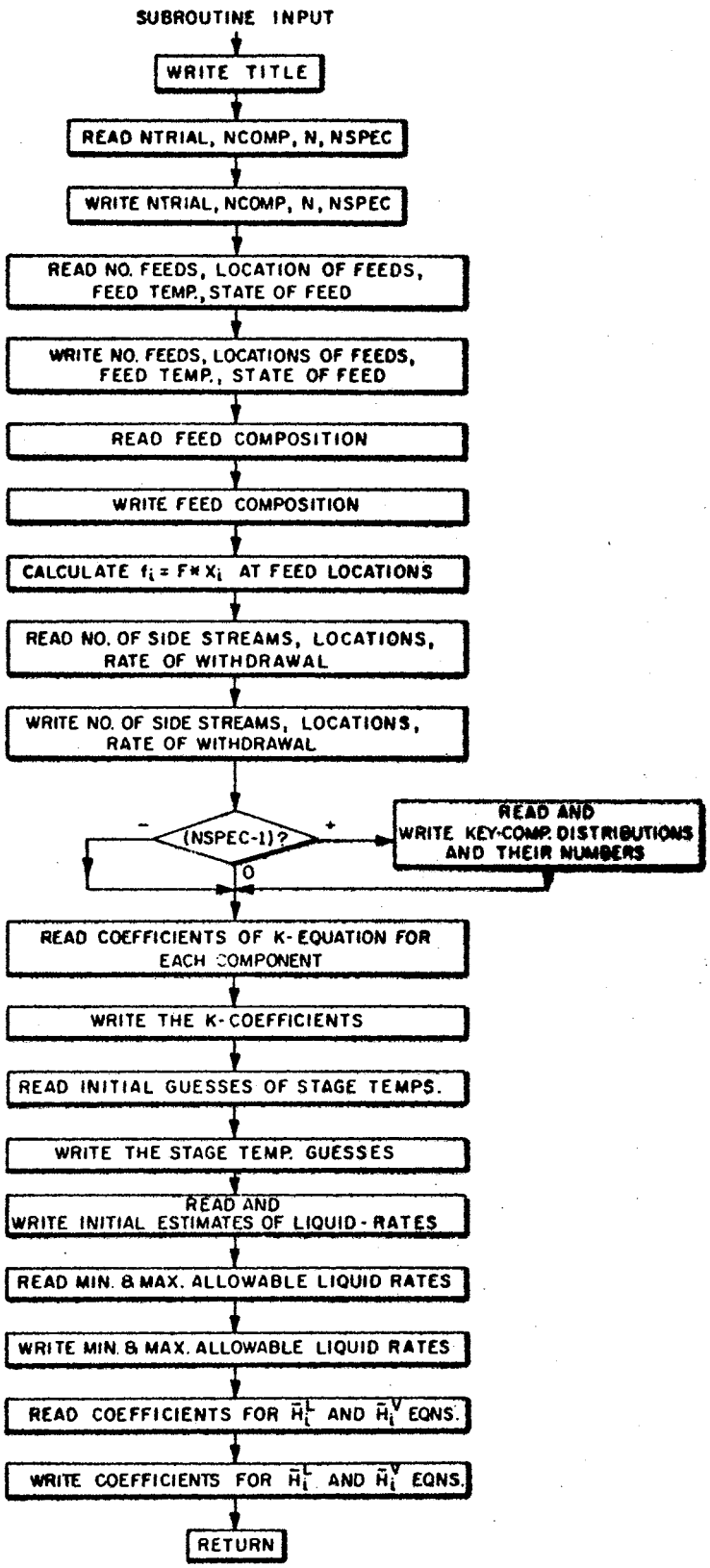
liquid), location of feed, etc. It should be noted here that a partially vaporized feed is treated as two-feeds, the saturated vapor going to the plate above while the saturated liquid going to the plate below. Additional variables include number of side streams, their locations, rates, assumed temperature profile for the column, assumed liquid rates, maximum and minimum allowable values of liquid rates, coefficients of K_i's and $\overline{H}_i$'s for all components at the column conditions. In addition to reading and supplying these values to the main program, this subroutine also sends the tolerance specified on heat balance and equilibrium functions. (i.e., Equations (3.20) and (3.21)). It is desired to have the values of these functions on all stages near to zero.

The subroutine MATBAL serves an important purpose of numerical accuracy: i.e., for the component material balance on all stages one has two sets of equations. (Equations (3.11) and (3.12). For relatively light components, i.e., components characterized by large stripping-factors (in the program they are defined as $\prod_{j=1}^{N} A_{ji} \leq 1$ where $\prod$ denotes the product on N stages), the use of equation sets 11 yields a better accuracy. Similar argument holds for heavy components $\left(\prod_{j=1}^{N} A_{ji} > 1\right)$ by using equation set 13. In the subroutine, the accuracy is achieved by using the arrangement of defining the quantities σ_{ji} and α_{ji} for lights and heavies, respectively. (Arrangement is given in Equations (3.24) and (3.25)). Arrangements have also been provided for the extreme cases such as all the components being light or all being heavy. After performing the separation task described above, the subroutine computes vapor and liquid rates of all components on all stages. The values are finally returned to the main program. The subroutine

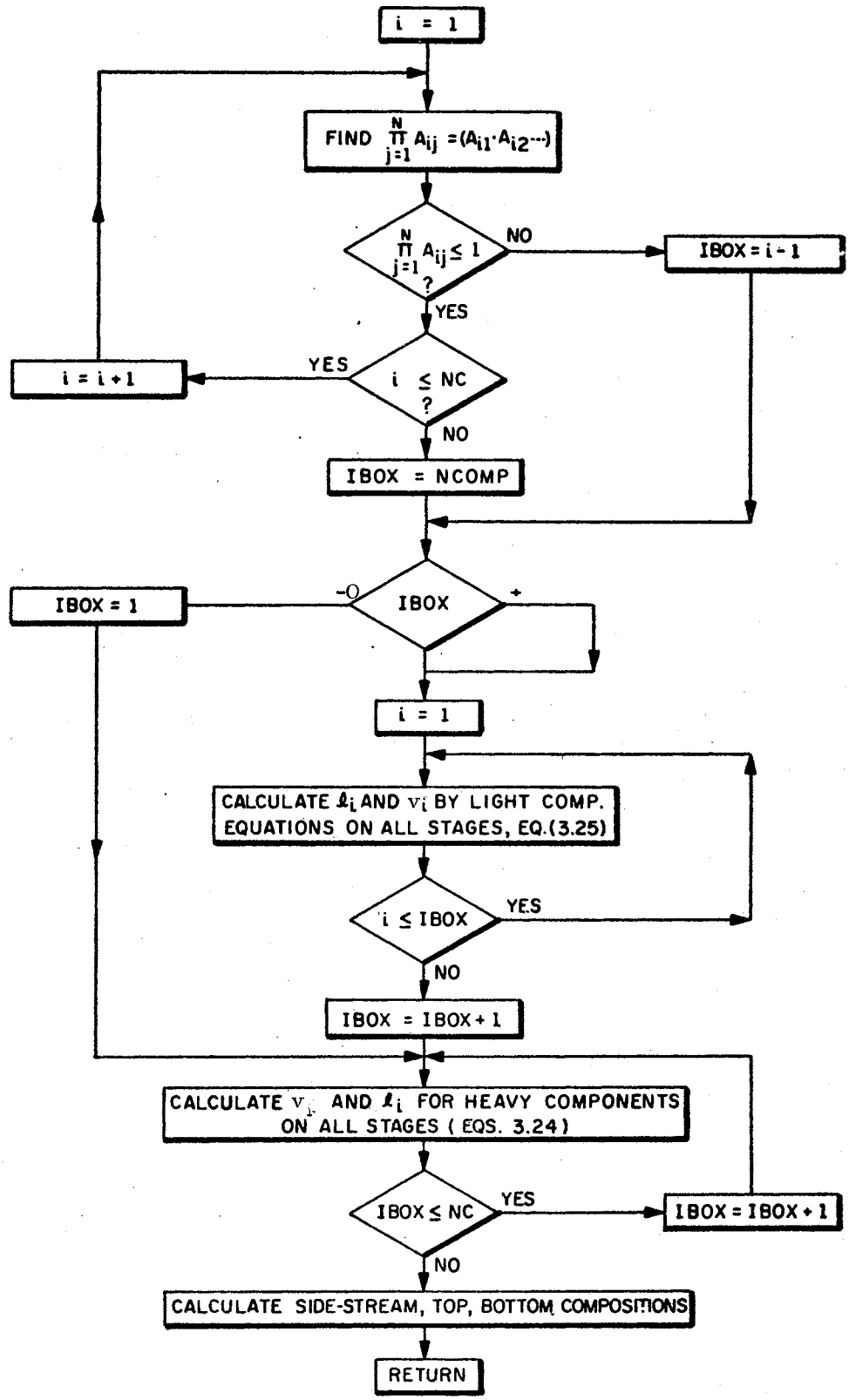
FCAL calculates the equilibrium and heat balance functions from the component - molar flow rates obtained from the subroutine MATBAL via the main program. Calculation of heat balance functions is not initiated until the equilibrium functions on each plate are less than or equal to 0.20. This is achieved by means of KHB, i.e., heat-balance index. KHB = 0 means no heat balance and KHB = 1 means heat balance inclusion. The subroutine DERCAL finds the derivatives of the functions calculated by the FCAL subroutine. These derivatives are needed to form the equation set (3.22).

The derivative values are returned to the main program. The subroutine SIMQ gets the values of the derivatives from the subroutine DERCAL via the main program. It solves the equation set (3.22) by the Gauss successive elimination and back substitution method. The values are sent to the main program which then updates the temperature and flow profile by adding ΔT_j and ΔL_j to the previous T_j and L_j, respectively. The calling and calculating and updating of the independent variables is repeated until desired accuracy is obtained. The program prints each trial, its temperature profile, and liquid-vapor traffics. As written, it can handle maximum of 52 stages, maximum 11 components, with temperature limits 100°F - 500°F. By changing the dimensions concerned, the program may handle even bigger columns and more components. The necessary block diagrams will now be presented.

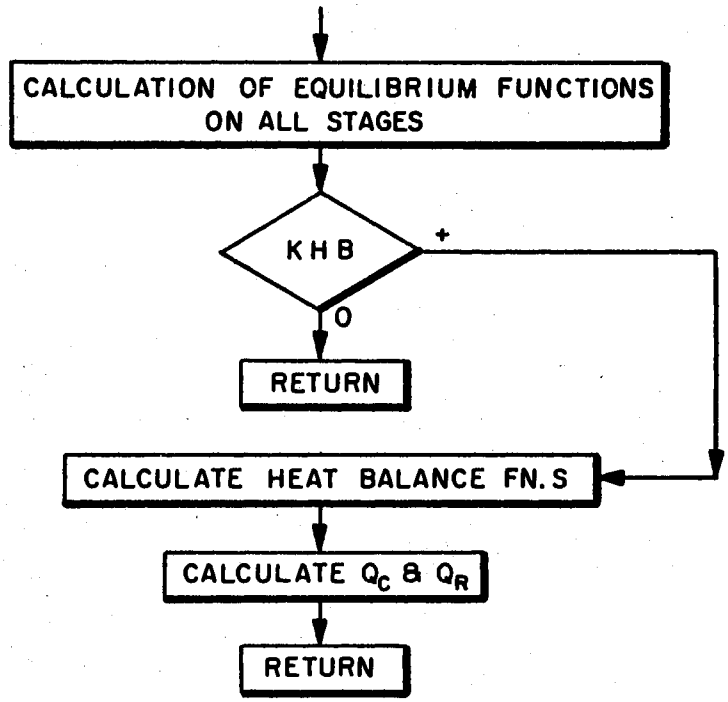

MAIN PROGRAM
JAX =0
FUNCTION STATEMENTS- $K_i, \bar{H}_i$
T,L,N, NFEED, NSD, IFD ISD, ETC.
CALL INPUT
SETUP B_j, b_j, KHB, CALC. TOTAL FEED, TOTAL SIDE DRAW
J=1
CALC. ENTHALY OF EACH FEED V_j AND b_j's
CALCULATE H OF EACH STREAM & A-S FACTORS
COMPONENT MOLAL FLOW RATES ON ALL STAGES
CALL MATBAL
JOKE>1 JAX=0
YES
NO
WRITE N TRIAL, PROD. T(J), L(J), V(J)
VALUES OF THE FUNCTIONS ACCORDING TO HEAT-BALANCE INDEX
CALL FCAL
DERIVATIVES OF THE FUNCTIONS ACCORDING TO HEAT-BALANCE INDEX
CALL DERCAL
j ≤ NNP2
NO
j=j+1
YES
ALL FUNCTIONS ≤ TOLERANCE ?
YES
STOP
NO
CALL SIMQ
ΔT_j AND ΔL_j
$\Delta T_j \leq 50°F$
$.5L_j \leq \Delta L_j \leq .5L_j$?
NO
SET $\Delta T_j = 50$
$\Delta L_j = .5L_j$
YES
$100 \leq T_j \leq 500$ AND MIN ≤ L_j ≤ MAX
NO
SET TO THE NEAREST LIMIT
YES
TEMPS. AND FLOW RATES UPDATED
$T_j = T_j + \Delta T_j$
$L_j = L_j + \Delta L_j$
DO THE TRIALS EXCEED THOSE SPECIFIED ?
YES
STOP
NO
GO TO JAX = 0

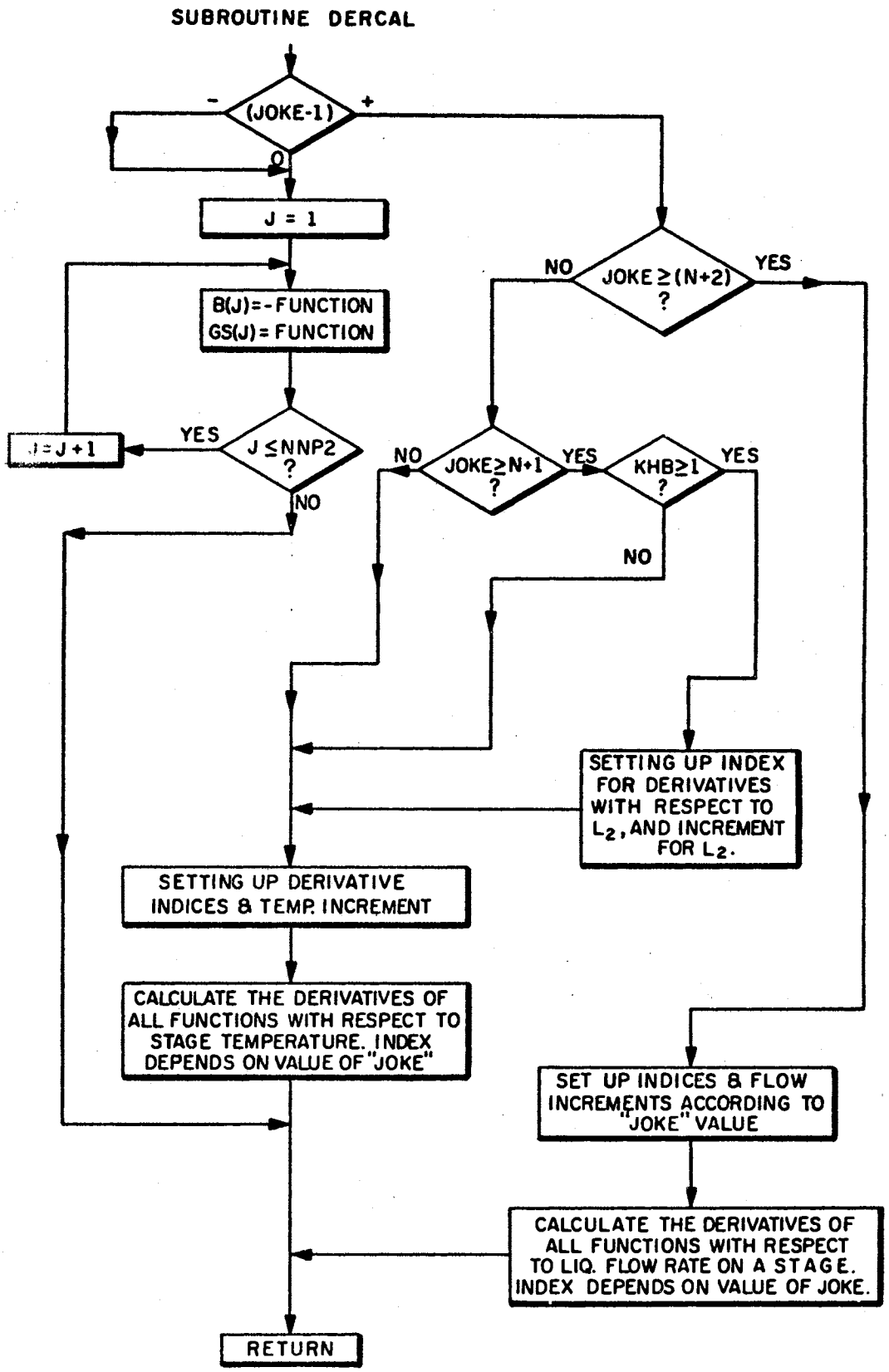

SUBROUTINE INPUT
WRITE TITLE
READ NTRIAL, NCOMP, N, NSPEC
WRITE NTRIAL, NCOMP, N, NSPEC
READ NO. FEEDS, LOCATION OF FEEDS, FEED TEMP., STATE OF FEED
WRITE NO. FEEDS, LOCATIONS OF FEEDS, FEED TEMP., STATE OF FEED
READ FEED COMPOSITION
WRITE FEED COMPOSITION
CALCULATE $f_i = F * X_i$ AT FEED LOCATIONS
READ NO. OF SIDE STREAMS, LOCATIONS, RATE OF WITHDRAWAL
WRITE NO. OF SIDE STREAMS, LOCATIONS, RATE OF WITHDRAWAL
(NSPEC-1)?
-
+
0
READ AND WRITE KEY-COMP. DISTRIBUTIONS AND THEIR NUMBERS
READ COEFFICIENTS OF K-EQUATION FOR EACH COMPONENT
WRITE THE K-COEFFICIENTS
READ INITIAL GUESSES OF STAGE TEMPS.
WRITE THE STAGE TEMP. GUESSES
READ AND WRITE INITIAL ESTIMATES OF LIQUID-RATES
READ MIN. & MAX. ALLOWABLE LIQUID RATES
WRITE MIN. & MAX. ALLOWABLE LIQUID RATES
READ COEFFICIENTS FOR $\bar{H}_i^L$ AND $\bar{H}_i^V$ EQNS.
WRITE COEFFICIENTS FOR $\bar{H}_i^L$ AND $\bar{H}_i^V$ EQNS.
RETURN

SUBROUTINE MATBAL

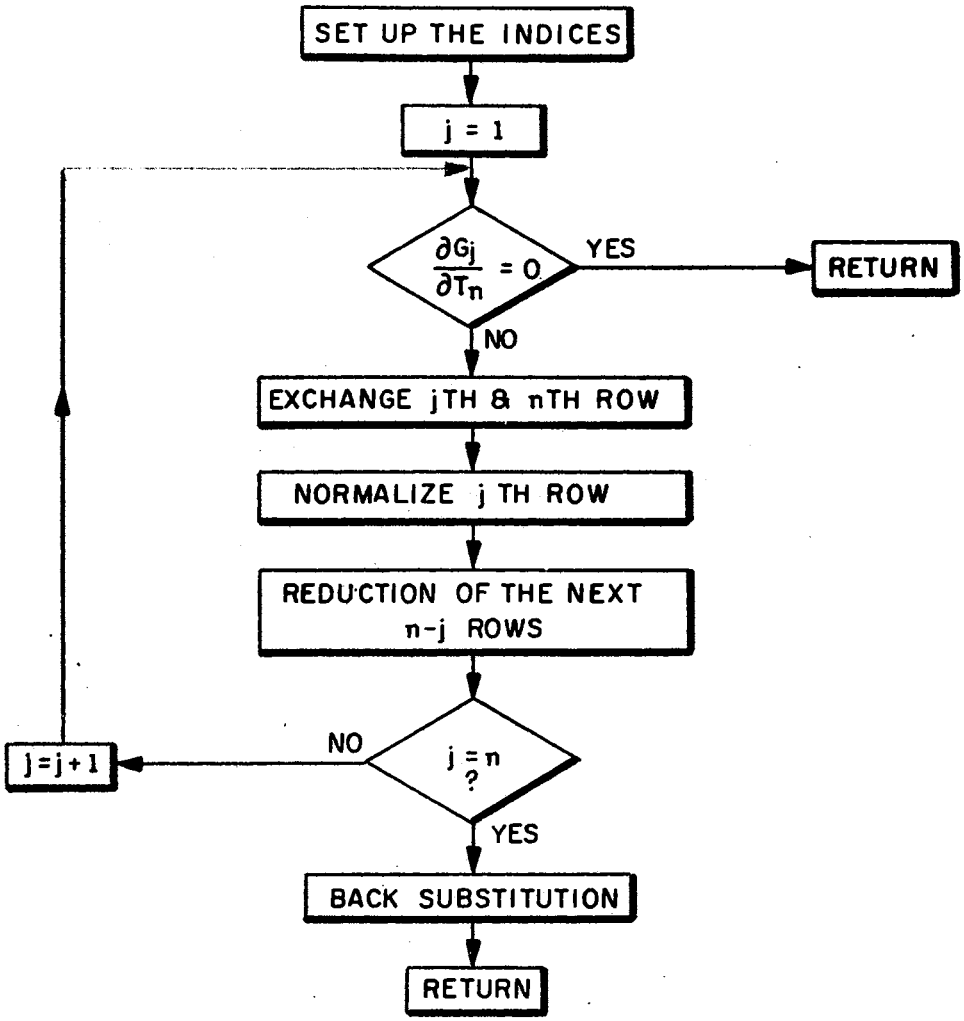


SUBROUTINE FCAL




SUBROUTINE DERCAL
(JOKE-1)
-
+
0
J = 1
B(J)=-FUNCTION
GS(J)=FUNCTION
J ≤ NNP2 ?
YES
NO
J=J+1
JOKE ≥ (N+2) ?
NO
YES
JOKE ≥ N+1 ?
NO
YES
KHB ≥ 1 ?
YES
NO
SETTING UP INDEX FOR DERIVATIVES WITH RESPECT TO L2, AND INCREMENT FOR L2.
SETTING UP DERIVATIVE INDICES & TEMP. INCREMENT
CALCULATE THE DERIVATIVES OF ALL FUNCTIONS WITH RESPECT TO STAGE TEMPERATURE. INDEX DEPENDS ON VALUE OF "JOKE"
SET UP INDICES & FLOW INCREMENTS ACCORDING TO "JOKE" VALUE
CALCULATE THE DERIVATIVES OF ALL FUNCTIONS WITH RESPECT TO LIQ. FLOW RATE ON A STAGE. INDEX DEPENDS ON VALUE OF JOKE.
RETURN

SUBROUTINE SIMQ



APPENDIX E

INPUT AND OUTPUT FOR TAYLOR'S PROGRAM

This section presents the details of preparing the input for the program. Data consistency is of prime importance in the input preparation. Frequently, the troubles arise because of the invalid input information. Equally important is reasonable specification of parameters, i.e., number of stages and reflux rate should be sufficient for producing the desired products.

Format Specifications

I, F, and E type formats are used in the program. The I and E type of formats should always be right justified, while the F type format must have a decimal point punched in their respective fields.

The discussion of input preparation follows.

Card Title	Variable Name	Input Format	No. of Cards Required	Minimum Value for Variable	Maximum Value for Variable	Remarks
Control Card 1	Max. no. of trials	I	1	1	-	Some integer number must be specified.
	Number of components	I	-	2	25	"
	Number of stages	I	-	3	52	This number includes both the partial condenser and a reboiler.
	Problem specification	I	-	1	2	1 = calculation of product distribution for a given reflux ratio and given number of stages. 2 = calculation of reflux ratio for a given key-component distribution and given number of stages.
Control Card 2	Total no. of feeds	I	1	1	4	
Feeds location and state identification cards.			NFD	1	4	NFD = Total number of feed streams to column.

(Continued)

Card Title	Variable Name	Input Format	No. of Cards Required	Minimum Value for Variable	Maximum Value for Variable	Remarks
	Entry for the first feed.	I	1			
	State of feed no. 1	I	-	1	2	1 = Liquid feed; 2 = 2 = vapor feed
	Temperature of feed 1	F	-	-	-	Temperature should be in degrees fahrenheit. Be sure to punch the decimal point. After finishing this first card for first feed, other cards must be filled in this order.
Feed rate Card	Molal rate of first feed.	F	1	-	-	
Feed composition Card(s)	Composition of first feed in mole fraction units.	F	?	0	1.0	Here the number of cards depends on the number of components. One card contains composition for 12 components. These should be repeated for other feeds, in the same order.
Number of side-stream cards.	Number of sidestreams	I	1	0	4	Only liquid sidestreams are allowed.

(Continued)

Card Title	Variable Name	Input Format	No. of Cards Required	Minimum Value for Variable	Maximum Value for Variable	Remarks
Locations of side-streams.	Stage numbers from where the streams are withdrawn.	I	1	0	4	
Sidestream rates	Molar rates of side-streams.	F	1	0	-	
Key component card.	Key component number.	I	1	-	-	Components are numbered starting with the lightest. The same should be repeated in this order for another key in bottom. Use this card only if problem specification = 2.
	Key component composition in distillate.	F	-	-	-	
K-coefficients card.	Coefficients a_0', a_1', and a_2'.	E	NC	-	-	NC means number of components in feed mixture. Arrange 3 coefficients per card; the components should be arranged in order of decreasing volatility. The constants describe the effect of temperature and pressure on K's.

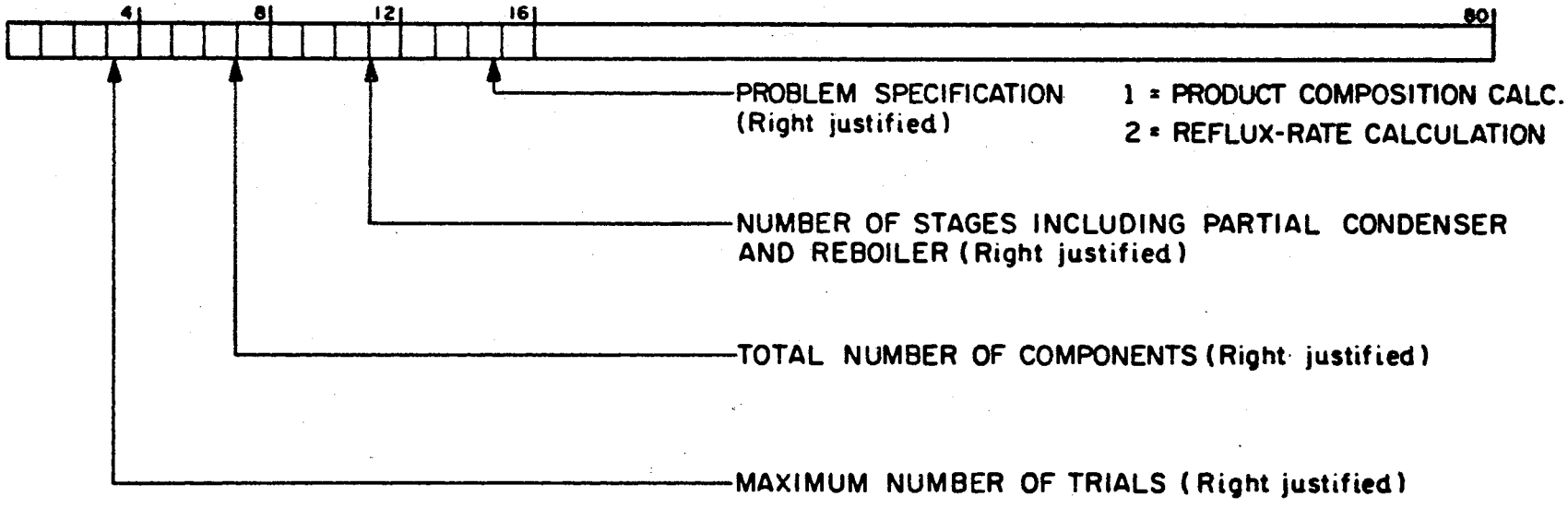
(Continued)

Card Title	Variable Name	Input Format	No. of Cards Required	Minimum Value for Variable	Maximum Value for Variable	Remarks
Temperature-profile card.	Temperature (Initially assumed profile)	F	NC	-	-	Temperature is in degrees fahrenheit. The number of cards depends on the number of stages. One card contains maximum of 12 entries.
Liquid-flow profile	Liquid-flow rate (Initially assumed)	F	?	-	-	Same as for temperature profile, except that the rate is in mole/time basis.
Minimum allowable liquid flow rates	Liquid flow	F	?	-	-	Some reasonable figure should be used. Same remarks as in temperature profile.
Maximum flow rate card.	Maximum flow rate	F	?	-	-	Use some big reasonable number. Rest of the comments are the same as in temperature profile.

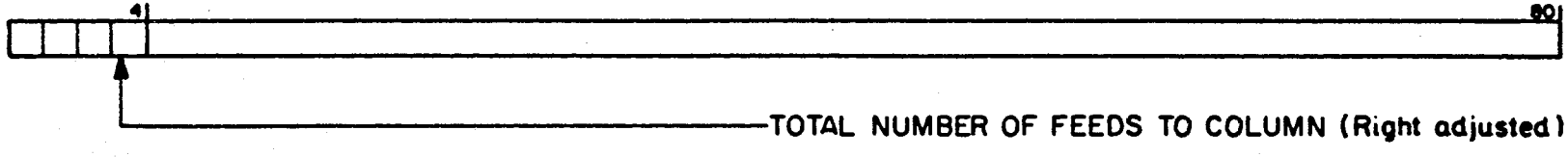
(Continued)

Card Title	Variable Name	Input Format	No. of Cards Required	Minimum Value for Variable	Maximum Value for Variable	Remarks
Enthalpy coefficients cards.	Coefficients b_0', b_1', b_2', c_0', c_1', c_2'	E	2NC	-	-	Total number of cards for this section are 2 times the number of components. One component will need two cards, one for its liquid-state coefficients and another for its vapor state coefficients. The components should be arranged from lightest to heaviest. These constants describe the effects of temperature, pressure, and composition on partial molal enthalpies.

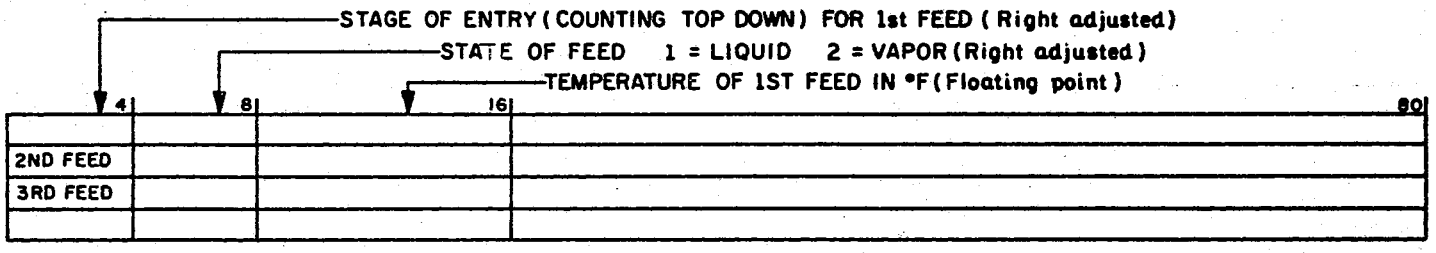
CONTROL CARD 1



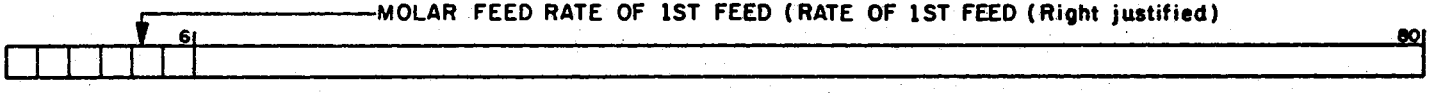
CONTROL CARD 2



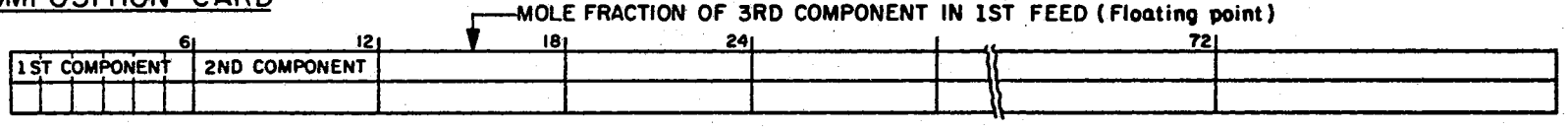
FEED IDENTIFICATION CARD



FEED RATE CARD

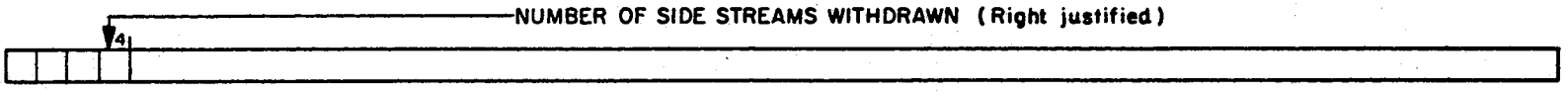


COMPOSITION CARD

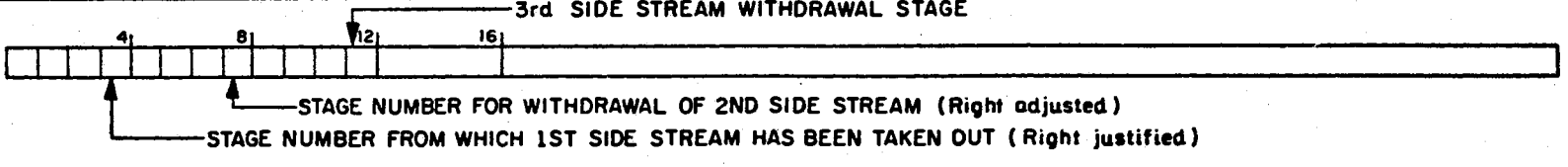


*REPEAT FEED RATE AND COMPOSITION CARDS FOR OTHER FEEDS

NUMBER OF SIDE STREAMS-CARD



SIDE STREAM LOCATION CARD



KEY COMPONENT CARD *(Use only if problem specification = 2, otherwise skip this card)*

MOLE FRACTION OF HEAVY IN DISTILLATE (Floating point)

LIGHT KEY NUMBER (FIRST IS THE LIGHTEST AND LAST IS HEAVIEST COMP.) (Right adjust)

MOLE FRACTION OF 2ND KEY IN BOTTOM (Floating point)

6	20	26	40
HEAVY KEY	HEAVY KEY	LIGHT KEY	LIGHT KEY

HEAVY KEY NUMBER (NO. 1 BEING FOR THE LIGHTEST) (Right justify)

COEFFICIENTS OF K EQUATION *(Proposed new form Eq. 4.4)*

a_0' (OBTAINED BY CURVE FIT) (USE 'E' FORMAT)

a_1' (E FORMAT)

a_2' (E FORMAT)

16	32	48	
FIRST COMPONENT a'	FIRST COMPONENT a'	FIRST COMPONENT a'	
SECOND COMPONENT a	SECOND COMPONENT a'	SECOND COMPONENT a'	
3RD COMPONENT			
4TH COMPONENT			
5TH COMPONENT			
6TH COMPONENT			

TEMPERATURE PROFILE CARD *(Initially estimated profile)*

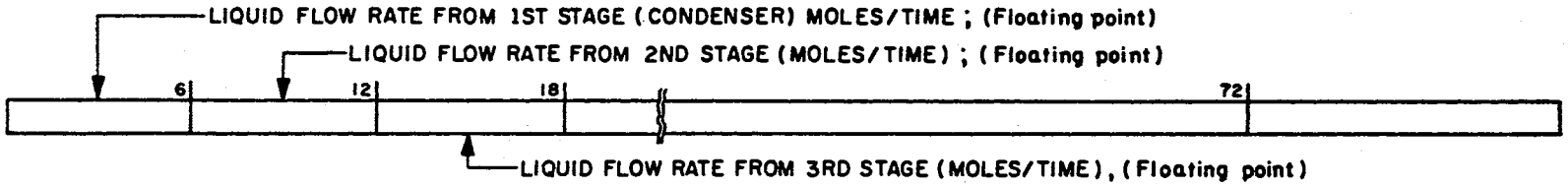
TEMPERATURE ON THE FIRST STAGE (CONDENSER) IN DEGREES FAHRENHEIT (Floating point)

6	12	18	24	30		72	

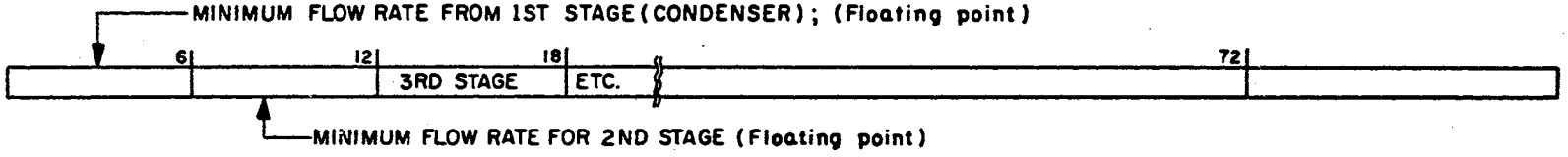
3RD STAGE

TEMPERATURE ON 2ND STAGE (DEGREES FAHRENHEIT) (Floating point)

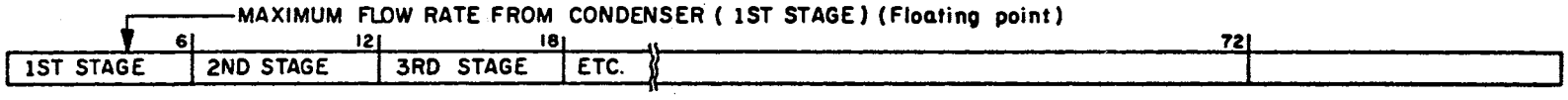
FLOW PROFILE CARD



MINIMUM ALLOWABLE FLOW RATE CARD



MAXIMUM ALLOWABLE FLOW RATE CARD



COEFFICIENTS OF ENTHALPY EQUATIONS CARDS *(Proposed new forms Eqs.(4-5),(4-6)* 'E' FORMAT

16	32	48	
COMPONENT 1 b_0'	COMPONENT 1 b_1'	COMPONENT 1 b_2'	COMPONENT 1 LIQUID COEFFICIENTS
COMPONENT 1 c_0'	COMPONENT 1 c_1'	COMPONENT 1 c_2'	COMPONENT 1 VAPOR COEFFICIENTS
COMPONENT 2 b_0'	COMPONENT 2 b_1'	COMPONENT 2 b_2'	
COMPONENT 2 c_0'	COMPONENT 2 c_1'	COMPONENT 2 c_2'	

Explanation of Print-Out Results

This section deals with the explanation of the print-out results from Taylor's program for "General-Solution".

Print-Out of Input Data

All the input data is printed. It is essential to check the input data to make sure that they are correct. The format for this print-out is identical to that given in input.

Print-Out of Results

The results are printed in the following order:

1. Iteration number, starting with "zero", i.e., the first iteration. This iteration is based on the initial values of temperature and flow-profiles supplied.
2. Product-distributions, starting with the distillate distribution, XD(I), and ending with the bottoms distributions, XB(I). The order in which the compositions are reported for a particular product is the same as in the input, i.e., starting with the lightest component and ending with the heaviest "E" format has been used for this print.
3. Temperature and flow profiles. Temperatures are reported in degrees fahrenheit units while the flow profiles are in molar-rate units. "F" format has been used here.
4. Condenser duty Q(C) and reboiler duty A(R) in Btu/time units. "E" format has been employed for this.

The foregoing will be made clear by some typical print-out presentation. This is only a qualitative representation.

Data

Data appears in the same order as that described in the INPUT section of this appendix. Trial results are shown below.

Trial No. 0

XD(I)	0.600000E00	0.200000E00	0.10000E00	0.100000E00
XS(J)	0.500000E00	0.40000E00	0.050000E00	0.049000E00

(If there are more than one sidestreams, they are printed in the same format. The order of their print is from top toward bottom.)

XB(I)	0.700000E00	0.100000E00	0.050000	0.150000E00

J	T(J)	L(J)	V(J)
1	122.7	102.0	28.0
2	126.2	102.0	130.0
3	127.0	102.0	130.0
4	127.8	102.0	130.0
.	.		
.	.		
.	.		
N	225.8	64.0	130.0

(Note that the column labeled J shows the numbering for the stages. "1" refers to the partial condenser while "N" refers to the reboiler.)

Q(C) = 0.0 Q(R) = 0.0

(For the first trial (Trial No. 0), this program usually does not take the heat balance and, thus, Q(C) and Q(R) are reported as zero.)

Trial No. 1

XD(I)

XS(J)

*REPEAT IN THE SAME ORDER AS FOR TRIAL '0', BUT DO NOT PRINT THE INPUT DATA.

APPENDIX F

NOMENCLATURE

A_{ji} = Absorption factor component i on stage j., $A_{ji} = L_j/(K_{ji}V_j)$.

β = Convergence-controller in Burman's method.

$\left.\begin{matrix} B_j \\ b_j \end{matrix}\right\}$ = Quantities defined by Equations (2.7) and (2.8).

dm = Mole fraction of complex-fraction in a mixture.

F_j^L = Total molal rate of flow of liquid feed that enters above stage j.

f_{ji}^V = Molal rate at which component "i" enters the column in the vapor part of feed below stage j.

f_{ji}^L = Molal rate at which component i enters the column in the liquid part of the feed above stage j.

F_j^V = Total molal rate of flow of vapor feed that enters below stage j.

G_r = Set of functions defined by Equations (2.20) and (2.21) also used in Equation (2.22).

$\left.\begin{matrix} \overline{H}_{ji} \\ \overline{h}_{ji} \end{matrix}\right\}$ = Partial molal enthalpies of component i, in vapor and liquid state, respectively, on the stage j.

$\left.\begin{matrix} H_{ji}^F \\ h_{ji}^F \end{matrix}\right\}$ = Partial molal enthalpies of component i in the vapor feed and liquid feed, respectively, on the stage j.

K_{ji} = Vapor-liquid equilibrium constant for the component i on the stage j.

L_j = Total molal rate of flow of liquid from stage j.

ℓ_{ji} = Molal rate of flow of component i from stage j.

N = Number of stages including the reboiler and partial condenser.

Q(C) = Condenser duty., Btu/hr.

Q(R) = Reboiler duty., Btu/hr.

S_{ji} = Stripping factor for component i on stage j.

T_j = Temperature of stage j.

V_j = Total molal flow rate of vapor from stage j.

v_{ji} = Molal rate of flow of component i from stage j.

W_j^L = Total molal rate of withdrawal of liquid sidestream that leaves below stage j.

W_j^V = Total molal rate of flow of vapor sidestream that leaves the column above stage j.

w_{ji}^L = Molal rate at which component i leaves the column in the liquid sidestream below stage j.

w_{ji}^V = Molal rate at which component "i" leaves the column in the vapor sidestream from stage j.

x_{ji} = Mole fraction of component "i" in the liquid stream leaving stage j.

x_{d_i} = Mole fraction of component "i" in the distillate; mole fraction of pseudo-component "i" in distillate for Simpson's rule application in Example 5.

x_{b_i} = Mole fraction of component "i" in the bottoms' mole fraction of pseudo-component "i" in bottoms for Simpson's rule use in Example 5.

x_{w_j} = Composition in mole-fraction units for the liquid sidestream from stage j. Mole-fraction of pseudo-component "i" in liquid sidestream from stage j. (for Simpson's rule, Example 5)

x_f = Feed composition on mole fraction basis; pseudo-feed composition for Simpson's rule in Example 5.

y_{ji} = Mole fraction of component "i" in the vapor stream leaving stage j.

$\left.\begin{matrix}\alpha\\ \sigma\end{matrix}\right\}$ = Quantities defined by Equations (2.24) and (2.25).

Φ_{ji} = Total molal flow-rate of component "i" in the vapor and liquid feeds that enter stage j.

φ_{ji} = Functions used in Equations (5.3), (5.4), and (5.5).

Subscripts

i = Component number. i = 1....c 1 designates the lightest component and c designates the heaviest one.

j = Stage number. Stages are numbered from top-down. Stage "1" is the partial condenser and N is the reboiler.

r = index used for functions, G_r, in Equations (3.20) and (3.21).

q, t = Summation and product indices, respectively, used in Equations (2.24) and (2.25).

D = Distillate

B = Bottoms

W = Sidestreams

F = Feed

Superscripts

F = Specifies that the associated enthalpy is for a feed stream.

L, V = Specifies that the associated quantity is for a liquid and vapor stream, respectively.

′ = Denotes the pseudo-compositions of feed in Example 5, and denotes the new equilibrium and heat balance functions in Chapter VI.

VITA

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