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A NEW METHOD FOR MULTISTAGE MULTICOMPONENT SEPARATION CALCULATIONS

by

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A THESIS

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ABSTRACT

A new calculational method for multistage, multicomponent separation processes is presented and evaluated in this thesis. A modified Newton-Raphson procedure is used to solve all the model equations simultaneously for corrections to temperatures, flow rates and compositions.

A detailed description of the method proposed by Tomich is given and the new method is compared with Tomich's method and with Bubble Point and Sum Rates procedures. These comparisons indicate that the new method is a significant improvement on current procedures.

The method is reliable for both distillation and absorber type problems, is particularly effective for reboiled absorber calculations and readily handles complex column configurations and the direct calculation of composition dependent equilibrium and enthalpy data.

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

7

CHAPTER I

INTRODUCTION

Multicomponent, multistage separation processes are commonly used in the chemical, natural gas, petroleum and related industries and the simulation and the design of these processes are often based on the steady state solution of the equations describing an equilibrium stage model. The model equations can be numerous and are nonlinear so that solution procedures are complex and numerical methods must be employed. As a consequence, many calculational methods have been proposed.

The traditional approach to designing a procedure for the rigorous solution of the model equations has been to avoid the larger problem of attempting to solve all equations simultaneously by partitioning the problem into smaller sub-problems. This is accomplished by decoupling the effects of certain variables and solving selected groups of equations in a particular order for compositions, temperatures and flow rates. The equations are grouped in such a way that solutions of the subsets are readily obtained after assuming certain variables. A convergence technique is used to link the subsets so that over-all consistency is obtained. Well known procedures such as those proposed by Lewis and Matheson (1), Holland (2), Thiele and Geddes (3), Wang and Henke (4) and Sujata (5) are in this category. Such methods, based on decoupling, have inherent difficulties in that the ability to converge will vary widely from application to application and there is no assurance that such methods will converge except experience with particular classes of problems.

A general algorithm that would be reliable for a broad range of feed components or column configuration involved, has been desired and it has been recognized that a method based on solving all equations simultaneously would probably provide the ultimate solution procedure. However this is a formidable problem because of the computational effort involved.

The Newton-Raphson technique is an effective method for solving complicated sets of non-linear algebraic equations and several authors have recently reported on the use of Newton-Raphson procedures in iterative methods designed to solve the equilibrium stage model equations for several or all variables simultaneously. Examples are the methods proposed by Tomich (6), Gentry (7), Naphtali and Sandholm (8), (9), Goldstein and Stahfield (10), Billingsley and Boynton (11), and Tierney and coworkers (12), (13). These methods generally require fewer iterations for solution than do the traditional methods and exhibit good convergence characteristics for a wide range of problems. However they have the disadvantage that the large number of partial derivatives that must be evaluated and the methods used for solving the linearized sets of equations generally result in large computer storage requirements and long computational time. The methods may become particularly unwieldy when composition dependent enthalpy and equilibrium data are employed. In addition several of these methods still decouple the effect of composition in that the component material balance equations are solved separately. Thus, there is still plenty of scope for devising more efficient methods for solving the equilibrium stage model equations. While working at Chiyoda Chemical Engineering and Construction Co. Ltd., the author developed the bsic theory for a new calculational procedure that showed promise of being an improvement on the procedures presently available.

The objectives of this investigation are:

(i) to elaborate the basic theory for practical use.

(ii) to prepare a computer program based on the new method and evaluate its performance for distillation and absorption type problems.

(iii) to prepare a computer program based on the algorithm suggested by Tomich (6), which appears to be one of the most promising of the recent methods, and to compare its performance with the new algorithm.

The new method makes use of a linearization technique which is actually a multivariate Newton-Raphson procedure. The method solves all the linearized equilibrium stage model equations simultaneously. Convenient matrix structures are formulated by the use of prudent assumptions when selecting the linearized equations and these matrices are solved using a procedure for inverting tri-diagonal matrices that had previously been developed by the author. The method is characterized by the simultaneous solution of the linearized equations and by the use of new matrix manipulation procedures. In addition the new algorithm takes into account the composition dependency of enthalpy and equilibrium data.

In the computer programs the Chao-Seader correlation was used exclusively. It is representative of generalized correlation procedures and it has been widely accepted for use in the hydrocarbon processing industries.

CHAPTER 2

LITERATURE REVIEW

2.1 Equilibrium Stage Model

A generalized equilibrium stage model is shown as Figure 1. This model may be used to represent a wide range of separation devices including complex column configurations where multiple feeds, side streams and/or side heaters and coolers may be employed. Each stage in the model is assumed to be an equilibrium stage, that is, the streams leaving a stage are assumed to be in thermodynamic equilibrium.

The steady state model equations for any stage j and any component i may be represented as follows.

(1) Equilibrium Relations:

$$y_{i,j} = K_{i,j}x_{i,j} \qquad (2\text{-}1)$$

(2) Component Material Balances:

$$F_jZ_{i,j} + L_{j-1}x_{i,j-1} + V_{j+1}y_{i,j+1} - (L_j+SL_j)x_{i,j} - (V_j+SV_j)y_{i,j} \equiv C_{i,j} \qquad (2\text{-}2)$$

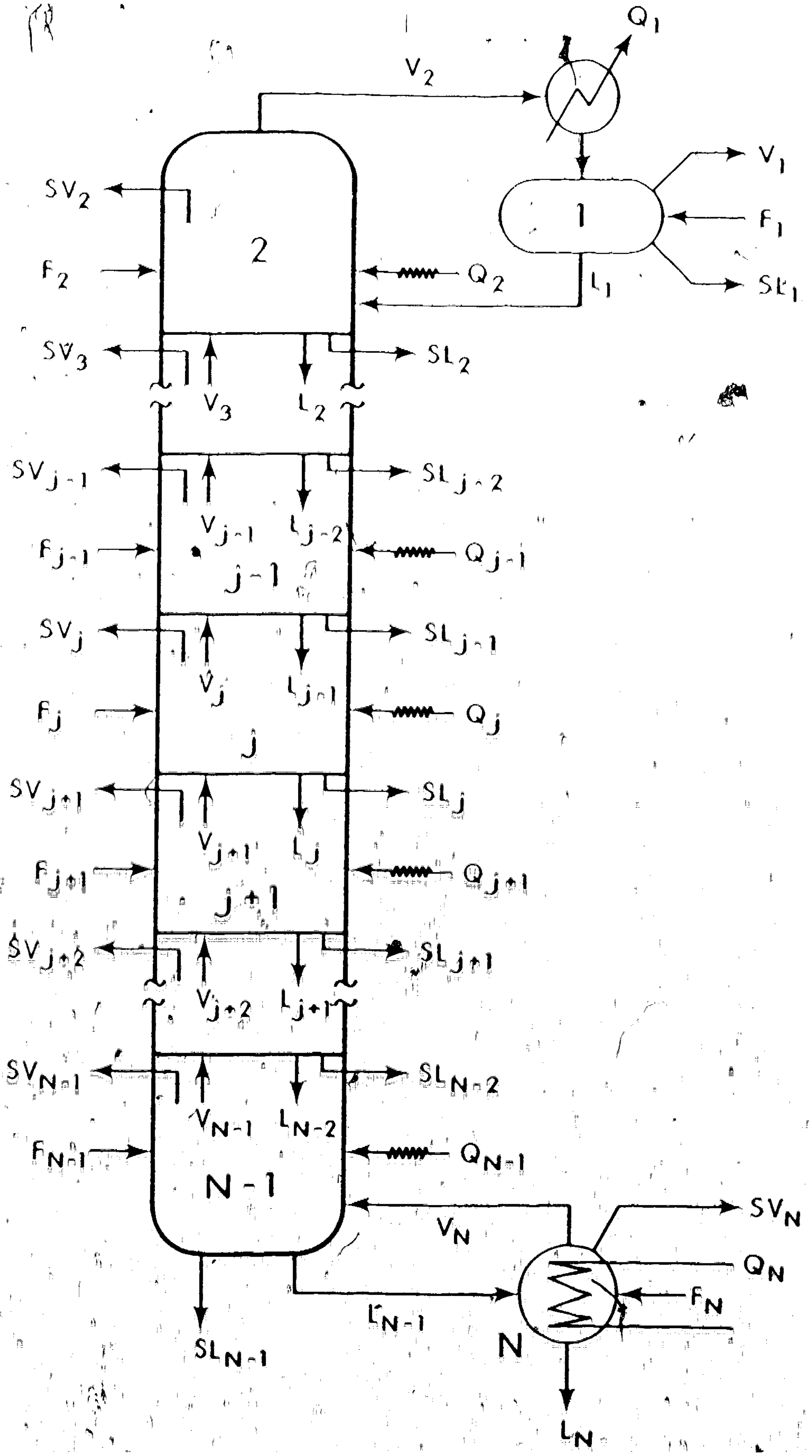
(3) Energy Balance:

$$F_jH_{F,j} + Q_j + L_{j-1}h_{j-1} + V_{j+1}H_{j+1} - (L_j+SL_j)h_j - (V_j+SV_j)H_j \equiv E_j \qquad (2\text{-}3)$$

(4) Summation Equation:

$$\sum_{i=1}^{NCP} x_{i,j} - 1.0 \equiv S_j \quad \text{or} \quad \sum_{i=1}^{NCP} y_{i,j} - 1.0 \equiv S_j \qquad (2\text{-}4)$$

FIGURE 1: Generalized Equilibrium Stage Model



(5) Over-all Material Balance:

$$F_j + L_{j-1} + V_{j+1} - (L_j+SL_j) - (V_j+SV_j) = M_j \quad , \qquad (2\text{-}5)$$

The component material balance equations are often combined with the equilibrium relations as,

$$F_j Z_{i,j} + L_{j-1}x_{i,j-1} + V_{j+1}K_{i,j+1}x_{i,j+1} - (L_j+SL_j)x_{i,j} - (V_j+SV_j)K_{i,j}x_{i,j} = C_{i,j} \qquad (2\text{-}6)$$

There are $N \times (2 \times NCP+3)$ independent equations and $N \times (2 \times NCP+3)$ unknowns provided that the following quantities are specified,

(i) the number of equilibrium stages

(ii) the pressure at each stage

(iii) the rates, compositions and conditions of all feed streams

(iv) the rates of all side streams

(v) the amount of heat added or removed from each stage including any condenser or reboiler.

The solution of the model equations then requires finding values for the temperatures, T_j's, the liquid and vapor flow rates, L_j's and V_j's, and the phase compositions, $x_{i,j}$'s and $y_{i,j}$'s, at each stage such that M_j, $C_{i,j}$, E_j and S_j are all equal to zero.

The specifications listed above are those normally made for an absorber type problem. It is permissible and often desirable to interchange some of the specified variables with the unknown variables. For distillation problems it is usual to specify the amount of top product and the reflux ratio and to treat the reboiler and condenser loads as unknowns. Similarly, the top vapor flow rate, V_1, is usually specified for reboiled absorber problems and the reboiler load is treated as an unknown.

2.2 Solution Methods

In general, the equilibrium stage model equations form a quite complicated and nonlinear system so that numerical techniques are required in order to obtain solutions. One approach, and perhaps the most mathematically desirable approach, to solving the equations is to linearize all of the model equations and to solve them simultaneously. Successive solutions would be obtained until a satisfactory convergence is achieved. This is referred to as a Newton-Raphson procedure. However, the general Newton-Raphson procedure requires the evaluation of a large number of partial derivatives and a prohibitively large amount of computer storage and calculation time. Consequently considerable effort has been directed toward finding more tractable methods.

Friday and Smith (14) do an excellent job of analyzing and categorizing traditional calculation methods that are based on decoupling the model equations and clearly outline six decisions that must be made to formulate a solution procedure. Published methods differ because of the different approaches taken in making these decisions.

The first decision is to choose one of two formulation procedures which concern the grouping of the model equations, namely grouping by stage or by type. Greenstadt et all (15) and Bergamini (16) group the equations by stage. However most methods group the equations by type. Generally grouping by type is preferable because grouping by stage essentially makes the method susceptible to build up of truncation error.

The second decision involves the order of satisfaction of the equations. The order (1-2)-4-3 is most common. Equations (2-1) and (2-2) are always combined and satisfied simultaneously. Also equation (2-5) is used to eliminate one set of the phase rates, V_j's or L_j's.

The third decision concerns the selection of the appropriate type of equation to provide a given variable. Any set of compositions, which are obtained by simultaneous solution of the material balance equations and equilibrium relationships, can be used to estimate the new flow rates through the summation of the unnormalized compositions, or they can be used to supply the new temperatures. The former procedure is called the Sum Rates method and it has been applied to absorber problems. The latter is called the Bubble Point method. Most methods use the latter procedure to obtain the new temperatures and then energy balances to generate the new flow rates.

The fourth decision is the selection of a method to solve the material balance equations for the new stage compositions. One is the stage-to-stage method which usually calculates from both ends of a column toward the middle. The second makes use of a matrix which describes all material balance equations simultaneously for each component. Stage-to-stage methods are often numerically unstable because of the build up of truncation error. This is especially serious for a system which contains components whose relative volatilities differ widely in magnitude.

The Lewis-Matheson (1) and the Thiele-Geddes (3) method are representative of stage-to-stage procedures. In the former method the feed, reflux and the separation of two key components are specified and the number of theoretical stages required for a desired separation is calculated. The feed plate is determined by comparing the composition obtained by calculating from both the top and the bottom of the column. The mismatch at the feed stage is used to correct the assumed end compositions. The Lewis-Matheson method is advantageous for design work since it computes directly the required number of stages for a specified separation and also determines the optimum point for feed introduction. However it is difficult to obtain the solution for a complex column where multiple feeds or side streams are involved. In the Thiele-Geddes method the number of the theoretical stages in each section of the column, feed flow rate, reflux rate and the quantity of the distillate must be specified. The two methods differ in that the Thiele-Geddes method initially calculates the ratio of the stage composition to end composition rather than stage composition. Then using the material balance equation, the ratio of composition at the top plate to that at the bottom for each component is calculated. The flow rate of top product, which can be calculated from the above ratios, is compared with the specified one. If matching is not obtained, the same procedure is performed successively. Holland and coworkers (17), (2) have developed a convergence technique called "the Theta method" which they have used with the Thiele-Geddes method to improve the performance of the Thiele-Geddes method and to extend its range of application.

Matrix methods have been used widely. They are not susceptible to truncation error and they work equally well for any number of feeds and side streams, and handle nondistributed components in the same manner as distributed ones. In these methods specifications are the same as those in the Thiele-Geddes method. The first rigorous computational procedure for the simultaneous solution of the material balance equations was proposed by Amundson and Pontinen (18). Later the tridiagonal matrix method incorporating Thomas' algorithm was proposed by Wang and Henke (4).

The fifth decision concerns the stage temperatures. They are usually determined by bubble point or dew point calculations. In these calculations, the Regula-Falsi method or the Newton-Raphson method have been often used. Wang and Henke (4) recommend the Muller method for bubble point or dew point calcualtions. However it is quite time-consuming to do those iterative calcualtions. To avoid bubble or dew point calcualtions, Holland and coworkers (19) developed the K_b method which uses relative volatilities to a reference component. Newman (20) has proposed the use of the Newton-Raphson method for solving the stage temperatures so as to satisfy all material balance and equilibrium relationships. In this case Thomas' tridiagonal matrix algorithm can be used. A similar concept has been exclusively used in the Sum Rates procedures (5), (21), (22) to calculate temperatures so as to satisfy the energy balance equations.

The sixth decision is the method of obtaining the new flow rates. In the Sum Rates method the new flow rates are immediately determined from the calculated compositions. In the Bubble Point method the flow rates are determined so as to satisfy the energy balance equations.

The above six decisions deal with the calculation at each iteration. Solutions are attained by successive approximation until a certain convergence criterion is satisfied. The following sequence is usually employed.

(1) Assume a set of temperatures and flow rates.
(2) Calculate phase compositions.
(3) Correct flow rates and temperatures.
(4) Return to step (2).

However, there is no assurance that these decoupled methods will converge. For example, computational procedures which are very effective for a close boiling point distillation may have difficulty converging for a wide boiling point feed and procedures that work well for absorber and extration problems often fail on ordinary close boiling point distillation problems.

For a mixture which consists of extremely volatile and extremely nonvolatile components, phase flow rates may be completely dominated by the relative volatilities and may not be affected relatively by temperatures. If the temperatures are determined by the Bubble Point method in this case, a slight change in compositions will lead to much temperature fluctuation. Then the ordinary Bubble Point method is not suitable for solving this type of problem. This is often the case for absorber problems.

Sum Rates procedures have been proposed for such problems. McNeese (21), Sujata (5), Burningham and Otto (22), and Friday and Smith (14) presented methods which successfully solve absorber type problems. These methods are based on the Sum Rates procedure as described in <u>the third decision</u>. However the methods usually cannot solve problems dealing with close boiling point mixtures. In addition the Sum Rate methods do not appear to work well for reboiled absorber problems (22), (23).

Holland and coworkers (2), (17) have utilized exclusively the Thiele-Geddes method in conjunction with the theta convergence procedure to solve absorber and reboiled absorber problems. However, in order to obtain convergent solutions of these problems, they found it is necessary to employ special techniques to handle the energy balances. These are the Q-method and the constant composition method. The Q-method introduces side heaters or coolers on each stage so as to maintain specified flow rates. However, it does not necessarily give a practical solution. The constant composition method of calculating stream enthalpy is introduced to avoid round-off errors associated with conventional enthalpy balances. This method cannot be applied correctly for systems utilizing composition dependent enthalpy data. However, their method has been one of the successful procedures for solving reboiled absorber problems. Another possibility to solve reboiled absorber problems may be to make use of relaxation methods (24), (25), (26). Prowse and Johnson (27) have successfully employed a relaxation procedure to solve a reboiled absorber problem. The characteristics of these methods will be described later.

Friday and Smith in their analysis pointed out that an improvement in reliability could probably be obtained by solving the C-matrix equations (2-6) for phase compositions and then solving the E_j and S_j equations, (2-3) and (2-4), simultaneously for corrections to temperatures and flow rates. Algorithms based on this approach have been presented by Tierney and Bruno (12), Tierney and Yanoski (13), and Tomich (6). Their methods make use of the Newton-Raphson procedure.

Namely, functions which show material imbalance or energy imbalance are approximated by expanding as functions of flow rates and temperatures using a Taylor series expansion truncating after the first order derivatives. These functions are then set equal to zero and solved to obtain corrections to temperatures and flow rates simultaneously. In this case the Jacobian matrix must be evaluated numerically rather than analytically.

Tomich (6) applied Broyden's procedure (28), which is actually an improved Newton-Raphson method, to obtain corrections for temperatures and flow rates simultaeously. Broyden's procedure updates the inverse of the approximate Jacobian matrix using residuals calculated at the preceding iteration level instead of evaluating a large number of partial derivatives numerically and inverting the rigorous Jacobian matrix at each iteration. Tomich's method reduces the amount of computation required significantly in that only one matrix inversion is required per problem solution.

Billingsley and Boynton (11) suggest another method to reduce the amount of computational effort in the Newton-Raphson procedure. They assume temporarily that the material imbalance equations are functions of only temperatures and then solve for temperatures by the Newton-Raphson method as proposed by Newman (20). These temperatures are then substituted into the original equations which are generated from the material imbalances and energy imbalances by the Newton-Raphson procedure. However, this decoupling assumption seems to be often serious, especially for a wide boiling point range mixture.

Friday and Smith also suggested that the ultimate method could be to linearize all the model equations first and then solve simultaneously for all variables. Even though this concept has been recognized as desirable, it has been difficult to find a practical algorithm because of the inherent computational effort. Naphtali and Sandholm (8), (9) have proposed a method based on this concept of linearization and solving all variables simultaneously. In their method all equations are grouped according to stage rather than type. The method may take composition dependent data into account. A similar method has been proposed by Gentry (7). However these new methods are still accompanied by several difficulties. Namely, a large amount of computer storage and a tremendous amount of calculational effort for the evaluation of partial derivatives are required. These problems have restricted the exact application of the methods. For example Gentry (7) solved only problems with composition independent data. To avoid such restriction of computer storage Goldstein and Stanfield (10) present a new algorithm. In their method enthalpy and equilibrium relationships are assumed to be functions of temperatures only and all equations are grouped by type and then linearized. When a problem involves a relatively large number of theoretical stages, the method makes use of a special technique to cope with the limitation of computer storage. For such a problem, a sectioning procedure, which calculates for a group of stages assuming linearity of variables in the group, is applied.

Other representative solution procedures are the so called "relaxation methods" and the methods based on an analytical approach.

"Relaxation methods", in principle, calculate the transient behavior of the stage variables until steady state operation is approached. Flow rates, stage compositions and temperatures are first assumed and then the variables corresponding to each stage are calculated so as to compensate imbalances in enthalpy and material balance at each stage. These procedures are continued until all equations are satisfied. Rose, Sweeny and Schrodt (24) have successfully developed this approach. Applications and improvements have been proposed by Hanson, Duffin and Somerville (29), Ball (25), Ishikawa and Hirata (26), and Prowse and Johnson (27). Relaxation methods are highly stable numerically. Their high stability can be helpful when the system contains a wide boiling point range mixture or a highly non-ideal mixture. However, the rate of convergence of relaxation methods is quite slow, especially as the solution is approached.

Acrivos and Amundson (30) present the analytical solution of an ideal distillation problem for the case when constant molar overflow and constant relative volatility can be assumed. Acrivos and Amundson (31) utilized perturbation techniques to extend the method to non-ideal systems. This idea has been further extended by combining the concept of the theta convergence procedure by Yamada and Sugie (32). However the methods for a non-ideal system are quite complicated and it does not seem to be practical. Furthermore it is not easy to take account of energy calculations to generate new flow rates

CHAPTER 3

THE TOMICH METHOD

The procedure proposed by Tomich (6) for solving the equilibrium stage model appears to be one of the most promising of the recent methods. Thus it was selected as an appropriate method to use as a basis of comparison when evaluating the performance of the calculational procedure proposed by the author. In Tomich's method the effect of composition is decoupled in that the component material balances are solved separately. Corrections to temperatures and flow rates are then determined simultaneously using a multivariate Newton scheme. Broyden's procedure is effectively applied to reduce the computational effort required for the evaluation of partial derivatives. Details of this method follow.

The component material balance equations combined with the equilibrium relationships, that is equations (2-6) with $C_{i,j} = 0$, may be expressed in a tridiagonal matrix form.

$$\begin{bmatrix} b_{i,1} & c_{i,1} & & & \\ a_{i,2} & b_{i,2} & c_{i,2} & & \\ & a_{i,j} & b_{i,j} & c_{i,2} & 0 \\ & & a_{i,N-1} & b_{i,N-1} & c_{i,N-1} \\ & & & a_{i,N} & b_{i,N} \end{bmatrix} \begin{bmatrix} x_{i,1} \\ x_{i,2} \\ x_{i,j} \\ x_{i,N-1} \\ x_{i,N} \end{bmatrix} = \begin{bmatrix} m_{i,1} \\ m_{i,2} \\ m_{i,j} \\ m_{i,N-1} \\ m_{i,N} \end{bmatrix} \quad (3\text{-}1)$$

where.

$$b_{i,1} = -(L_1+SL_1) - V_1K_{i,1}$$

$$c_{i,1} = V_2K_{i,2}$$

$$m_{i,1} = -F_1Z_{i,1}$$

$$a_{i,j} = L_{j-1}$$

$$b_{i,j} = -(L_j+SL_j) - (V_j+SV_j)K_{i,j}$$

$$c_{i,j} = V_{j+1}K_{i,j+1}$$

$$m_{i,j} = -F_jZ_{i,j}$$

$$a_{i,N} = L_{N-1}$$

$$b_{i,N} = -L_N - (V_N+SV_N)K_{i,N}$$

$$m_{i,N} = -F_NZ_{i,N}$$

For given liquid and vapor profiles and equilibrium ratios these equations are a linear set which may readily be solved by using the Thomas algorithm for a tridiagonal matrix as described by Wang and Henke (4).

Imbalances for energy and the summations of compositions at each stage are given by,

$$E_j = F_jH_{F,j} + Q_j + L_{j-1}h_{j-1} + V_{j+1}H_{j+1} - (L_j+SL_j)h_j - (V_j+SV_j)H_j \qquad (3\text{-}2)$$

and

$$S_j = \sum_{i=1}^{NCP} y_{i,j} - \sum_{i=1}^{NCP} x_{i,j} \quad . \qquad (3\text{-}3)$$

In the Tomich method the temperatures, T_j's, the flow rates,

V_j's, L_j's, and the compositions, $x_{i,j}$'s, $y_{i,j}$'s, are calculated by using the Newton-Raphson method so as to satisfy the following conditions:

$$E_j = 0 \;, \tag{3-4}$$

$$S_j = 0 \;. \tag{3-5}$$

A multivariable nonlinear function may be approximated in a linearized form by expanding the function as a Taylor series truncated after the first order derivatives. That is,

$$f^{k+1}(x_1,x_2,\ldots,x_n) \simeq f^k(x_1,x_2,\ldots,x_n) + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i} \Delta x_i \tag{3-6}$$

where k is the iteration number and the x_i's are variables.

E_j and S_j are assumed to be functions of the temperatures and the vapor flow rates only, and are approximated as follows:

$$E_j^{k+1} = E_j^k + \sum_{i=1}^{N} \left(\frac{\partial E_j}{\partial V_i}\right)\Delta V_i + \sum_{i=1}^{N} \left(\frac{\partial E_j}{\partial T_i}\right)\Delta T_i \;, \tag{3-7}$$

$$S_j^{k+1} = S_j^k + \sum_{i=1}^{N} \left(\frac{\partial S_j}{\partial V_i}\right)\Delta V_i + \sum_{i=1}^{N} \left(\frac{\partial S_j}{\partial T_i}\right)\Delta T_i \;. \tag{3-8}$$

Since the S_j and E_j are errors or residuals in the summation and heat balance equations and are equal to zero when a solution is reached, these relations are set equal to zero at the new iteration level. The equation set (3-7) and (3-8) with $E_j^{k+1} = 0$ and $S_j^{k+1} = 0$ can be written in a matrix form,

$$\begin{bmatrix} \frac{\partial S_1}{\partial V_1} & \cdots & \frac{\partial S_1}{\partial V_N} & \frac{\partial S_1}{\partial T_1} & \cdots & \frac{\partial S_1}{\partial T_N} \\ \vdots & & \vdots & \vdots & & \vdots \\ \frac{\partial S_N}{\partial V_1} & \cdots & \frac{\partial S_N}{\partial V_N} & \frac{\partial S_N}{\partial T_1} & \cdots & \frac{\partial S_N}{\partial T_N} \\ \frac{\partial E_1}{\partial V_1} & \cdots & \frac{\partial E_1}{\partial V_N} & \frac{\partial E_1}{\partial T_1} & \cdots & \frac{\partial E_1}{\partial T_N} \\ \vdots & & \vdots & \vdots & & \vdots \\ \frac{\partial E_N}{\partial V_1} & \cdots & \frac{\partial E_N}{\partial V_N} & \frac{\partial E_N}{\partial T_1} & \cdots & \frac{\partial E_N}{\partial T_N} \end{bmatrix} \begin{bmatrix} \Delta V_1 \\ \vdots \\ \Delta V_N \\ \Delta T_1 \\ \vdots \\ \Delta T_N \end{bmatrix} = \begin{bmatrix} -S_1 \\ \vdots \\ -S_N \\ -E_1 \\ \vdots \\ -E_N \end{bmatrix} \qquad (3\text{-}9\text{-}a)$$

The strict application of equation (3-9-a) is to an absorber type problem where all the flow rates, V_j's are unknowns. For normal reboiled absorber and distillation type problems slight modifications are required. Matrix expressions for these problems are as follows,

For a reboiled absorber where V_1 is specified,

$$\begin{bmatrix} \frac{\partial S_1}{\partial V_2} & \cdots & \frac{\partial S_1}{\partial V_N} & \frac{\partial S_1}{\partial T_1} & \cdots & \frac{\partial S_1}{\partial T_N} \\ \vdots & & \vdots & \vdots & & \vdots \\ \frac{\partial S_N}{\partial V_2} & \cdots & \frac{\partial S_N}{\partial V_N} & \frac{\partial S_N}{\partial T_1} & \cdots & \frac{\partial S_N}{\partial T_N} \\ \frac{\partial E_1}{\partial V_2} & \cdots & \frac{\partial E_1}{\partial V_N} & \frac{\partial E_1}{\partial T_1} & \cdots & \frac{\partial E_1}{\partial T_N} \\ \vdots & & \vdots & \vdots & & \vdots \\ \frac{\partial E_{N-1}}{\partial V_2} & \cdots & \frac{\partial E_{N-1}}{\partial V_N} & \frac{\partial E_{N-1}}{\partial T_1} & \cdots & \frac{\partial E_{N-1}}{\partial T_N} \end{bmatrix} \begin{bmatrix} \Delta V_2 \\ \vdots \\ \Delta V_N \\ \Delta T_1 \\ \Delta T_2 \\ \vdots \\ \Delta T_N \end{bmatrix} = \begin{bmatrix} \text{[illegible]}_1 \\ \vdots \\ -S_N \\ -E_1 \\ \vdots \\ -E_{N-1} \end{bmatrix} \qquad (3\text{-}9\text{-}b)$$

For a distillation problem where V_1 and V_2 are specified.

$$\begin{bmatrix} \frac{\partial S_1}{\partial V_3} & \cdots & \frac{\partial S_1}{\partial V_N} & \frac{\partial S_1}{\partial T_1} & \cdots & \frac{\partial S_1}{\partial T_N} \\ \vdots & & \vdots & \vdots & & \vdots \\ \frac{\partial S_N}{\partial V_3} & \cdots & \frac{\partial S_N}{\partial V_N} & \frac{\partial S_N}{\partial T_1} & \cdots & \frac{\partial S_N}{\partial T_N} \\ \frac{\partial E_2}{\partial V_3} & \cdots & \frac{\partial E_2}{\partial V_N} & \frac{\partial E_2}{\partial T_1} & \cdots & \frac{\partial E_2}{\partial T_N} \\ \vdots & & \vdots & \vdots & & \vdots \\ \frac{\partial E_{N-1}}{\partial V_3} & \cdots & \frac{\partial E_{N-1}}{\partial V_N} & \frac{\partial E_{N-1}}{\partial T_1} & \cdots & \frac{\partial E_{N-1}}{\partial T_N} \end{bmatrix} \begin{bmatrix} \Delta V_3 \\ \vdots \\ \Delta V_N \\ \Delta T_1 \\ \Delta T_2 \\ \vdots \\ \Delta T_N \end{bmatrix} = \begin{bmatrix} -S_1 \\ \vdots \\ -S_N \\ -E_2 \\ \vdots \\ -E_{N-1} \end{bmatrix} \qquad (3\text{-}9\text{-}c)$$

From equation (3-9-a-b-c) the corrections, ΔV_j's and ΔT_j's, are calculated. Then V_j's and T_j's are corrected as follows,

$$V_j^{k+1} = V_j^k + t\Delta V_j \qquad (3\text{-}10)$$

$$T_j^{k+1} = T_j^k + t\Delta T_j \qquad (3\text{-}11)$$

where t is a weighting factor. The determination of t will be shown later.

In equations (3-9-a-b-c) E_j and S_j are calculated from the definitions (3-2) and (3-3). The partial derivatives in the Jacobian matrix must be evaluated by a finite difference method. The equation sets (3-1) and (3-9-a-b-c) are then solved and the same calculations are performed iteratively. The basic procedure may be as follows,

(1) Some initial set of V_j's and T_j's is assumed.

(2) The L_j's are computed from equation (2-5) with $M_j = 0$.

(3) The equation set (3-1) is solved by using the tridiagonal matrix algorithm to give the $x_{i,j}$'s.

(4) The $y_{i,j}$'s are calculated from equation (2-1).

(5) The E_j's and S_j's, and then partial derivatives are evaluated.

(6) Equation (3-9-a-b-c) is solved for ΔV_j's and ΔT_j's.

(7) The V_j's and T_j's are calculated from equations (3-10) and (3-11).

(8) By using this new set of V_j's and T_j's, steps (2) through (7) are repeated until an appropriate convergence criterion is satisfied.

However, the procedure mentioned requires the evaluation of the Jacobian matrix numerically at each iteration. In this case it is quite time-consuming to compute all partial derivatives in the Jacobian. Furthermore a large computer effort is required to obtain the inversion of the Jacobian matrix. To cope with these difficulties Tomich applied the Broyden procedure (28). The Broyden procedure is a modified version of the Newton method and is designed to reduce the number of function evaluations required and to update the inverse of the approximate Jacobian matrix. An outline of this procedure follows.

Consider the set of n nonlinear equations,

$$f_j(x_1, x_2, \ldots, x_n) = 0 , \qquad j = 1, 2, \ldots, n. \tag{3-12}$$

These may be written more concisely as,

$$\bar{f}(\bar{x}) = 0 . \qquad (3\text{-}13)$$

If $\bar{x}^k$ is the k^{th} approximation of the solution of equation (3-13), then the next variables are defined as follows according to Newton's method;

$$\bar{x}^{k+1} = \bar{x}^k - \bar{A}^{k^{-1}} \bar{f}^k , \qquad (3\text{-}14)$$

where $\bar{A}^k$ is the Jacobian matrix.

Let $\bar{p}^k$ be defined as

$$\bar{p}^k = -\bar{B}^{k^{-1}} \bar{f}^k , \qquad (3\text{-}15)$$

where $\bar{B}^k$ is some approximation to the Jacobian matrix $\bar{A}^k$.

Then a simple modification to Newton's algorithm gives $\bar{x}^{k+1}$ by

$$\bar{x}^{k+1} = \bar{x}^k + t\bar{p}^k . \qquad (3\text{-}16)$$

Let $\bar{H}^k$ and $\bar{y}^k$ be defined by

$$\bar{H}^k = \bar{B}^{k^{-1}} \qquad (3\text{-}17)$$

$$\bar{y}^k = \bar{f}^{k+1} - \bar{f}^k . \qquad (3\text{-}18)$$

$\bar{B}^{k+1}$ is chosen so that the change in $\bar{f}$ predicted by $\bar{B}^{k+1}$ in a direction orthogonal to $\bar{p}^k$ is the same as would be predicted by $\bar{B}^k$. Then the next relation is obtained by using Householder's formula.

$$\bar{H}^{k+1} = \bar{H}^k - \frac{(\bar{H}^k \bar{y}^k + t\bar{p})\bar{p}^{k^T} \bar{H}^k}{\bar{p}^{k^T} \bar{H}^k \bar{y}^k} , \qquad (3\text{-}19)$$

where t is a weighting factor and $\bar{p}^{k^T}$ is a transpose vector of $\bar{p}^k$.

$\bar{H}^k$ is actually an approximate inverse form of the Jacobian matrix $\bar{A}^k$. Then the new $\bar{x}$ is calculated as,

$$\bar{x}^{k+1} = \bar{x}^{k} + t\bar{H}^{k}\bar{f}^{k} \quad (3\text{-}20)$$

The determination of a weighting factor t, which moves the solution toward convergence, is described by Broyden as follows.

The first value of a weighting factor $t^{(1)}$ at each iteration is chosen to be unity since this is the value arising naturally in Newton's method. The second value, if required, is given by the semi-empirical relation,

$$t^{(2)} = \frac{(1+6\theta)^{\frac{1}{2}} - 1}{3\theta} \quad (3\text{-}21)$$

where

$$\theta = \frac{\phi(1)}{\phi(0)} \quad (3\text{-}22)$$

and where $\phi(t)$ is the square of the Euclidean norm of $\bar{f}(t)$.

If further improvement to ϕ is required, it is approximated by a quadratic function whose ordinates are specified at $t = 0, 1$ and $t^{(2)}$. If this function is convex, then $t^{(3)}$ is chosen to be the value of t that minimize ϕ, and a new quadratic is formed whose ordinates are specified at $t^{(3)}$ and two of the previous trial values of t. If there is no value of t, $(0 < t \leq 1)$, such that $\phi(t)$ is smaller than $\phi(0)$, then t will be searched for between 0 and -1.

Functions, f_j's, in the general equation (3-12) represent the residuals in the model equations, namely, E_j's and S_j's. The vector, $\bar{x}$, in the general equation corresponds to the temperatures, T_j's, and the vapor flow rates, V_j's, in the model equations. Consequently the approximated inverse of the Jacobian matrix, which is calcualted from equation (3-19), is expressed in terms of E_j's,

S_j's, T_j's and V_j's at present and previous iteration levels.

Now for succeeding iterations, Broyden's procedure is effectively used for updating the inverse of the Jacobian matrix using information at preceding iteration levels. Thus there is no need for more than one evaluation of partial derivatives and matrix inversion per problem solution and the computation time may be greatly reduced.

The improved calculation procedure may be summarized as follows,

(1) Some initial set of V_j's and T_j's is assumed.

(2) The L_j's are computed from equation (2-5) with $M_j = 0$.

(3) The equation set (3-1) is solved by using the tridiagonal matrix algorithm to give, the $x_{i,j}$'s.

(4) The $y_{i,j}$'s are calculated from equation (2-1).

(5) The E_j's and S_j's are calculated by substituting the above information into equations (3-4) and (3-5).

(6) The approximate inverse of the Jacobian matrix is calculated based on the Broyden procedure and the new variables are calculated from equation (3-20).

(7) By using this new set of V_j's and T_j's, steps (2) through (6) are repeated until an appropriate convergence criterion is satisfied.

However, at the first iteration only, all the partial derivatives must be evaluated and the inversion of the Jacobian matrix must be obtained. The procedure for doing this is the same as the general Newton-Raphson method. The evaluations of the partial derivatives are performed numerically, because the E_j's in equation (3-2) and the S_j's in equation (3-3), which show the residuals in the energy balance equations and the component material balance equations, cannot be expressed analytically. If K-values and enthalpies which are dependent on compositions are employed initial phase compositions must be assumed at step (1). The initial assumptions are often provided by substituting ideal K-values into equation (2-6) and solving the C-matrix equations with $C_{i,j} = 0$ by the Thomas algorithm.

In the computer program developed calcualtions are continuied until a convergence criterion such as the following is satisfied,

$$\frac{[CRIT]}{N} < 10^{-6} \tag{3-23}$$

where [CRIT] is defined as follows according to Tomich (6),

$$[CRIT] = \sum_{j=1}^{N} (S_j^2 + E_j'^2) \tag{3-24}$$

and where

$$E_j' = \frac{E_j}{F_j H_{F,j} + Q_j + L_{j-1} h_{j-1} + V_{j+1} H_{j+1}} \tag{3-25}$$

In equation (3-25), E_j is normalized by dividing by the total heat input to any stage j so that it is of the order of magnitude 1. ϕ, the square of the Euclidean norm of $\bar{f}$, in equation (3-22) corresponds to [CRIT] in the program. Then a weighting factor, t, is searched for to satisfy the following relation according to Broyden (28) as stated before.

$$[CRIT]^{k+1} < [CRIT]^k . \tag{3-26}$$

CHAPTER 4

EQUILIBRIUM AND ENTHALPY DATA

In the range of low or moderate pressures remote from the critical conditions, equilibrium K-ratios can be closely approximated by using the vapor pressure of each component and the system pressure. For a non-ideal system K-ratios are often modified by liquid phase activity coefficients. The Wilson correlation (33) is typical of such a modification.

Phase equilibria at high pressures such as encountered in petroleum or natural gas processing industries are more complicated. The convergence pressure concept has been used commonly to correlate K-ratios in a multicomponent hydrocarbon system at high pressure. The N.G.P.S.A. charts (34) are the most common source for the prediction of K-ratios. The B.W.R. equation (35), (36), which is one of the first analytical methods to correlate composition dependency, has been often used to predict equilibrium K-ratios. A general correlation for calculating equilibria in hydrocarbon mixtures was first proposed by Chao and Seader (37) and has been widely accepted in the hydrocarbon processing and related industries. Attempts to elaborate a general correlation are continuing. The Prausnitz and Chueh method (38), (39), and the Lee and Edmister method (40) are typical of those.

The enthalpy of a pure component is often expressed as a function of the temperature and pressure of the system and the enthalpy of a mixture can be evaluated from these pure component enthalpies. Yen and Alexander (41) have proposed general enthalpy correlations based on the theory of corresponding state. Edmister et al (42) have developed procedures for enthalpy calculations based on thermodynamic relationships and the Chao-Seader correlation.

4.1 Chao-Seader K-ratio Correlation

The Chao-Seader correlation has been widely accepted in hydrocarbon processing industries. In this thesis the correlation is exclusively employed to generate equilibrium and enthalpy data.

Physical properties used with the Chao-Seader correlation to calculate equilibrium and enthalpy data are shown in Appendix I.

This correlation utilizes vapor fugacity coefficients, liquid fagacity coefficients and liquid activity coefficients. The vapor fugacity coefficients are calculated by the Redlich-Kwong equation of state (43). The liquid fugacity coefficients are evaluated by the curve fitted relationship and the acentric factor concept of Pitzer. The solubility parameter and the theory of regular solutions are applied for calculating the liquid activity coefficients. In the correlation there are no parameters which depend on interactions among the molecules in a multicomponent system.

The equilibrium K-ratios may be defined as follows by setting the fugacity of any component i in the vapor phase equal to that in the liquid.

$$K_i \equiv \frac{y_i}{x_i} = \frac{\gamma_i f^{o}_{i,L}}{\psi_i P} \qquad (4\text{-}1)$$

Chao and Seader correlated the non-ideality of each component in both the liquid and vapor phase to the properties of pure components. The vapor phase fugacity coefficient, ψ_i, is calculated based on the Redlich-Kwong equation of state. The liquid phase activity coefficient, γ_i, is calculated from the Scatchard-Hildebrand equation for regular solutions. The liquid fugacity coefficient, $\nu_i = f^o_{i,L}/P$, is curvefitted in terms of reduced pressure, reduced temperature and the acentric factor.

4.1.1 Evaluation of Vapor Fugacity Coefficient ψ_i

In the Chao-Seader correlation the basic equation for calculating the vapor phase properties is the Redlich-Kwong equation of state (43), namely,

$$Z = \frac{1}{1-h} - \frac{A^2}{B} \times \frac{h}{1+h} \qquad (4\text{-}2\text{-}a)$$

$$h = \frac{BP}{Z} \qquad (4\text{-}2\text{-}b)$$

where Z is the compressibility factor, and A and B are constants expressed in terms of the critical properties of a component as,

$$A_i = \left(\frac{0.4278}{P_c \, T_R^{2.5}}\right)^{\frac{1}{2}} \qquad (4\text{-}3\text{-}a)$$

$$B_i = \left(\frac{0.0867}{T_R \, P_c}\right) \qquad (4\text{-}3\text{-}b)$$

$$A = \sum_{i=1}^{NCP} y_i A_i \qquad (4\text{-}3\text{-}c)$$

$$B = \sum_{i=1}^{NCP} y_i B_i \quad . \qquad (4\text{-}3\text{-}d)$$

The fugacity coefficient ψ_i is commonly expressed as,

$$\ln\psi_i = \frac{1}{RT} \int_v^{\infty} \left[\left(\frac{\partial P}{\partial n_i}\right)_{T,v,n_j} - \frac{RT}{v}\right] dv - \ln z \quad . \qquad (4\text{-}4)$$

This equation is combined with the Redlich-Kwong equation and then the fugacity coefficient of any component i in the vapor phase is obtained,

$$\ln\phi_i = (Z-1)\frac{B_i}{B} - \ln(Z-BP) - \frac{A^2}{B}\left(\frac{2A_i}{A} - \frac{B_i}{B}\right)\ln\left(1 + \frac{BP}{Z}\right) \qquad (4\text{-}5)$$

4.1.2 Evaluation of Activity Coefficient γ_i

The liquid phase activity coefficient γ_i is calculated from the Hildebrand and Scatchard equation,

$$\ln\gamma_i = \frac{V^*(\delta_i - \bar{\delta}_m)^2}{RT} \qquad (4\text{-}6)$$

$$\delta_i = \left(\frac{\Delta H}{V^*_i}\right)^{\frac{1}{2}} \qquad (4\text{-}7\text{-}a)$$

$$\bar{\delta}_i = \frac{\delta_i x_i V^*_i}{\sum x_i V^*_i} \qquad (4\text{-}7\text{-}b)$$

where V^*_i is the molal volume of the liquid phase of component i, ΔH is the heat of vaporization and δ_i is the solubility parameter.

The equation for calculating γ_i is based on the assumption of the regular solution for which the excess entropy of mixing is zero. The Gibbs excess free energy consists of enthalpy and entropy of mixing. Therefore the non-ideality in a regular solution is entirely due to its heat of mixing only. Generally, the assumption of the regular solution is not valid. However, systems of non-polar fluids such as hydrocarbon mixtures behave close to the regular solution theory over a relatively large range of pressure, temperature and composition. The characteristic of the method is that the evaluation of the activity coefficient γ_i is performed from the assumption that

γ_i is a function only of the properties of the individual pure components.

4.1.3 Evaluation of Liquid Fugacity Coefficient ν_i

The theory of corresponding states has been extended by Pitzer introducing the third parameter ω_i which is called an acentric factor. Any property of a fluid is then assumed to be given as function of reduced pressure, reduced temperature and the acentric factor.

Chao and Seader applied this concept to correlate the liquid fugacity coefficient, ν_i, as,

$$\log \nu_i = \log \nu_i^{(0)} + \omega_i \log \nu_i^{(1)} \qquad (4\text{-}8)$$

where $\nu_i^{(0)}$ is ν_i of a simple fluid state and $\nu_i^{(1)}$ accounts for the departure of ν_i from that of a simple fluid state.

However, when the pure liquid of any component i of the mixture becomes hypothetical at a given system condition, ν_i cannot be evaluated. In order to overcome this difficulty they extended the liquid fugacity coefficient correlation into the hypothetical region using experimental equilibrium data. Then they curvefitted the expression $\nu_i^{(0)}$ and $\nu_i^{(1)}$ with approximating functions of reduced properties,

$$\log \nu_i^{(0)} = A_1 + A_2/T_R + A_3 T_R + A_4 T_R^2 + A_5 T_R^3 + (A_6 + A_7 T_R + A_8 T_R^2) P_R + (A_9 + A_{10} T_R) P_R^2 - \log P_R \qquad (4\text{-}9)$$

$$\log \nu_i^{(1)} = A_{11} + A_{12} T_R + A_{13}/T_R + A_{14} T_R^3 + A_{15} (P_R - 0.6) \qquad (4\text{-}10)$$

where all the constants A, which are common for all components, were obtained for frequently occurring hydrocarbons.

The liquid fugacity coefficient for any component i is then calculated only from the reduced pressure, the reduced temperature and the acentric factor using equations (4-8), (4-9) and (4-10).

4.2 Enthalpy Calculation From the Chao-Seader Correlation

The general correlation of enthalpy data based on the thermodynamic relationships and the Chao-Seader correlation has been developed by Edmister, Persy and Erbar (42), and Erbar (44).

The ideal partial molar heat of vaporization is given by,

$$h_i^* - H_i^0 = -RT^2 \left(\frac{\partial \ln \nu_i^0}{\partial T}\right)_{P_i} \qquad (4\text{-}11)$$

The enthalpy of mixing due to the non-ideal solution, assuming the excess entropy of mixing is zero is obtained from,

$$\bar{h}_i - h_i^* = -RT^2 \left(\frac{\partial \ln \gamma_i}{\partial T}\right)_{P_i, x_i} \qquad (4\text{-}12)$$

Then the partial molar enthalpy of component i in the liquid is obtained from equations (4-11) and (4-12).

$$\bar{h}_i = H_i^0 - RT_R^2 T_C \left\{\left(\frac{\partial \ln \nu_i^0}{\partial T_R}\right)_{P_i} + \left(\frac{\partial \ln \gamma_i}{\partial T_R}\right)_{P_i, x_i}\right\} \qquad (4\text{-}13)$$

$$\log \nu_i^{(0)} = A_1 + A_2/T_R + A_3T_R + A_4T_R^2 + A_5T_R^3 + (A_6 + A_7T_R + A_8T_R^2)P_R + (A_9 + A_{10}T_R)P_R^2 - \log P_R \qquad (4\text{-}9)$$

$$\log \nu_i^{(1)} = A_{11} + A_{12}T_R + A_{13}/T_R + A_{14}T_R^3 + A_{15}(P_R - 0.6) \qquad (4\text{-}10)$$

where all the constants A, which are common for all components, were obtained for frequently occurring hydrocarbons.

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$$\bar{h}_i = H_i^0 - RT_R^2 T_C \left\{\left(\frac{\partial \ln \nu_i^0}{\partial T_R}\right)_{P_i} + \left(\frac{\partial \ln \gamma_i}{\partial T_R}\right)_{P_i, x_i}\right\} \qquad (4\text{-}13)$$

include the ability to handle complex hydrocarbon fractions as well as pure components. Erbar (44) and Cavett (45) have developed procedures to predict the properties of complex mixtures to provide data for the equilibrium and enthalpy calculations. The minimum information required for the calculations is the API gravity, the molecular weight and either the mean average boiling point or the molal average boiling point and the cubic average boiling point of the fraction. From this minimum information the equilibrium and enthalpy calculations are performed as,

(1) If the mean boiling point is not specified it is calculated from the molal average boiling point and the cubic average boiling point by,

$$BP_{mn} = \frac{BP_{ca} + BP_{mba}}{2.0} \qquad (4\text{-}20)$$

(2) The specific gravity of the fraction at 60° F is calculated by means of,

$$\text{specific gravity} = \frac{141.5}{131.5 + {}^{o}API} \qquad (4\text{-}21)$$

and the density is adjusted by 25° C by,

$$d_{25} = 0.98907 \times \text{specific gravity at } 60^\circ\text{ F.} \qquad (4\text{-}22)$$

(3) The liquid molal volume at 25° C is calculated by,

$$V^{*}_{i} = \frac{\text{molecular weight}}{d_{25}} \qquad (4\text{-}23)$$

(4) The pseudo-critical temperature of the hypothetical component is calculated by,

$$T_C = a_0 - a_1T + a_2T^2 + a_3T^3 + a_4AT + a_5AT^2 + a_6A^2T^2 \qquad (4\text{-}24)$$

where T is the molal average boiling point, if available, or the mean average boiling point in °R, and A is API gravity.

(5) The pseudo-critical pressure (psia) of the hypothetical component is calculated from,

$$\log P_C = b_0+b_1T+b_2T^2+b_3T^3+b_4AT+b_5AT^2$$
$$+b_6A^2T+b_7A^2T^2 \qquad (4\text{-}25)$$

If the critical pressure has been specified this calculation is by-passed.

(6) The acentric factor ω is computed from Edmister's equation,

$$\omega = \frac{3}{7}\ \frac{\log (P_c/14.7)}{T_b/T_c - 1.0} - 1.0 \qquad (4\text{-}26)$$

where T_b is mean average boiling point in °R.

(7) The latent heat of vaporization at the normal boiling point is calculated by Kistiakowsky's equation,

$$\frac{\Delta H}{T_b} = 7.58 + 4.571 \log T_b \qquad (4\text{-}27)$$

and adjusted to 25°C by means of Watson's equation,

$$\frac{\Delta H_{25°C}}{\Delta H} = (\frac{T_c - 537}{T_c - T_b})^{0.38} \qquad (4\text{-}28)$$

The solubility parameter is calculated by,

$$\delta_i = \frac{(\Delta H_{25°C} - RT)^{1/2}}{V^*} \qquad (4\text{-}29)$$

(8) The constants required for the ideal gas state enthalpy equation,

$$H_i^o = (AH)_i+(BH)_iT+(CH)_iT^2+(DH)_iT^3 \qquad (4\text{-}30)$$

are calculated from the following equations,

$$AH = \overline{MW}(C_0+C_1A+C_2A^2+C_3A^3+C_4K+C_5K^2+C_6K^3+C_{18}AK) \qquad (4\text{-}30\text{-}a)$$

$$BH = \overline{MW}(C_7+C_8A+C_9A^2+C_{10}A^3+C_{11}K+C_{12}K^2+C_{13}K^3) \qquad (4\text{-}30\text{-}b)$$

$$CH = \overline{MW}(C_{14} + C_{15}A) \qquad (4\text{-}30\text{-}c)$$

$$DH = \overline{MW}(C_{16} + C_{17}A) \qquad (4\text{-}30\text{-}d)$$

where

A = °API

K = the U.O.P. characterization factor

$\overline{MW}$ = Molecular Weight.

4.4 Limitations of the Chao-Seader Correlation

The general Chao-Seader correlation has been widely used and extensively evaluated. The method is characterized by a generalization based on sound thermodynamic relations. Furthermore the non-ideality is related to the properties of pure components only. Then the calculation procedures are greatly simplified. On the other hand the existence of some limitations due to the simplified assumptions is indispensable. Lenoir (46) has summarized the conditions under which the correlation can give satisfactory predictions as follows,

(1) The pressure should not exceed 1000 psia and should not be greater than 0.8 of the system critical pressure.

(2) The reduced temperature of any hydrocarbon other than methane should be between 0.5 and 1.3.

(3) The methane content in the liquid phase should not exceed 0.3 mole fraction, and for any system containing hydrogen or methane, the reduced temperature should not exceed 0.93, and the temperature should be between 100 and 500°F.

(4) When predicting paraffins or olefinic equilibrium ratios, the aromatic content should be less than 0.5 mole fraction.

4.5 Partial Derivatives of K-ratio and Enthalpy

The general algorithm for multistage multicomponent separation calculations proposed by the author requires the following partial derivatives,

$$\frac{\partial K_{i,j}}{\partial T_j}, \quad \frac{\partial K_{i,j}}{\partial x_{i,j}}, \quad \frac{\partial H_j}{\partial T_j} \quad \text{and} \quad \frac{\partial h_j}{\partial T_j} .$$

Either numerical or analytical techniques may be used to evaluate these partial derivatives. The computer effort is generally large for numerical evaluation. As far as complicated correlations such as the Chao-Seader method are concerned, it is especially advantageous to determine partial derivatives analytically.

K-ratio is expressed in the form,

$$K_i = \frac{\gamma_i}{\psi_i} \frac{f^o_{i,L}}{P} \tag{4-31}$$

Then the partial derivatives of K with respect to T and x are,

$$\frac{\partial K_i}{\partial T} = \frac{\gamma_i}{\psi_i} \frac{\partial}{\partial T} \left(\frac{f^o_{i,L}}{P}\right) + \frac{f^o_{i,L}}{P} \left\{\gamma_i \frac{\partial}{\partial T} \left(\frac{1}{\psi_i}\right) + \frac{1}{\psi_i} \frac{\partial \gamma_i}{\partial T}\right\} \tag{4-32}$$

$$\frac{\partial K_i}{\partial x_i} = \frac{\gamma_i}{\psi_i} \frac{\partial}{\partial x_i} \left(\frac{f^o_{i,L}}{P}\right) + \frac{f^o_{i,L}}{P} \left\{\gamma_i \frac{\partial}{\partial x_i} \left(\frac{1}{\psi_i}\right) + \frac{1}{\psi_i} \frac{\partial \gamma_i}{\partial x_i}\right\} \tag{4-33}$$

where analytical expressions for the derivatives of the vapor phase fugacity coefficient, ψ_i, the liquid phase fugacity coefficient, $f^o_{i,L}/P$, and of the activity coefficient, γ_i, can be derived from the relations making up the Chao-Seader correlation.

$\frac{\partial}{\partial T}\left(\frac{f^{o}_{i,L}}{P}\right)$, which is defined as $\frac{\partial \nu_i}{\partial T}$, is derived from equation (4-8)

$$\frac{\partial \nu_i}{\partial T} = \nu_i^{(0)} \omega_i \nu_i^{(1)} \frac{\omega_i - 1 \partial \nu_i^{(1)}}{\partial T} + \nu_i^{(1)} \frac{\omega_i \partial \nu_i^{(0)}}{\partial T} \quad . \qquad (4\text{-}34)$$

Now define $f(T)$ and $g(T)$ as follows,

$$f(T) = \log \nu_i^{(0)} = A_1 + \frac{A_2}{T_R} + A_3 T_R + A_4 T_R^2 + A_5 T_R^3 + (A_6 + A_7 T_R + A_8 T_R^2) P_R + (A_9 + A_{10} T_R) P_R^2 - \log P_R \qquad (4\text{-}35)$$

$$g(T) = \log \nu_i^{(1)} = A_{11} + A_{12} T_R + \frac{A_{13}}{T_R} + A_{14} T_R^3 + A_{15}(P_R - 0.6) \quad . \qquad (4\text{-}36)$$

Then $\frac{\partial \nu_i}{\partial T}$ is given by,

$$\frac{\partial \nu_i}{\partial T} = 2.303\, \nu_i \left\{\frac{\partial f(T)}{\partial T} + \omega_i \frac{\partial g(T)}{\partial T}\right\} \qquad (4\text{-}37)$$

$$\frac{\partial f(T)}{\partial T} = \frac{1}{T_C} \left\{- \frac{A_2}{T_R^2} + A_3 + 2A_4 T_R + 3A_5 T_R^2 + (A_7 + 2A_8 T_R) P_R + A_{10} P_R^2\right\} \qquad (4\text{-}38)$$

$$\frac{\partial g(T)}{\partial T} = \frac{1}{T_C} \left(A_{12} - \frac{A_{13}}{T_R^2} + 3A_{14} T_R^2\right) \quad . \qquad (4\text{-}39)$$

$\frac{\partial \nu_i}{\partial x_i}$ is zero, since ν_i is a function of only the reduced temperature and pressure.

The partial derivatives of the activity coefficient are evaluated as follows,

$$\frac{\partial \gamma_i}{\partial T} = - \frac{\gamma_i}{T} \ln \gamma_i \tag{4-40}$$

$$\frac{\partial \gamma_i}{\partial x_i} = 2T \frac{v_i^*}{\sum x_i v_i^*} \frac{\partial \gamma_i}{\partial T} \tag{4-41}$$

$\frac{\partial}{\partial T} (\frac{1}{\psi_i})$ is given by,

$$\frac{\partial}{\partial T} (\frac{1}{\psi_i}) = - \frac{1}{\psi_i} [\frac{B_i}{B} \frac{\partial Z}{\partial T} + (Z-1)(\frac{1}{B} \frac{\partial B_i}{\partial T} - \frac{B_i}{B^2} \frac{\partial B}{\partial T})$$

$$- \frac{1}{(Z-BP)} (\frac{\partial Z}{\partial T} - P \frac{\partial B}{\partial T}) - (\frac{2A_i}{A} - \frac{B_i}{B}) \frac{A^2}{B} \frac{P}{1 + \frac{BP}{Z}} (\frac{1}{Z} \frac{\partial B}{\partial P} - \frac{B}{Z^2} \frac{\partial Z}{\partial T})$$

$$- \ln (1 + \frac{BP}{Z}) \{\frac{2A}{B} \frac{\partial A_i}{\partial A} - \frac{2A_i}{B} \frac{\partial A}{\partial T} - \frac{A^2}{B^2} \frac{\partial B_i}{\partial T}$$

$$+ (\frac{2A_i}{A} - \frac{B_i}{B}) (\frac{2A}{B} \frac{\partial A}{\partial T} - \frac{A^2}{B^2} \frac{\partial B}{\partial T}) \}] \tag{4-42}$$

where

$$\frac{\partial A_i}{\partial T} = - 1.25 \frac{A_i}{T} \tag{4-43}$$

$$\frac{\partial B_i}{\partial T} = - \frac{B_i}{T} \tag{4-44}$$

$$\frac{\partial A}{\partial T} = - 1.25 \frac{A}{T} \tag{4-45}$$

$$\frac{\partial B}{\partial T} = - \frac{B}{T} \tag{4-46}$$

$$\frac{\partial Z}{\partial T} = (2ABP^2 \frac{\partial A}{\partial T} + A^2P^2 \frac{\partial B}{\partial T} + 2BP^2Z \frac{\partial B}{\partial T}$$

$$- 2APZ \frac{\partial A}{\partial T} + PZ \frac{\partial B}{\partial T}) / \{3Z^2 - 2Z - (BP)^2 + A^2P - BP\} . \tag{4-47}$$

$\frac{\partial}{\partial x_i}\left(\frac{1}{\psi_i}\right)$ is given by,

$$\frac{\partial}{\partial x_i}\left(\frac{1}{\psi_i}\right) = \frac{1}{\psi_i}\left[\frac{1}{Z-BP}\frac{\partial}{\partial x_i}(Z-BP) + \frac{1}{(1+\frac{BP}{Z})^m}\frac{\partial}{\partial x_i}\left(1+\frac{BP}{Z}\right)^m + \frac{\partial}{\partial x_i}\left\{(1-Z)\frac{B_i}{B}\right\}\right] \tag{4-48}$$

where

$$m = \frac{A^2}{B}\left(\frac{2A_i}{A} - \frac{B_i}{B}\right) \tag{4-49}$$

$$\frac{\partial}{\partial x_i}(Z-BP) = \frac{\partial Z}{\partial x_i} - P\frac{\partial B}{\partial x_i} \tag{4-50}$$

$$\frac{\partial}{\partial x_i}\left(1+\frac{BP}{Z}\right)^m = m\left(1+\frac{BP}{Z}\right)^{m-1}\left\{\frac{P}{Z}\frac{\partial B}{\partial x_i} - \frac{BP}{Z^2}\frac{\partial Z}{\partial x_i}\right\} \tag{4-51}$$

$$\frac{\partial}{\partial x_i}\left\{(1-Z)\frac{B_i}{B}\right\} = (Z-1)\frac{B_i}{B^2}\frac{\partial B}{\partial x_i} - \frac{B_i}{B}\frac{\partial Z}{\partial x_i} \tag{4-52}$$

$$\frac{\partial Z}{\partial x_i} = \left(A^2P^2\frac{\partial B}{\partial x_i} + 2ABP^2\frac{\partial A}{\partial x_i} + 2BP^2Z\frac{\partial B}{\partial x_i} - 2APZ\frac{\partial A}{\partial x_i} + ZP\frac{\partial B}{\partial x_i}\right)/\{3Z^2-2Z-(BP)^2+A^2P-BP\} \tag{4-53}$$

However, $\frac{\partial A_i}{\partial x_i}$ $\frac{\partial A}{\partial x_i}$ $\frac{\partial B_i}{\partial x_i}$ and $\frac{\partial B}{\partial x_i}$ may be taken to be negligible, since constants A_i, A, B_i and B are functions of vapor phase compositions, y_i's and those constants are approximated to be functions of normalized y_i's at the previous iteration. $\frac{\partial}{\partial x}\left(\frac{1}{\psi_i}\right)$ is expressed in terms of partial derivatives of the constants with respect to x_i's. Consequently,

$$\frac{\partial}{\partial x_i}\left(\frac{1}{\psi_i}\right) \simeq 0 \text{ .} \tag{4-54}$$

$\frac{\partial H}{\partial T}$, $\frac{\partial h}{\partial T}$ are expressed as follows:

$$\frac{\partial H}{\partial T} = \sum_{i=1}^{NCP} x_i H_i^o \frac{\partial K_i}{\partial T} + \sum_{i=1}^{NCP} Y_i \frac{\partial H_i}{\partial T}$$

$$- \frac{3}{2} \frac{A^2}{B} \frac{1}{1 + \frac{BP}{Z}} \left(\frac{P}{Z} \frac{\partial B}{\partial T} - \frac{BP}{Z^2} \frac{\partial Z}{\partial T}\right)$$

$$- \frac{3}{2} \ln \left(1 + \frac{BP}{Z}\right)\left(- \frac{A^2}{B^2} + \frac{2A}{B} \frac{\partial A}{\partial T}\right) + \frac{\partial Z}{\partial T} , \tag{4-55}$$

$$\frac{\partial h}{\partial T} = \sum_{i=1}^{NCP} x_i \left[\frac{\partial H_i}{\partial T} - 2.303R\{2A_3 T_R + 6A_4 T_R^2 + 12A_5 T_R^3\right.$$

$$+ (2A_7 T_R + 6A_8 T_R^2) P_R + 2A_{10} P_R^2 T_R$$

$$\left. + \omega_i (2A_{12} T_R + 15A_{14} T_R^4)\}\right] \tag{4-56}$$

where

$$\frac{\partial H_i}{\partial T} = (BH)_i + 2(CH)_i T + 3(DH)_i T^2 . \tag{4-57}$$

CHAPTER 5

THE NEW METHOD

A new general calculational method for equilibrium stage processes is described in this chapter. The method employs the Taylor approximation procedure for the total linearization of all the model equations. This linearization technique, which is actually a modified Newton-Raphson method, has been widely applied for solving nonlinear equations numerically. For example, Lee (47) has solved successfully various kinds of nonlinear differential equations. The present author (48) applied the technique to solving complicated partial differential equations which represent the reactor problem where chemical reaction takes place between gas and liquid reactants on solid catalysts. In this case simultaneous heat and mass transfer with fluid mixing was taken into account. Roche and Staffin (49), (50) applied this linearization technique to calculations for a ternary liquid - liquid extraction problem. The present author (51) extended the same concept to a multicomponent extraction problem. Recently Gentry (7) has proposed the application of this linearization technique to distillation processes.

In the method proposed by the author all the model equations, namely, over-all material balances, component material balances, energy balances and the summations of compositions, are approximated in a linearized form. The linearized equations are then solved simultaneously, without decoupling, for corrections to temperatures, flow rates and compositions. In Tomich's method only the energy balance and summation equations are linearized decoupling the material balance equations. The methods are significantly different in that the linearized equations of the method proposed by the author are expressed analytically. However, those of Tomich's method cannot be expressed analytically since the functional relationships of the equations with related variables are implicit.[1]

5.1 Linearization of Equations

A multivariable nonlinear function, f, is often approximated as follows,

$$f(x_1+\Delta x_1,\ x_2+\Delta x_2,\ \ldots,\ x_n+\Delta x_n) \simeq f(x_1,x_2,\ldots,x_n) + \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}\Delta x_i \quad . \qquad (5\text{-}1)$$

Equations (2-3), (2-4), (2-5) and (2-6) are approximated in the same manner as equation (5-1), then linearized setting,

$$f(x_1+\Delta x_1,\ x_2+\Delta x_2,\ \ldots,\ x_n+\Delta x_n) = 0 \quad , \qquad (5\text{-}2)$$

However, slight modification of standard linearization procedures will be utilized in this thesis to obtain convenient matrix structures and manipulation. Namely, only the partial derivatives that have a dominant influence on the solution are included in the linearized equations. The details will be discussed later. The linearized equations are:

Over-all material balances

$$\Delta L_{j-1} + \Delta V_{j+1} - \Delta L_j - \Delta V_j = -M_j, \quad j = 2 \rightarrow N-1 \qquad (5\text{-}3)$$

from which it follows that

$$\Delta L_j = \sum_{k=1}^{j} M_k + \Delta V_{j+1} - \Delta V_1, \quad j = 2 \rightarrow N \qquad (5\text{-}4)$$

At $j = 1$

$$\Delta V_2 - \Delta L_1 - \Delta V_1 = -M_1 \tag{5-5}$$

where $\Delta V_1 = 0$ for a reboiled absorber problem when V_1 is specified and $\Delta V_2 = \Delta L_1 = \Delta V_1 = M_1 = 0$ for a distillation problem when V_1 and V_2 are specified.

At $j = N$

$$\Delta L_{N-1} - \Delta L_N - \Delta V_N = -M_N \tag{5-6}$$

where $\Delta L_N = 0$ except for the usual absorber problem.

Component material balances

$$\begin{aligned} L_{j-1}\Delta x_{i,j-1} &- \{(L_j+SL_j) + (V_j+SV_j)(K_{i,j}+x_{i,j}\frac{\partial K_{i,j}}{\partial x_{i,j}})\}\Delta x_{i,j} \\ &+ V_{j+1}(K_{i,j+1}+x_{i,j+1}\frac{\partial K_{i,j+1}}{\partial x_{i,j+1}})\Delta x_{i,j+1} \\ &- (V_j+SV_j)x_{i,j}\frac{\partial K_{i,j}}{\partial T_j}\Delta T_j + V_{j+1}x_{i,j+1}\frac{\partial K_{i,j+1}}{\partial T_{j+1}}\Delta T_{j+1} \\ &+ \Delta L_{j-1}x_{i,j-1} - \Delta L_j x_{i,j} - \Delta V_j K_{i,j}x_{i,j} + \Delta V_{j+1}K_{i,j+1}x_{i,j+1} \\ &= -C_{i,j}, \qquad j = 2 \to N-1 . \end{aligned} \tag{5-7}$$

At $j=1$

$$\begin{aligned} &-\{(L_1+SL_1)+V_1(K_{i,1}+x_{i,1}\frac{\partial K_{i,1}}{\partial x_{i,1}})\}\Delta x_{i,1}+V_2(K_{i,2}+x_{i,2}\frac{\partial K_{i,2}}{\partial x_{i,2}})\Delta x_{i,2} \\ &- V_1 x_{i,1}\frac{\partial K_{i,1}}{\partial T_1}\Delta T_1+V_2 x_{i,2}\frac{\partial K_{i,2}}{\partial T_2}\Delta T_2 - L_1 x_{i-1} - \Delta V_2 K_{i,1}x_{i,1} \\ &+ \Delta V_2 K_{i,2}x_{i,2} = -C_{i-1} . \end{aligned} \tag{5-8}$$

At $j = N$

$$L_{N-1}\Delta x_{i,N-1} - \{L_N+(V_N+SV_N)(K_{i,N}+x_{i,N}\frac{\partial K_{i,N}}{\partial x_{i,N}}))\}\Delta x_{i,N} - (V_N+SV_N)x_{i,N}\frac{\partial K_{i,N}}{\partial T_N}\Delta T_N+\Delta L_{N-1}x_{i,N-1}-\Delta L_N x_{i,N} - \Delta V_N K_{i,N}x_{i,N} = C_{i,N} \qquad (5\text{-}9)$$

Energy balances

$$L_{j-1}\frac{\partial h_{j-1}}{\partial T_{j-1}}\Delta T_{j-1}-\{(V_j+SV_j)\frac{\partial H_j}{\partial T_j}+(L_j+SL_j)\frac{\partial h_j}{\partial T_j}\}\Delta T_j - V_{j+1}\frac{\partial H_{j+1}}{\partial T_{j+1}}\Delta T_{j+1}+\Delta L_{j-1}h_{j-1}-\Delta V_j H_j-\Delta L_j h_j + \Delta V_{j+1}H_{j+1} = -E_j\,, \qquad j = 2 \rightarrow N-1\,. \qquad (5\text{-}10)$$

At $j = 1$

$$-\{V_1\frac{\partial H_1}{\partial T_1}+(L_1+SL_1)\frac{\partial h_1}{\partial T_1}\}\Delta T_1+V_2\frac{\partial H_2}{\partial T_2}\Delta T_2-\Delta L_1 h_1 - \Delta V_1 H_1 + \Delta V_2 H_2 + \Delta Q_1 = -E_1 \qquad (5\text{-}11)$$

where

$\Delta Q_1 = 0$ for an absorber problem

$\Delta V_1 = \Delta Q_1 \leq 0$ for a reboiled absorber problem

$\Delta V_1 = \Delta L_1 = \Delta V_2 = 0$ for a distillation problem.

At $j = N$

$$L_{N-1}\frac{\partial h_{N-1}}{\partial T_{N-1}}\Delta T_{N-1}-\{(V_N+SV_N)\frac{\partial H_N}{\partial T_N}+L_N\frac{\partial h_N}{\partial T_N}\}\Delta T_N + \Delta L_{N-1}h_{N-1}-\Delta V_N H_N-\Delta L_N h_N+\Delta Q_N = -E_N \qquad (5\text{-}12)$$

where

$\Delta Q_N = 0$ for an absorber problem

$\Delta L_N = 0$ except for an absorber problem.

Summation equations

$$\sum_{i=1}^{NCP} \Delta x_{i,j} = -S_j \ , \qquad j = 1 \rightarrow N \ . \tag{5-13}$$

The equilibrium ratios, and the liquid and vapor enthalpies are functions of temperature, pressure and phase compositions and may be calculated as such at each iteration. However, for the purpose of linearization only, the following relations were assumed.

$$K_{i,j} \simeq K_{i,j}(P_j, T_j, x_{i,j}) \tag{5-14}$$

$$H_j \simeq H_j(P_j, T_j) \tag{5-15}$$

$$h_j \simeq h_j(P_j, T_j) \ , \tag{5-16}$$

The number of partial derivatives to be evaluated follows.

$$\frac{\partial K_{i,j}}{\partial T_j} : N \times NCP \ , \qquad \frac{\partial K_{i,j}}{\partial x_{i,j}} : N \times NCP$$

$$\frac{\partial H_j}{\partial T_j} : N \qquad \text{and} \qquad \frac{\partial h_j}{\partial T_j} : N \ .$$

Then the total number of partial derivatives is $2N \times (1+NCP)$.

The linearized equations then only include the partial derivatives that have the strongest influence on the solution and this in turn greatly reduces the computer storage required. If the standard linearization procedure is employed directly without modification, simple matrix structures as in this thesis cannot be obtained and the matrix manipulation will encounter prohibitive difficulty. However, this practical simplification of the linearized equation need not affect the rigor of the final result in that the equilibrium ratios and enthalpies are calculated at each iteration as functions of temperature, pressure and normalized phase compositions.

Either numerical or analytical techniques may be used to evaluate the partial derivatives which appear in the linearized equations. The amounts of computer storage and calculational time required are generally large for numerical evaluation. The computer program developed in this thesis employs the Chao-Seader correlation. The partial derivatives are evaluated analytically in the program. The analytical expressions for the partial derivatives are given in Chapter 4.

Equation (5-4), the linearized over-all material balance, may be substituted into the component material balance equations and the energy balance equations to eliminate all ΔL_j terms. The linearized component and energy balances may then be expressed in matrix form as follows.

Component material balances for an absorber problem

$$\begin{bmatrix} b_{i,1} & c_{i,1} & & & \\ a_{i,2} & b_{i,2} & c_{i,2} & & \\ & a_{i,j} & b_{i,j} & c_{i,j} & \\ & & a_{i,N-1} & b_{i,N-1} & c_{i,N-1} \\ & & & a_{i,N} & b_{i,N} \end{bmatrix} \begin{bmatrix} \Delta x_{i,1} \\ \Delta x_{i,2} \\ \Delta x_{i,j} \\ \Delta x_{i,N-1} \\ \Delta x_{i,N} \end{bmatrix} +$$

$$\begin{bmatrix} d_{i,1} & e_{i,1} & & & \\ & d_{i,2} & e_{i,2} & & \\ & & d_{i,j} & e_{i,j} & \\ & & & d_{i,N-1} & e_{i,N-1} \\ & & & & d_{i,N} \end{bmatrix} \begin{bmatrix} \Delta T_1 \\ \Delta T_2 \\ \Delta T_j \\ \Delta T_{N-1} \\ \Delta T_N \end{bmatrix} +$$

$$\begin{bmatrix} \alpha_{i,1} + f_{i,1} & g_{i,1} & & & \\ \alpha_{i,2} & f_{i,2} & g_{i,2} & & \\ \alpha_{i,j} & & f_{i,j} & g_{i,j} & \\ \alpha_{i,N-1} & & & f_{i,N-1} & g_{i,N-1} \\ \alpha_{i,N} & & & & f_{i,N} \end{bmatrix} \begin{bmatrix} \Delta V_1 \\ \Delta V_2 \\ \Delta V_j \\ \Delta V_{N-1} \\ \Delta V_N \end{bmatrix} = \begin{bmatrix} m_{i,1} \\ m_{i,2} \\ m_{i,j} \\ m_{i,N-1} \\ m_{i,N} \end{bmatrix}$$

$$1 \leq i \leq NCP \qquad (5\text{-}17)$$

where

$$b_{i,1} = -\{(L_1 + SL_1) + V_1(K_{i,1} + x_{i,1} \frac{\partial K_{i,1}}{\partial x_{i,1}})\}$$

$$c_{i,1} = -V_2(K_{i,2} + x_{i,2} \frac{\partial K_{i,2}}{\partial x_{i,2}})$$

$$d_{i,1} = - V_1 x_{i,1} \frac{\partial K_{i,1}}{\partial T_1}$$

$$e_{i,1} = V_2 x_{i,2} \frac{\partial K_{i,2}}{\partial T_2}$$

$$\alpha_{i,1} = x_{i,1}$$

$$f_{i,1} = -K_{i,1} x_{i,1}$$

$$g_{i,1} = -(x_{i,1} - K_{i,2} x_{i,2})$$

$$m_{i,1} = -C_{i,1} + M_1 x_{i,1}$$

$$a_{i,j} = L_{j-1}$$

$$b_{i,j} = - \{ (L_j + SL_j) + (V_j + SV_j)(K_{i,j} + x_{i,j} \frac{\partial K_{i,2}}{\partial x_{i,j}}) \}$$

$$c_{i,j} = V_{j+1} (K_{i,j+1} + x_{i,j+1} \frac{\partial K_{i,j+1}}{\partial x_{i,j+1}})$$

$$d_{i,j} = - (V_j + SV_j) x_{i,j} \frac{\partial K_{i,j}}{\partial T_j}$$

$$e_{i,j} = V_{j+1} x_{i,j+1} \frac{\partial K_{i,j+1}}{\partial T_j}$$

$$\alpha_{i,j} = x_{i,j} - x_{i,j-1}$$

$$f_{i,j} = x_{i,j-1} - K_{i,j} x_{i,j}$$

$$g_{i,j} = -(x_{i,j} - K_{i,j+1} x_{i,j+1})$$

$$m_{i,j} = \sum_{k=2}^{j} M_k x_{i,j} - \sum_{k=2}^{j-1} M_k x_{i,j-1} - C_{i,j} - M_1 (x_{i,j-1} - x_{i,j})$$

$$a_{i,N} = L_{N-1}$$

$$b_{i,N} = -\{L_N + (V_N + SV_N)(K_{i,N} + x_{i,N}\frac{\partial K_{i,N}}{\partial x_{i,N}})\}$$

$$d_{i,N} = -(V_N + SV_N)x_{i,N}\frac{\partial K_{i,N}}{\partial T_N}$$

$$\alpha_{i,N} = x_{i,N} - x_{i,N-1}$$

$$f_{i,N} = x_{i,N-1} - K_{i,N}x_{i,N}$$

$$m_{i,N} = \sum_{k=2}^{N} M_k x_{i,N} - \sum_{k=2}^{N-1} M_k x_{i,N-1} - C_{i,N} - M_1(x_{i,N-1} - x_{i,N}) .$$

Component material balances for a reboiled absorber where V_1 is specified.

Equation (5-17) is modified as,

$$\alpha_{i,j} = 0 , \quad j = 1 \to N$$

$$f_{i,1} = 0$$

$$\Delta V_1 = 0 .$$

Component material balances for distillation where V_1 and V_2 are specified.

Equation (5-17) is modified as

$$\alpha_{i,j} = 0 , \quad j = 1 \to N$$

$$f_{i,1} = 0$$

$$f_{i,2} = 0$$

$$g_{i,1} = 0$$

$$\Delta V_1 = 0$$

$$\Delta V_2 = 0 .$$

Energy balances for an absorber

$$\begin{bmatrix} q_1 & r_1 & & & & \\ p_2 & q_2 & r_2 & & & \\ & p_j & q_j & r_j & & \\ & & p_{N-1} & q_{N-1} & r_{N-1} \\ & & & p_N & q_N \end{bmatrix} \begin{bmatrix} \Delta T_1 \\ \Delta T_2 \\ \Delta T_j \\ \Delta T_{N-1} \\ \Delta T_N \end{bmatrix} +$$

$$\begin{bmatrix} \beta_1+s_1 & t_1 & & & \\ \beta_2 & s_2 & t_2 & & \\ \beta_j & & s_j & t_j & \\ \beta_{N-1} & & & s_{N-1} & t_{N-1} \\ \beta_N & & & & s_N \end{bmatrix} \begin{bmatrix} \Delta V_1 \\ \Delta V_2 \\ \Delta V_j \\ \Delta V_{N-1} \\ \Delta V_N \end{bmatrix} = \begin{bmatrix} u_1 \\ u_2 \\ u_j \\ u_{N-1} \\ u_N \end{bmatrix} \qquad (5\text{-}18\text{-}a)$$

where

$$q_1 = -\{V_1 \frac{\partial H_1}{\partial T_1} + (L_1+SL_1)\frac{\partial h_1}{\partial T_1}\}$$

$$r_1 = V_2 \frac{\partial H_2}{\partial T_2}$$

$$\beta_1 = h_1$$

$$s_1 = -H_1$$

$$t_1 = H_2 - h_1$$

$$u_1 = -E_1 + M_1 h_1$$

$$p_j = L_{j-1} \frac{\partial h_{j-1}}{\partial T_{j-1}}$$

$$q_j = -\{(V_j+SV_j) + (L_j+SL_j)\frac{\partial h_j}{\partial T_j}\}$$

$$r_j = V_{j+1} \frac{\partial H_{j+1}}{\partial T_{j+1}}$$

$$\beta_j = h_j - h_{j-1}$$

$$s_j = h_{j-1} - H_j$$

$$t_j = H_{j+1} - h_j$$

$$u_j = -E_j + \sum_{k=2}^{j} M_k h_j - \sum_{k=2}^{j-1} M_k h_{j-1} - M_1 (h_{j-1} - h_j)$$

$$p_N = L_{N-1} \frac{\partial h_{N-1}}{\partial T_{N-1}}$$

$$q_N = \{(V_N + SV_N) \frac{\partial H_N}{\partial T_N} + L_N \frac{\partial h_N}{\partial T_N}\}$$

$$\beta_N = h_N - h_{N-1}$$

$$s_N = h_{N-1} - H_N$$

$$u_N = -E_N + \sum_{k=2}^{N} M_k h_N - \sum_{k=2}^{N-1} M_k h_{N-1} - M_1 (h_{N-1} - h_N) \quad .$$

Energy balances for a reboiled absorber

$$\begin{bmatrix} q_1 & r_1 & & & \\ p_2 & q_2 & r_2 & & \\ & p_j & q_j & r_j & \\ & & p_{N-1} & q_{N-1} & r_{N-1} \\ & & & p_N & q_N \end{bmatrix} \begin{bmatrix} \Delta T_1 \\ \Delta T_2 \\ \Delta T_j \\ \Delta T_{N-1} \\ \Delta T_N \end{bmatrix} +$$

$$\begin{bmatrix} 0 & t_1 & & & \\ & s_2 & t_2 & & \\ & & s_j & t_j & \\ & & & s_{N-1} & t_{N-1} \\ 1 & & & & s_N \end{bmatrix} \begin{bmatrix} \Delta Q_N \\ \Delta V_2 \\ \Delta V_j \\ \Delta V_{N-1} \\ \Delta V_N \end{bmatrix} = \begin{bmatrix} u_1 \\ u_2 \\ u_j \\ u_{N-1} \\ u_N \end{bmatrix} \tag{5-18-b}$$

where p, q, r, s, t, and u are the same as those in equation (5-18-a).

<u>Energy balances</u> for distillation

$$\begin{bmatrix} q_1 & r_1 & & & \\ p_2 & q_2 & r_2 & & \\ & p_j & q_j & r_j & \\ & & p_{N-1} & q_{N-1} & r_{N-1} \\ & & & p_N & q_N \end{bmatrix} \begin{bmatrix} \Delta T_1 \\ \Delta T_2 \\ \Delta T_j \\ \Delta T_{N-1} \\ \Delta T_N \end{bmatrix} + \begin{bmatrix} 1 & 0 & & & \\ & 0 & t_2 & & \\ & & s_j & t_j & \\ & & & s_{N-1} & t_{N-1} \\ & 1 & & & s_N \end{bmatrix} \begin{bmatrix} \Delta Q_1 \\ \Delta Q_N \\ \Delta V_j \\ \Delta V_{N-1} \\ \Delta V_N \end{bmatrix} = \begin{bmatrix} u_1 \\ u_2 \\ u_j \\ u_{N-1} \\ u_N \end{bmatrix} \tag{5-18-c}$$

where p, q, r, s, t and u are the same as those in equation (5-18-a).

Now the component material balances combined with the equilibrium relationships and the energy balances are expressed simultaneously in matrix forms as equations (5-17) and (5-18).

5.2 Solution Procedure

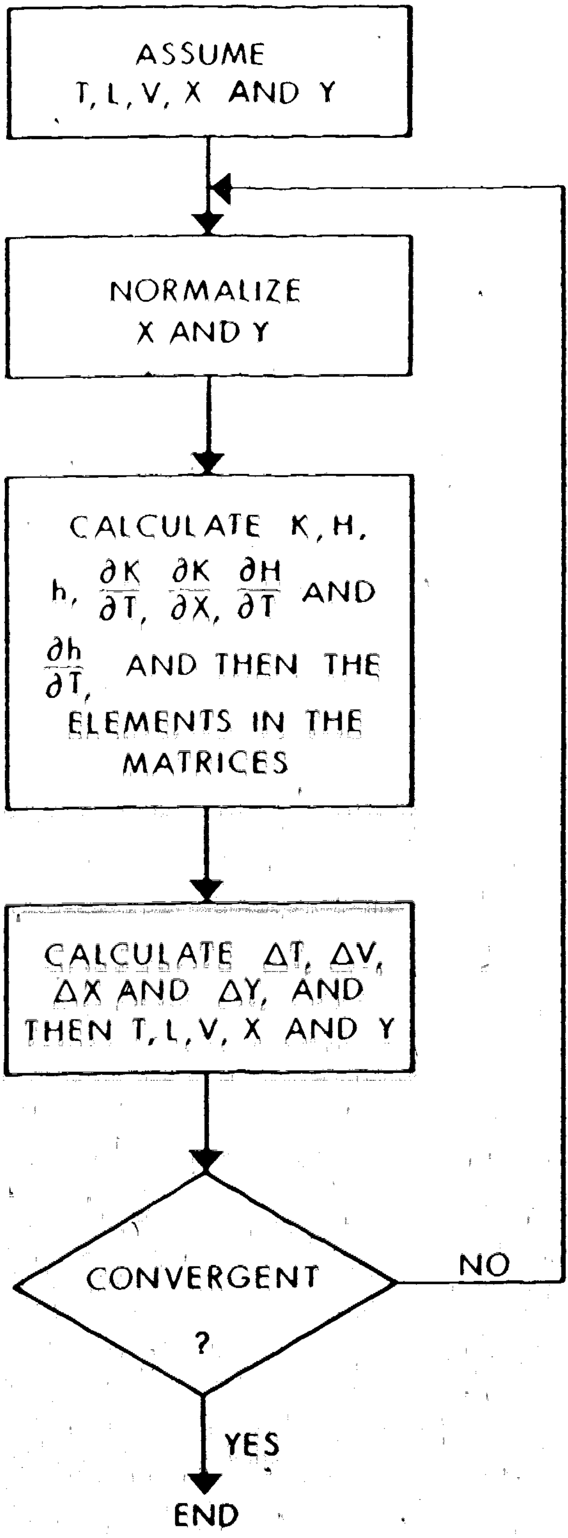
The solution procedure is iterative. Figure 2 shows the flow diagram for computation. As seen in the figure all unknown variables of temperatures, flow rates and phase compositions are solved simultaneously in a single convergence loop. This is a significant characteristic of the new method.

At first appropriate specifications are made and initial values are selected for the flow rates, L_j's and V_j's, the temperatures, T_j's and the phase compositions, $x_{i,j}$'s and $y_{i,j}$'s. Substitution of ideal K-ratios into equation (2-6) and solving the C-matrix with $C_{i,j} = 0$ by the Thomas algorithm such as described by Wang and Henke (4) will readily provide initial estimate of $x_{i,j}$'s. Then the phase compositions are normalized and K, H, h, $\frac{\partial K}{\partial T}$, $\frac{\partial K}{\partial x}$, $\frac{\partial H}{\partial T}$ and $\frac{\partial h}{\partial T}$ are calculated as described in Chapter 4. All the elements in the matrices of equations (5-17) and (5-18) can then be calculated. From equations (5-17), (5-18) and the summation equation (5-13) with $S_j = 0$, the correction terms for the unknown variables are obtained. If the corrected variables satisfy a certain convergence criterion, then the computation will stop. Otherwise the procedure will be performed again iteratively.

The detail computation procedure for obtaining the solution is as follows,

FIGURE 2

FLOW DIAGRAM FOR COMPUTATIONAL PROCEDURE



(1) Convert the first matrices in equations (5-17) and (5-18) to unit matrices and obtain matrix equations of the form,

$$\bar{I}\,\overline{\Delta x}_i + \bar{B}_i\overline{\Delta T} + \bar{C}_i\overline{\Delta V} = \bar{D}_i \qquad (5\text{-}19)$$

and

$$\bar{I}\,\overline{\Delta T} + \bar{P}\overline{\Delta V} = \bar{Q} \quad . \qquad (5\text{-}20)$$

The following algorithm was derived for inverting the tridiagonal matrices (51).

$$\begin{bmatrix} b_1 & c_1 & & & & \\ a_2 & b_2 & c_2 & & & \\ & a_j & b_j & c_j & & \\ & & a_{N-1} & b_{N-1} & c_{N-1} \\ & & & a_N & b_N \end{bmatrix}^{-1} = \begin{bmatrix} G_{1,1} & G_{1,2} & \cdot & \cdot & G_{1,N} \\ G_{2,1} & G_{2,2} & \cdot & \cdot & G_{2,N} \\ G_{j,1} & \cdot & \cdot & \cdot & \cdot \\ G_{N-1,1} & \cdot & \cdot & \cdot & \cdot \\ G_{N,1} & \cdot & \cdot & \cdot & G_{N,N} \end{bmatrix} \qquad (5\text{-}21)$$

where

$\varepsilon_1 = b_1$

$\varepsilon_j = b_j - a_j c_{j-1}/\varepsilon_{j-1}$, $\quad j = 2 \rightarrow N$

$G_{N,N} = 1/\varepsilon_N$

$G_{N,j} = -G_{N,j+1}a_{j+1}/\varepsilon_N$ $\quad j = N-1 \rightarrow 1$

$G_{k,j} = -G_{k+1,j}c_k/\varepsilon_k$, $\quad k = N-1 \rightarrow 1$, $\quad j = N \rightarrow k+1$

$G_{k,k} = (1-G_{k,k+1}a_{k+1})/\varepsilon_k$, $\quad k = N-1 \rightarrow 1$

$G_{k,j} = G_{k,k+1}a_{j+1}/\varepsilon_j$, $\quad k = N-1 \rightarrow 1$, $\quad j = 2 \rightarrow N$.

However, one could also use the Gauss-Jordan elimination procedure. The algorithm will be simplified by the use of the new procedure. A numerical example which illustrates the application of this procedure is shown in Appendix 2.

(2) Sum equation (5-19) over $i = 1 \rightarrow NCP$

$$\hat{I}\overline{\Sigma\Delta x_i} + \hat{B}\overline{\Delta T} + \hat{C}\overline{\Delta V} = \bar{D} \quad . \tag{5-22}$$

(3) Eliminate the Δx_i term from equation (5-19) by substituting equation (5-13) with $S_j = 0$ to obtain,

$$\hat{B}\overline{\Delta T} + \hat{C}\overline{\Delta V} = \bar{D} \quad . \tag{5-23}$$

(4) Substitute equation (5-20) into equation (5-23) to obtain ΔV_j's and then ΔT_j's are calculated from equation (5-20). The values are substituted into equation (5-17) which is then solved for the $\Delta x_{i,j}$'s using the Thomas algorithm.

(5) Compute new V_j's, T_j's and $x_{i,j}$'s as,

$$V_j^{k+1} = V_j^k + t\Delta V_j \tag{5-24}$$

$$T_j^{k+1} = T_j^k + t\Delta T_j \tag{5-25}$$

$$x_{i,j}^{k+1} = x_{i,j}^k + t\Delta x_{i,j} \tag{5-26}$$

where t, $(0 < t \leq 1)$ is a weighting factor.

A weighting factor, t, is chosen so as to satisfy the following relation.

$$[CRIT]^{k+1} < [CRIT]^k \tag{5-27}$$

where [CRIT] is defined as,

$$[CRIT] = \sum_{j=1}^{N} \{ (\sum_{i=1}^{NCP} y_{i,j} - 1)^2 + (\frac{E_j}{F_j H_{F,j} + Q_j + L_{j-1} h_{j-1} + V_{j+1} H_{j+1}})^2 \} \tag{5-28}$$

(6) $y_{i,j}$'s are obtained from equation (2-1) and then normalize the phase compositions, $x_{i,j}$'s and $y_{i,j}$'s. Theoretically the normalization of $x_{i,j}$'s is not required. However they are normalized to avoid truncation error. Again calculate

$$K_{i,j},\quad H_j,\quad h_j,\quad \frac{\partial K_{i,j}}{\partial T_j},\quad \frac{\partial K_{i,j}}{\partial x_{i,j}},\quad \frac{\partial H_j}{\partial T_j} \text{ and } \frac{\partial h_j}{\partial T_j}$$

These values and the new stage variables are used to obtain the elements in the matrices.

(7) Continue calculations until a convergence criterion such as the following is satisfied.

$$\frac{[\text{CRIT}]}{N} < 10^{-6} \qquad (5\text{-}29)$$

One possible definition of the convergence criterion may be,

$$[\text{CRIT}] = \sum_{j=1}^{N} \{M_j^2 + (\sum_{i=1}^{NCP} C_{i,j})^2 + E_j^2 + S_j^2\} \qquad (5\text{-}30)$$

This represents the summation of imbalances in over-all material balances (2-5), component material balances (2-6), energy blances (2-3) and summation equations (2-4) over an entire column. However, in the computer program flow rates are calculated so as to satisfy equation (2-5) with $M_j = 0$. In addition, the liquid phase compositions, $x_{i,j}$'s always satisfy equation (2-4) with $S_j = 0$. Then equation (5-30) is expressed as,

$$[\text{CRIT}] = \sum_{j=1}^{N} \{(\sum_{i=1}^{NCP} C_{i,j})^2 + E_j^2\} \qquad (5\text{-}31)$$

In place of equation (5-31) the convergence criterion may be defined as,

$$[CRIT] = \sum_{j=1}^{N} \{(\sum_{i=1}^{NCP} y_{i,j} - 1)^2 + E_j^2\} \quad . \qquad (5\text{-}32)$$

Since if the following conditions are satisfied,

$$\sum_{i=1}^{NCP} y_{i,j} = 1, \quad \sum_{i=1}^{NCP} x_{i,j} = 1 \quad \text{and} \quad M_j = 0$$

then the component matrerial balance equations should be satisfied, namely, $C_{i,j} = 0$.

The second term in equation (5-32) is normalized by dividing by the total heat input to any stage j so that it is of the order of magnitude 1. Consequently equation (5-28) can be defined as a convergence criterion.

The weighting factor, t, in step (5) is chosen as follows. First a weighting factor, $t^{(1)}$, at each iteration is determined so as to satisfy the following conditions.

$$T_j^k - 60.0°F \le T_j^k + t\Delta T_j \le T_j^k + 60.0\ °F, \quad j = 1 \to N \qquad (5\text{-}33)$$

$$0.5\ V_j^k \le V_j^k + t\Delta V_j \le 2.0\ V_j^k\ , \quad j = 1 \to N\ . \qquad (5\text{-}34)$$

Then $t^{(1)}$ is the smallest value of t which satisfies the above conditions. If the condition (5-27) is not satisfied, the next factor is set as $t^{(2)} = 0.5\ t^{(1)}$. It has been the author's experience that the condition (5-27) is usually satisfied with the first weighting factor, $t^{(1)}$. The conditons (5-33) and (5-34) are selected so as to give a steady solution. For example, in case the temperature correction at any stage is over 1000°F, obviously one cannot expect a converged solution.

Some flexibility in specifications exists in that the algorithm for an absorber may be used for distillation problems where all heat loads including the condenser and the reboiler are specified, and for a reboiled absorber where the reboiler load is specified.

CHAPTER 6

EVALUATION OF THE NEW METHOD

The calculational procedure described in Chapter 5 has been used to prepare a general program for the solution of multicomponent, multistage separation problems. The new algorithm has been tested on a number of problems including absorbers, reboiled absorbers and distillation columns typical of those used in natural gas processing industries, and complex hydrogen rich demethanizers used at the Canadian Industry Limited polyethylene plant in Edmonton and at the Polymer Corporation Limited synthetic rubber plant in Sarnia, Ontario. Comparisons have been made with the results obtained using algorithms prepared by the author based on Tomich's method (6) and the tridiagonal matrix-Bubble Point procedure described by Wang and Henke (4), and with the results obtained by Burningham and Otto (22) for programs based on (i) the Sum-Rates-Thiele-Geddes procedure, (ii) the Sum-Rates-Tridiagonal matrix procedure and (iii) the Bubble Point-Thiele-Geddes method with θ convergence.

Composition dependent equilibrium and enthalpy data were calculated directly in all programs using the Chao-Seader correlation. Computations were made on the I.B.M. 360-67 system at the University of Alberta.

Descriptions of the problems utilized in evaluating the new algorithm follow. Complete computed results obtained with the new algorithm are given in Appendix 3.

6.1 Test Problems

6.1.1 Example Problem No. 1 - Absorber

This absorber problem is described by Holland et al (2).

The problem specifications and initial assumptions are as follows.

Compositions of Entering Streams

Component	Feed (moles/time)	Lean Oil (moles/time)
methane	70	0
ethane	15	0
propane	10	0
n-butane	4	0
n-pentane	1	0
n-octane	0	20

Pressure = 300 psia

Number of theoretical stages = 8

Lean oil temperature = 90° F

Feed temperature = dew point

Initial Assumptions

Stage No.	Temperature (° F)	Vapor Rate (moles/time)
1	100.0	85.0
2	100.0	90.0
3	100.0	90.0
4	100.0	90.0
5	100.0	90.0
6	100.0	90.0
7	100.0	90.0
8	100.0	95.0

6.1.2 Example Problem No. 2 - Absorber

This problem is described by Burningham and Otto (22), and is typical of absorbers in natural gas processing plants.

The problem specifications and initial assumptions are as follows.

Compositions of Entering Streams

Component	Feed (moles/time)	Lean Oil (moles/time)
nitrogen	206.7	0.0
CO_2	152.5	0.0
methane	8721.5	0.0
ethane	1767.8	0.0
propane	686.8	0.0
i-butane	72.8	0.0
n-butane	136.7	0.0
i-pentane	19.7	0.0
n-pentane	19.5	0.0
n-hexane	13.1	0.0
hypth-1	8.4	0.7
hypth-2	2.5	2.9
hypth-3	0.5	129.9
hypth-4	0.1	204.3
hypth-5	0.1	24.7

Pressure = 1310.0 psia

Number of theoretical stages = 6

Lean oil temperature = -5.0° F

Feed temperature = 45.0° F

Inter cooler duty on plate 6 = -5,800,000.0 BTU

Hypothetical Component Data

	Normal Boiling Point (° F)	API Gravity	Molecular Weight
hypth-1	200	63.2	89.6
hypth-2	265	57.3	103.6
hypth-3	325	52.8	127.0
hypth-4	380	47.3	145.0
hypth-5	425	44.6	166.0

Initial Assumptions

Stage	Temperature (° F)	Vapor Rate (moles/time)
1	20.0	9398.6
2	29.0	9500.0
3	25.0	9759.0
4	25.0	10000.0
5	25.0	10500.0
6	20.0	11000.0

6.1.3 Example Problem No. 3 - Reboiled Absorber

This problem is described by Holland and et al (2).

The specifications and initial assumptions are:

Compositions of Entering Streams

Component	Feed (moles/time)	Lean Oil (moles/time)
methane	80.0	0.0
ethane	6.7	0.0
propane	6.7	0.0
n-butane	6.7	0.0
n-octane	0.0	30.0

Pressure = 300 psia

Top product (vapor) = 95.0 moles

Liquid side stream from 9th plate = 15.0 moles

Lean oil temperature = 90°F

Feed temperature = dew point

Number of theoretical stages = 10

Feed stage number = 6.

Initial Assumptions

Stage No.	Temperature (°F)	Vapor Rate (moles/time)
1	100.0	95.0
2	150.0	105.0
3	150.0	105.0
5	150.0	110.0
6	220.0	75.0
7	280.0	50.0
8	350.0	50.0
9	400.0	50.0
10	480.0	65.0

6.1.4 Example Problem No. 4 - Reboiled Absorber

This reboiled absorber problem is described by Burningham and Otto (22), and is typical of reboiled absorbers utilized in natural gas processing plants.

The specifications and initial assumptions are:

Compositions of Entering Streams

Component	Feed (moles/time)	Lean Oil (moles/time)
nitrogen	0.7	0.0
CO_2	12.4	0.0
methane	167.4	0.0
ethane	474.5	0.0
propane	440.2	0.0
i-butane	64.3	0.0
n-butane	128.8	0.0
i-pentane	19.5	0.0
n-pentane	19.4	0.0
n-hexane	13.1	0.0
hypth-1	9.0	0.5
hypth-2	5.3	2.1
hypth-3	128.3	95.3
hypth-4	203.3	149.9
hypth-5	24.7	18.1

Pressure = 270.0 psia

Number of theoretical stages = 16

Lean oil temperature = -5.0°F

Feed temperature = 50.0°F

Side reboiler duty on plate 12 = 4,000,000 BTU

Feed stage number = 6

Top product (vapor) = 677.0 moles

Hypothetical Component Data

	Normal Boiling Point (°F)	API Gravity	Molecular Weight
hypth-1	200	63.2	89.6
hypth-2	265	57.3	103.6
hypth-3	325	52.8	127.0
hypth-4	380	47.3	145.0
hypth-5	425	44.6	166.0

Initial Assumptions

Stage No.	Temperature (°F)	Vapor Rate (moles/time)
1	75.0	677.0
2	90.0	750.0
3	100.0	800.0
4	110.0	850.0
5	120.0	900.0
6	135.0	950.0
7	150.0	900.0
8	160.0	900.0
9	175.0	900.0
10	190.0	900.0
11	200.0	950.0
12	210.0	1000.0
13	220.0	1000.0
14	230.0	1000.0
15	240.0	1000.0
16	250.0	1000.0

6.1.5 Example Problem No. 5 - Reboiled Absorber

This is the hydrogen rich demethanizer operating at the Canadian Industry Limited polyethylene plant in Edmonton.

The problem specifications and initial assumptions are as follows.

Compositions of Entering Feed

Component	Feed (moles/time)	Lean Oil (moles/time)
methane	127.920	0.0
ethane	278.870	0.0
ethylene	413.190	0.0
propane	1.279	0.0
hydrogen	0.0	0.0
benzene	0.0	792.610
toluene	0.0	70.980
xylene	0.0	23.660
propylene	0.0	59.150
ethylcyclohexane	0.0	23.660

Pressure = 464.7 psia
Number of theoretical stages = 20
Lean oil temperature = 5°F
Feed temperature = 50°F
Inter cooler duties
- on plate 4 = 840,000.0 BTU
- on plate 7 = 1,095,000.0 BTU

Feed stage number = 17
Top product (vapor) = 642.2 moles

Initial Assumptions

Stage No.	Temperature (°F)	Vapor Rate (moles/time)
1	0.0	642.0
2	5.0	650.0
3	10.0	650.0
4	5.0	700.0
5	10.0	900.0
6	15.0	920.0
7	10.0	930.0
8	12.0	1100.0
9	20.0	1150.0
10	30.0	1200.0
11	40.0	1200.0
12	50.0	1250.0
13	60.0	1250.0
14	70.0	1300.0
15	75.0	1300.0
16	80.0	1350.0
17	90.0	1400.0
18	120.0	250.0
19	130.0	350.0
20	150.0	400.0

6.1.6 Example Problem No. 6 - Reboiled Absorber

This problem is hydrogen rich three feed demethanizer operating at the Polymer Corporation Limited synthetic rubber plant in Sarnia, Ontario. It is taken from the information given by Prowse and Johnson (27), and Petryshuk and Johnson (52).

The problem specifications and initial assumptions are as follows.

Compositions of Entering Streams

Component	Feed - 1 (moles/time)	Feed - 2 (moles/time)	Feed - 3 (moles/time)
hydrogen	0.0	0.0	562.4
nitrogen	0.0	0.0	207.2
methane	0.0	28.9	651.2
ethylene	0.0	57.8	414.4
ethane	0.0	144.5	414.4
propylene	0.0	491.3	384.8
propane	23.66	317.9	118.4
i-butene	196.56	520.2	88.8
2-butene	444.08	173.4	14.8
n-butane	777.14	982.6	59.2
n-pentane	331.24	158.95	35.52
heptane	47.32	14.45	8.88

Pressure = 475.0 psia

Number of theoretical stages = 30

Lean oil temperature = -4°F

Feed - 1 temperature = -4°F

Feed - 2 temperature = -4°F

Feed - 1 stage number = 15

Feed - 2 stage number = 22

Top product (vapor) = 1520.0

The initial temperatures are assumed to be linear between 0°F and the top stage and 203°F at the reboiler.

Initial Assumptions

Stage No.	Temperature (°F)	Vapor Rate (moles/time)
1	0	1520
2	7	1600
3	14	1650
4	21	1700
5	28	1750
6	35	1800
7	42	1850
8	49	1900
9	56	1950
10	63	2000
11	70	2000
12	77	2000
13	84	2000
14	91	2000
15	98	2000
16	105	2000
17	112	2000
18	119	2100
19	126	2200
20	133	2300
21	140	2400
22	147	2500
23	154	1000
24	161	1200
25	168	1400
26	175	1600
27	182	1800
28	189	2000
29	196	2200
30	203	2400

6.1.7 Example Problem No. 7 - Distillation Column

This distillation column is described by Wang and Henke (4).

The problem specifications and initial assumptions are:

Compositions of Entering Streams

Component	Feed - 1 (moles/time)	Feed - 2 (moles/time)
methane	2.0	0.0
ethane	10.0	0.0
propylene	6.0	1.0
propane	12.0	7.0
i-butane	1.0	4.0
n-butane	3.0	17.0
n-pentane	0.5	15.2
n-hexane	0.0	9.0
heptane	0.0	4.5
octane	0.0	4.3
decane	0.0	3.5

Pressure = 264.7 psia

Number of theoretical stages = 21

Feed stage numbers = 7 and 13

Feed temperatures

stage 7 = dew point

stage 13 = bubble point

Vapor distillate rate = 23.0 moles

Reflux ratio = 3.122

Liquid side stream from 4th plate = 15.0

Vapor side stream from 16th plate = 25.0

Initial Assumptions

Plate No.	Temperature (°F)	Vapor Rate (moles/time)
1	80.0	23.0
2	98.5	94.806
3	117.0	94.806
4	135.5	94.806
5	154.0	94.806
6	172.5	94.806
7	191.0	94.806
8	209.5	60.306
9	228.0	60.306
10	246.5	60.306
11	265.0	60.306
12	283.5	60.306
13	302.5	60.306
14	320.5	60.306
15	339.0	60.306
16	357.5	60.306
17	376.0	85.306
18	394.5	85.306
19	413.0	85.306
20	431.5	85.306
21	450.0	85.306

6.1.8 Example Problem No. 8. Distillation Column

This is a two product condenser stabilizer which is presently operating in a natural gas processing plant in the province of Alberta.

The problem specifications and initial assumptions follow.

Composition of Entering Streams

Component	Feed (moles/time)
CO_2	0.419
nitrogen	0.211
methane	74.737
ethane	78.890
propane	130.060
i-butane	44.244
n-butane	90.173
i-pentane	41.344
n-pentane	43.606
2-methylpentane	15.143
hexane	14.955
heptane	25.817
octane	15.875
nonane	8.784
decane	2.392
undecane	0.443
dodecane	0.174
tridecane	0.088

Pressure = 350.0 psia

Number of theoretical stages = 25

Feed stage number = 9

Feed temperature = 250.0°F

Vapor distillate rate = 21.02 moles

Liquid distillate rate = 21.02 moles

Reflux ratio = 1.9

Initial Assumptions

Stage No.	Temperature (°F)	Vapor Rate (moles/time)
1	120.00	210.20
2	131.87	1219.20
3	143.75	1219.20
4	155.62	1219.20
5	167.50	1219.20
6	179.37	1219.20
7	191.25	1219.20
8	203.12	1219.20
9	215.00	1219.20
10	226.87	800.19
11	238.75	800.19
12	250.62	800.19
13	263.40	800.19
14	274.37	800.19
15	286.25	800.19
16	298.12	800.19
17	310.0	800.19
18	321.87	800.19
19	333.75	800.19
20	345.62	800.19
21	357.50	800.19
22	369.37	800.19
23	381.25	800.19
24	393.12	800.19
25	405.00	800.19

6.1.9 Example Problem No. 9 -- Distillation Column

This is a n-butane-i-butane splitter operating in the province of Alberta. A linear temperature profile and constant molar flow rates are assumed as initial assumptions.

The problem specifications are:

Feed Composition

Component	Feed (moles/time)
propane	10.0
i-butane	652.0
n-butane	1140.0
i-pentane	17.5

Pressure = 84.0 psia

Number of theoretical stages = 70

Feed stage number = 35

Feed temperature = boiling point

Vapor distillate = 670.0

Reflux ratio = 11.3

6.2 Comparison of the Results

The computed results obtained with the new algorithm are shown in Appendix 3. The computing time and number of iterations required are summarized in Table 1 and Table 2.

In Table 1 and Table 2, the methods compared are,

New:	New method proposed by the author.
Tomich:	Tomich's method.
BP-TRI:	Bubble Point method combined with the Tridiagonal Matrix procedure.

SR-TG: Sum Rates method combined with the Thiele-Geddes procedure.

SR-TRI: Sum Rates method combined with the Tridiagonal Matrix procedure.

BP-TG: Bubble Point method combined with the Thiele-Geddes and the Theta convergence procedure.

In Table 3, Table 4 and Table 5, typical comparisons of the rate of convergence between the new method and the Tomich method are shown.

Table I

Comparison of Computing Time

(Time is seconds on an IBM 360-67)

problem		NEW	TOMICH	BP-TRI	SR-TG	SR-TRI	BP-TG
Absorber	1	4.07	15.69	(118)$_{\Lambda\Lambda}$	(128)$_{\Lambda\Lambda}$	(18)$_{\Lambda\Lambda}$	(99)$_{\Lambda\Lambda}$
	2	6.46	21.66	X	(381)$_{\Lambda}$	12.58 (79)$_{\Lambda}$	X
Re[illegible]ed Absorber	3	4.67	24.08	X	X	(214)$_{\Lambda\Lambda}$	(237)$_{\Lambda\Lambda}$
	4	14.43	75.28	X	X	X	(767)$_{\Lambda\Lambda}$
	5	22.23	X				
	6	86.72	X				
Distillation	7	12.86	51.46	33.50			$**$
	8	27.10	>190.9*	>143.0*			
	9	21.35		123.84			

Table 1 Comments

X: divergent

( ): on an IBM 7040

A: Burningham and Otto (22)

AA: Otto, private communication

^{A}: not converged in specified time (180 sec.) or number of iterations (30 times)

^{AA}: Wang and Henke (4); they reported that BP-TRI is faster than BP-TG for problem 7 when polynomial data are employed.

Table 2

Comparison of Number of Iterations Required

problem \ method		NEW	TOMICH	BP-TRI	SR-TG	SR-TRI	BP-TG
Absorber	1	3	20	16	22	6	16
	2	7	24	X	18	18	X
Reboiled Absorber	3	5	29	X	X	52	33
	4	5	27	X	X	X	27
	5	10	X				
	6	16	X				
Distillation	7	4	14	12			**
	8	5	≥25*	≥30*			
	9	1		26			

X: divergent

*: not converged in specified time (180 sec.) or number of iterations (30 times)

**: see the comment in Table 1

Table 3

Comparison of Rate of Convergence with Tomich's Method

(Problem 1)

The New Method		The Tomich Method	
Iteration No.	[CRIT]	Iteration No.	[CRIT]
0	0.327×10^{-1}	0	0.453×10^{-1}
1	0.361×10^{-3}	1	0.919×10^{-2}
2	0.145×10^{-3}	5	0.633×10^{-3}
3	0.762×10^{-5}	10	0.583×10^{-3}
		15	0.343×10^{-3}
		20	0.908×10^{-6}

Table 4

Comparison of Rate of Convergence with Tomich's Method

(Problem 3)

The New Method		The Tomich Method	
Iteration No.	[CRIT]	Iteration No.	[CRIT]
0	0.545	0	0.424
1	0.197	1	0.270
2	0.446×10^{-1}	5	0.119
3	0.122×10^{-2}	10	0.434×10^{-2}
4	0.259×10^{-4}	15	0.289×10^{-3}
5	0.357×10^{-5}	20	0.155×10^{-3}
		25	0.139×10^{-3}
		29	0.145×10^{-4}

Table 5

Comparison of Rate of Convergence with Tomich's Method

(Problem 7)

The New Method		The Tomich Method	
Iteration No.	[CRIT]	Iteration No.	[CRIT]
0	0.873	0	0.983
1	0.199	1	0.675
2	0.198×10^{-2}	5	0.159×10^{-2}
3	0.461×10^{-3}	10	0.106×10^{-3}
4	0.140×10^{-4}	14	0.168×10^{-4}

6.3 Discussion

A comparison of the performance of the new method with Tomich's method and with Bubble Point and Sum Rates procedures is given in Table 1 and Table 2. The Sum Rates and Bubble Point procedures are based on traditional procedures and, in general, are not reliable for all types of problems. The Sum Rates procedures are more effective for absorber problems whereas the Bubble Point methods are more reliable for distillation problems. These observations are in agreement with the conclusions of Friday and Smith (14).

The Thiele-Geddes bubble point method with theta convergence has successfully solved some complex reboiled absorber problems. However there is no assurance that this method will converge for a particular problem (52), (22).

Both Tomich's method and the new method show promise of being reliable for all types of separation problems. However, Tomich's method requires longer computational time and has difficulty with complex reboiled absorber problems.

Demethanizer absorbers which handle a significant amount of hydrogen, such as described in problems 5 and 6, seem to be one of the more difficult types of problems to solve. Petryschuk and Johnson (52) were not able to solve a problem similar to example 6 with their program based on the Thiele-Geddes bubble point procedure. Prowse and Johnson (27) solved a problem similar to example 6 using a method based on Ball's relaxation procedure (25). Relaxation methods are characteristically stable but converge quite slowly. Prowse and Johnson (27) report using more than 60 iterations for a problem similar to example 6.

Problem 5 was formulated from information provided by C.I.L. (Canadian Industry Limited) for a column operating at the C.I.L. Edmonton polyethylene plant. The new method readily solves this complex column. However, attempts to simulate the column operation have, as yet, been unsuccessful because of uncertainties as to the identity of all the components present, the plant analyses and as to the proper equilibrium and enthalpy data.

The results obtained for problems 7, 8 and 9 indicate that the new method is the superior method of the procedures tested for distillation problems. The method was particularly effective for the iso-butane - n-butane splitter which contains a large number of equilibrium stages and is described in problem 9.

Comparisons of the convergence characteristics of the new method and of the Tomich method are shown in Table 3, Table 4 and Table 5. In general, the new method requires less computational time and fewer iterations than the Tomich method. However, the average computational time per iteration is less for the Tomich method. This illustrates the effectiveness of the Broyden procedure.

The initial assumptions of temperature and flow rate profiles can have a marked effect on the performance of any procedure, thus identical initial assumptions must be used for valid comparisons. The initial assumptions used for the test problems were moderately far from the final solutions and were selected as ones that could be easily calculated or assumed without prior knowledge of the problem solution. The new method shows promise of being relatively insensitive to the initial assumptions used, that is, it appears to give convergent solutions for a wider range of initial assumptions for any given problem than other methods. However, proper analysis of the relative sensitivity of the methods to initial assumptions is complex and must take into account the method of finding the weighting factor t. Additional work is required to clarify the effect that the choice of initial assumptions has on the convergence characteristics.

The method of selecting the weighting factor, t, has an important effect on the characteristics of the new method and Tomich's method. Further work is required to provide the optimum procedure for selecting the weighting facotr.

The new method obviously requires a larger amount of computer storage than the traditional decoupled methods such as those proposed by Lewis and Matheson (1), Thiele and Geddes (3), and Wang and Henke (4). However, singinficantly less computer storage is required than for the methods proposed by Gentry (7) and Naphtali et al (9). The methods of Gentry and Naphtali et al require a prohibitive amount of computer storage when the use of composition dependent equilibrium and enthalpy data is incorporated in the methods. The new method requires less storage than the Tomich method. A comparison of the sizes of the inverses of the Jacobian matrices can be used as a measure of the computer storage requirement. For example, for a 100 stage column the total number of elements in the inverse of the Jacobian matrix for the new method is 10^4 whereas 4×10^4 elements are required in the Tomich method.

The Chao-Seader correlation has been used exclusively for the direct calculation of equilibrium and enthalpy data for the problems reported in this thesis. Other correlations such as the ones proposed by Chueh and Prausnitz (38), Lee and Edmister (40), Wilson (33) as well as polynomial data correlations can be easily used with the new method.

It should be possible to develop analytical expressions for the partial derivatives required from the correlations mentioned above. Numerical evaluation of the partial derivatives will be required when analytical expressions are not available.

When linearizing the model equations, only the partial derivatives that were thought to have a dominant influence on the solution were employed. This concept is fundamental to the new method in that it allows convenient matrix structures to be formulated which in turn facilitate the simultaneous solution of all the model equations. The test of the method on a wide range of problems suggests that this strategy is quite successful.

CHAPTER 7

CONCLUSIONS

The new calculational procedure for multistage, multicomponent separation calculations that has been described and evaluated in this thesis is a reliable and efficient method for absorber, reboiled absorber and distillation calcualtions, typical of those encountered in the hydrocarbon processing industries and the chemical industries in general.

The new method is more reliable and requires less computational time than the Tomich method and Bubble Point and Sum Rates procedures, and would appear to be a significant improvement on current procedures.

The method seems to be relatively insensitive to initial assumptions, but additional work is required to clarify the influence of initial assumption and of the choice of the weighting factor on the convergence characteristics.

Structuring the equilibrium stage problem as described in this thesis, making effective use of matrix manipulation procedures to solve all the model equations simultantously, avoiding iterative bubble point calculations or other decoupling methods and the fa[illegible] that only 2N(1+NCP) partial derivatives need to be evaluated per iteration, all contribute to the significant reduction in computer storage requirement and computational time compared to other methods.

NOMENCLATURE

A	API gravity, or Chao-Seader coefficient
A, B	defined by equation (4-3)
$\bar{A}$	Jacobian matrix
AH, BH, CH, DH	ideal gas constants
a, b, c	elements of matrix
$\bar{B}$	matrix
C	function defined by equation (2-2)
$\bar{C}$	matrix
$\bar{D}$	matrix
d	density
d, e	elements of matrix
E	function defined by equation (2-3)
E'	normalized energy imbalance
f	general function
f	fugacity
f, g	defined by equations (4-35) and (4-36)
f, g	elements of matrix
$\bar{f}$	column vector defined by equation (3-13)
F	molar feed rate
G	element of matrix
h	enthalpy of liquid, or defined by equation (4-2)
H	enthalpy of vapor
$\bar{H}$	matrix defined by equation (3-19)
ΔH	heat of vaporization
$\bar{I}$	unit matrix

K	equilibrium K-ratio or U.O.P. characteristic factor
L	molar liquid flow rate
M	function defined by equation (2-5)
MW	molecular weight
m	element of column vector
N	total number of stages
NCP	number of components
$\bar{P}$	column vector defined by equation (3-15)
p, q, r	elements of matrix
P	pressure
$\bar{P}$	matrix
Q	heat duty
$\bar{Q}$	column vector
R	gas constant
s, t	elements of matrix
S	function defined by equation (2-4)
SL	molar flow rate of liquid side stream
SV	molar flow rate of vapor side stream
t	weighting factor
T	temperature
$\overline{\Delta T}$	column vector
u	element of column vector
v	molecular volume of gas
V	molar vapor flow rate, or liquid molar volume
$\overline{\Delta V}$	column vector
x	liquid composition
$\bar{x}$	colum vector defined by equation (3-13)

$\overline{\Sigma\Delta x}$	column vector whose element is $\bar{\Sigma}\,\bar{\Delta x}_i$
$\overline{\Delta x}$	column vector
y	vapor composition
$\tilde{y}$	column vector defined by equation (3-18)
z	feed composition, or compressibility factor

Greek Letters

α	element of matrix in equation (5-17)
β	element of matrix in equation (5-18)
γ	activity coefficient
δ	solubility parameter
Δ	"new value minus old value"
ϵ	defined by equation (5-21)
ν	liquid fugacity coefficient
ϕ	Euclidean norm
ψ	vapor phase fugacity coefficient
ω	acentric factor

Subscripts

F	feed
i	component number
j	stage number
L	liquid
N	bottom stage

Superscript

b	boiling point
c	critical condition
k	iteration number
o	pure component, or ideal state
R	reduced state

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APPENDIX 1.1

PHYSICAL PROPERTIES

```
            CODE   ACENT. FAC.    SOL. PARA.    MOLAL VOL.    CRIT. TEMP.   CRIT. PRES.
HYDROGEN     1     0.00000E 00   0.32500E 01   0.31000E 02   0.60200E 02   0.19[illegible]E 03
NITROGEN     3     0.21000E-01   0.44400E 01   0.53000E 02   0.22716E 03   0.4923[illegible]E 03
CO2          4     0.17700E 00   0.71200E 01   0.44000E 02   0.54756E 03   0.10713E 04
H2S          5     0.87000E-01   0.88000E 01   0.43100E 02   0.67248E 03   0.13[illegible]E 04
METHANE      2     0.00000E 00   0.56800E 01   0.57000E 02   0.34390E 03   0.6731[illegible]E 03
ETHANE       6     0.10600E 00   0.60500E 01   0.68000E 02   0.55050E 03   0.71[illegible]E 03
ETHYLENE     6     0.95000E-01   0.60800E 01   0.61000E 02   0.50950E 03   0.7421[illegible]E 03
PROPANE      6     0.15400E 00   0.64000E 01   0.84000E 02   0.66590E 03   0.6174[illegible]E 03
PROPYLEN     6     0.14500E 00   0.64300E 01   0.79000E 02   0.65720E 03   0.[illegible]7[illegible]E 03
IBUTANE      6     0.18250E 00   0.67300E 01   0.10550E 03   0.73470E 03   0.5[illegible]E 03
NBUTANE      6     0.19500E 00   0.67300E 01   0.10140E 03   0.76530E 03   0.55[illegible]7[illegible]E 03
CIS2BUTE     6     0.25750E 00   0.67600E 01   0.91200E 02   0.77[illegible]E 03   0.5[illegible]E 03
I-BUTENE     6     0.19750E 00   0.67600E 01   0.95400E 02   0.75220E 03   0.57[illegible]E 03
IPENTANE     6     0.21040E 00   0.70210E 01   0.11740E 03   0.82980E 03   0.4[illegible]E 03
NPENTANE     6     0.23900E 00   0.70210E 01   0.11610E 03   0.84560E 03   0.4[illegible]E 03
HEXANE       6     0.29700E 00   0.72660E 01   0.13160E 03   0.91420E 03   0.44[illegible]E 03
BENZENE      6     0.21300E 00   0.91580E 01   0.89400E 02   0.10127E 04   0.714[illegible]E 03
2MPENTAN     6     0.27700E 00   0.70180E 01   0.13290E 03   0.89550E 03   0.44[illegible]1[illegible]E 03
HEPTANE      6     0.34000E 00   0.74300E 01   0.14750E 03   0.97230E 03   0.39[illegible]E 03
TOLUENE      6     0.25900E 00   0.89150E 01   0.10680E 03   0.10692E 04   0.59[illegible]E 03
OCTANE       6     0.39900E 00   0.75510E 01   0.16350E 03   0.10249E 04   0.3621[illegible]E 03
O-XYLENE     6     0.29000E 00   0.86870E 01   0.12120E 03   0.11383E 04   0.53[illegible]E 03
ECHEXANE     6     0.30500E 00   0.77430E 01   0.14310E 03   0.10847E 04   0.453[illegible]E 03
NONANE       6     0.44400E 00   0.76490E 01   0.17950E 03   0.10730E 04   0.332[illegible]E 03
DECANE       6     0.48700E 00   0.77210E 01   0.19600E 03   0.11140E 04   0.304[illegible]E 03
UNDECANE     6     0.52100E 00   0.77900E 01   0.21220E 03   0.11540E 04   0.242[illegible]E 03
DODECANE     6     0.56100E 00   0.78400E 01   0.22860E 03   0.11860E 04   0.262[illegible]E 03
TRDECANE     6     0.60000E 00   0.78900E 01   0.24490E 03   0.12200E 04   0.250[illegible]E 03
```

APPENDIX 1.2

CONSTANTS FOR IDEAL GAS ENTHALPY

	A	B	C	D
HYDROGEN	0.31091E 04	0.68913E 01	0.16126E-03	-0.72242E-07
NITROGEN	0.31921E 04	0.69564E 01	-0.31038E-04	0.23500E-06
CO2	0.33577E 04	0.84401E 01	0.30405E-02	-0.78977E-06
H2S	0.36592E 04	0.80338E 01	0.55089E-03	0.32509E-06
METHANE	0.36839E 04	0.78808E 01	0.35057E-02	0.24465E-06
ETHANE	0.42201E 04	0.11202E 02	0.89381E-02	-0.80652E-05
ETHYLENE	0.37920E 04	0.91448E 01	0.78194E-02	-0.15227E-05
PROPANE	0.50686E 04	0.15108E 02	0.15406E-01	-0.29387E-05
PROPYLEN	0.47148E 04	0.13502E 01	0.11469E-01	-0.17973E-05
IBUTANE	0.60231E 04	0.19998E 02	0.20441E-01	-0.41461E-05
NBUTANE	0.66547E 04	0.20545E 02	0.18653E-01	-0.30157E-05
CIS2BUTE	0.57638E 04	0.16014E 02	0.17372E-01	-0.32793E-05
1-BUTENE	0.57975E 04	0.18815E 02	0.16076E-01	-0.30421E-05
IPENTANE	0.74756E 04	0.24654E 02	0.24462E-01	-0.44373E-05
NPENTANE	0.80398E 04	0.25190E 02	0.23486E-01	-0.41745E-05
HEXANE	0.94750E 04	0.29523E 02	0.29141E-01	-0.59119E-05
BENZENE	0.47399E 04	0.16158E 02	0.22386E-01	-0.53555E-05
2MPENTAN	0.85771E 04	0.28889E 02	0.32098E-01	-0.79119E-05
HEPTANE	0.10566E 05	0.33315E 02	0.32787E-01	-0.66961E-05
TOLUENE	0.59813E 04	0.20865E 02	0.26105E-01	-0.58166E-05
OCTANE	0.12262E 05	0.38991E 02	0.38411E-01	-0.79457E-05
O-XYLENE	0.77375E 04	0.27563E 02	0.28048E-01	-0.55709E-05
ECHEXANE	0.82914E 04	0.31816E 02	0.40773E-01	-0.72295E-05
NONANE	0.13661E 05	0.43736E 02	0.43017E-01	-0.89546E-05
DECANE	0.15052E 05	0.48486E 02	0.47562E-01	-0.98586E-05
UNDECANE	0.16463E 05	0.53067E 02	0.52624E-01	-0.11207E-04
DODECANE	0.17845E 05	0.57952E 02	0.56865E-01	-0.11944E-04
TRDECANE	0.19239E 05	0.62722E 02	0.61338E-01	-0.12815E-04

APPENDIX I.3

CHAO-SEADER COEFFICIENTS FOR LIQUID FUGACITY COEFFICIENTS

	HYDROGEN	METHANE	NITROGEN	CO_2	H_2S	GENERAL
A_1	1.967178	2.438000	2.736548	-30.060852	3.058120	5.757400
A_2	1.029718	-2.245500	-1.981830	6.140988	-2.649190	-3.017610
A_3	-0.0540[illegible]0	-0.340840	-0.514870	45.263214	0.374580	-4.985000
A_4	0.000530	-0.002120	0.042470	-27.302994	-1.464708	2.022988
A_5	0.0	-0.002230	-0.002810	5.915250	0.457350	0.0
A_6	0.008590	0.104860	-0.029470	0.368380	-0.957220	0.084270
A_7	0.0	-0.036910	0.023500	-0.679170	1.427258	0.266670
A_8	0.0	0.0	0.0	0.155460	-0.502420	-0.311380
A_9	0.0	0.0	0.0	0.0	0.335890	-0.026550
A_{10}	0.0	0.0	0.0	0.089560	-0.266780	0.028830
A_{11}	0.0	0.0	0.0	0.0	0.0	-4.238930
A_{12}	0.0	0.0	0.0	0.0	0.0	8.658078
A_{13}	0.0	0.0	0.0	0.0	0.0	-1.220590
A_{14}	0.0	0.0	0.0	0.0	0.0	-3.152240
A_{15}	0.0	0.0	0.0	0.0	0.0	-0.025000

APPENDIX 2

```
EXAMPLE OF USE OF NEW ALGORITHM
  FOR THE NUMERICAL SOLUTION OF TRIDIAGONAL MATRIX EQUATIONS

 EQUATIONS -

  1*X1 +1*X2                          = 3
  1*X1 +2*X2 -1*X3                    = 2
        3*X2 +2*X3 +1*X4              = 16
              1*X3 +2*X4 -3*X5        = -4
                   -1*X4 +1*X5        = 1


 RESULT

                      X1          X2          X3          X4          X5

 TRUE SOLUTION        1           2           3           4           5

 NEW METHOD          0.10000E 01 0.20000E 01 0.30000E 01 0.39999E 01 [illegible]

 THOMAS METHOD       0.10000E 01 0.19999E 01 0.30000E 01 0.40000E 01 [illegible]
```

```
APPENDIX 3-1   TEST PROBLEM NUMBER - 1


      ***** PROBLEM STATEMENT *****


 TYPE OF COLUMN         1

 NO. OF PLATES           8

 NO. OF COMPONENTS         6

 PRESSURE AT TOP PLATE (PSIA)          300.00

 PRESSURE DROP PER PLATE (PSIA)           0.0

 NO. OF FEEDS         2

     ENTERING PLATE OF FEED 1       1
     FEED QUANTITY          0.20000E 02
     PRESSURE OF FEED             300.00
     TEMPERATURE OF FEED (F)             90.00

     ENTERING PLATE OF FEED 2       8
     FEED QUANTITY          0.10000E 03
     PRESSURE OF FEED             300.00
     LIQUID RATIO OF FEED           0.0
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 0    SUM OF SQUARES OF RESIDUALS  0.32679E-01
TEMPERATURE
 0.55960E 03 0.55960E 03 0.55960E 03 0.55960E 03 0.55960E 03
 0.55960E 03 0.55960E 03 0.55960E 03
VAPOR FLOW RATE
 0.95000E 02 0.90000E 02 0.90000E 02 0.90000E 02 0.90000E 02
 0.90000E 02 0.90000E 02 0.95000E 02

 1    SUM OF SQUARES OF RESIDUALS  0.36086E-03
TEMPERATURE
 0.56296E 03 0.59013E 03 0.59172E 03 0.59047E 03 0.58676E 03
 0.58020E 03 0.57014E 03 0.55351E 03
VAPOR FLOW RATE
 0.85961E 02 0.91427E 02 0.91573E 02 0.92212E 02 0.94497E 02
 0.92951E 02 0.93739E 02 0.95105E 02

 2    SUM OF SQUARES OF RESIDUALS  0.14544E-03
TEMPERATURE
 0.57689E 03 0.58159E 03 0.58311E 03 0.58328E 03 0.58199E 03
 0.57837E 03 0.57080E 03 0.55555E 03
VAPOR FLOW RATE
 0.86080E 02 0.91885E 02 0.92603E 02 0.92957E 02 0.93245E 02
 0.93598E 02 0.94186E 02 0.95494E 02

 3    SUM OF SQUARES OF RESIDUALS  0.76246E-05
TEMPERATURE
 0.57911E 03 0.58466E 03 0.58581E 03 0.58488E 03 0.58216E 03
 0.57750E 03 0.56956E 03 0.55443E 03
VAPOR FLOW RATE
 0.86012E 02 0.91674E 02 0.92384E 02 0.92708E 02 0.93000E 02
 0.93388E 02 0.94028E 02 0.95387E 02
```

```
***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS     3

COLUMN PRESSURE (PSIA)    0.30000E 03

PRESSURE, TEMPERATURE, ENTHALPY AND LIQUID FRACTION OF FEED

 0.300E 03 PSIA  0.900E 02 F  0.[illegible]E 04 B.T.U.      1.000

 0.300E 03 PSIA  0.[illegible]E 02 F  0.432[illegible]E 0[illegible] B.T.U.      0.0

*** STAGE VARIABLES ***

   PLATE NO.  TEMPERATURE   LIQ. F. R.    VAP. F. R.    HEAT DUTY,
                   F        LB MOL/TIME   LB MOL/TIME    BTU/TIME
        1     0.11951E 03   0.25606E 02   0.90012E 02   0.0
        2     0.12506E 03   0.26372E 02   0.91674E 02   0.0
        3     0.12621E 03   0.26606E 02   0.92384E 02   0.0
        4     0.12524E 03   0.26988E 02   0.92270E 02   0.0
        5     0.12256E 03   0.27376E 02   0.93000E 02   0.0
        6     0.11790E 03   0.28016E 02   0.93388E 02   0.0
        7     0.10996E 03   0.29374E 02   0.94028E 02   0.0
        8     0.94824E 02   0.32988E 02   0.95387E 02   0.0
```

```
*** MATERIAL BALANCES ***

FEEDS

                    PLATE NO.    1                          PLATE NO.    2
                LB MOL/TIME      MOL FRC.          LB MOL/TIME      MOL FRC.
METHANE         0.0              0.0               0.70000E 02      0.70000E 00
ETHANE          0.0              0.0               0.15000E 02      0.15000E 00
PROPANE         0.0              0.0               0.10000E 02      0.10000E 00
NBUTANE         0.0              0.0               0.40000E 01      0.40000E-01
NPENTANE        0.0              0.0               0.10000E 01      0.10000E-01
OCTANE          0.20000E 02      0.10000E 01       0.0              0.0
TOTAL           0.20000E 02                        0.10000E 03

PRODUCTS

                      TOP PRODUCT                        BOTTOM PRODUCT
                LB MOL/TIME      MOL FRC.          LB MOL/TIME      MOL FRC.
METHANE         0.67326E 02      0.78275E 00       0.26796E 01      0.78839E-0[illegible]
ETHANE          0.12514E 02      0.14549E 00       0.24845E 01      0.73099E-01
PROPANE         0.54286E 01      0.63114E-01       0.45680E 01      0.13440E 00
NBUTANE         0.10626E 00      0.[illegible]E-02       0.36935E 01      0.10867E 00
NPENTANE        0.18415E-03      0.21409E-06       0.99981E 00      0.29417E-01
OCTANE          0.43764E 00      0.50881E-02       0.19562E 02      0.57557E 00
TOTAL           0.86012E 02                        0.33988E 02
```

```
APPENDIX 3-.    TEST PROBLEM NUMBER - 2


        ***** PROBLEM STATEMENT *****


TYPE OF COLUMN          1

NO. OF PLATES          6

NO. OF COMPONENTS        15

PRESSURE AT TOP PLATE (PSIA)           1310.00

PRESSURE DROP PER PLATE (PSIA)            0.0

NO. OF FEEDS        2

   ENTERING PLATE OF FEED 1         1
   FEED QUANTITY          0.36250E 02
   PRESSURE OF FEED           1310.00
   TEMPERATURE OF FEED (F)             -5.00

   ENTERING PLATE OF FEED 2         6
   FEED QUANTITY          0.11809E 04
   PRESSURE OF FEED           1310.00
   TEMPERATURE OF FEED (F)             45.00

NO. OF INTER COOLERS OR HEATERS         1

   PLATE NO. OF INTER COOLER OR HEATER 1         6
   HEAT LOAD OF INTER COOLER OR HEATER      -0.58000E 06
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 0    SUM OF SQUARES OF RESIDUALS  0.89902E-01
TEMPERATURE
 0.47960E 03 0.48460E 03 0.48460E 03 0.48460E 03 0.48460E 03
 0.47960E 03
VAPOR FLOW RATE
 0.93986E 03 0.95000E 03 0.97500E 03 0.10000E 04 0.10500E 04
 0.11000E 04

 1    SUM OF SQUARES OF RESIDUALS  0.85200E-02
TEMPERATURE
 0.49032E 03 0.48876E 03 0.48781E 03 0.48625E 03 0.48496E 03
 0.48290E 03
VAPOR FLOW RATE
 0.92373E 03 0.96618E 03 0.98453E 03 0.10045E 04 0.10374E 04
 0.10811E 04

      SUM OF SQUARES OF RESIDUALS  0.25760E-02
TEMPERATURE
 0.48915E 03 0.48606E 03 0.48416E 03 0.48322E 03 0.48367E 03
 0.48522E 03
VAPOR FLOW RATE
 0.93488E 03 0.99499E 03 0.10163E 04 0.10347E 04 0.10644E 04
 0.11052E 04

 3    SUM OF SQUARES OF RESIDUALS  0.77683E-03
TEMPERATURE
 0.49032E 03 0.48771E 03 0.48538E 03 0.48370E 03 0.48304E 03
 0.48367E 03
VAPOR FLOW RATE
 0.92874E 03 0.99307E 03 0.10151E 04 0.10353E 04 0.10627E 04
 0.11023E 04

 4    SUM OF SQUARES OF RESIDUALS  0.89358E-04
TEMPERATURE
 0.49077E 03 0.48985E 03 0.48828E 03 0.48690E 03 0.48563E 03
 0.48397E 03
VAPOR FLOW RATE
 0.93056E 03 0.99617E 03 0.10169E 04 0.10351E 04 0.10578E 04
 0.10929E 04

 5    SUM OF SQUARES OF RESIDUALS  0.52666E-04
TEMPERATURE
 0.48973E 03 0.48883E 03 0.48762E 03 0.48672E 03 0.4858[illegible]E 03
 0.48413E 03
VAPOR FLOW RATE
 0.93157E 03 0.99866E 03 0.10197E 04 0.10376E 04 0.10585E 04
 0.10912E 04
```

```
 6    SUM OF SQUARES OF RESIDUALS  0.86600E-05
TEMPERATURE
 0.49016E 03 0.48901E 03 0.48745E 03 0.48623E 03 0.48516E 03
 0.48384E 03
VAPOR FLOW RATE
 0.93008E 03 0.99697E 03 0.10181E 04 0.10361E 04 0.10571E 04
 0.10904E 04

 7    SUM OF SQUARES OF RESIDUALS  0.50215E-05
TEMPERATURE
 0.49060E 03 0.48953E 03 0.48799E 03 0.48662E 03 0.48525E 03
 0.48380E 03
VAPOR FLOW RATE
 0.92995E 03 0.99648E 03 0.10172E 04 0.10349E 04 0.10567E 04
 0.10895E 04
```

```
     ***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS     7

COLUMN PRESSURE (PSIA)    0.13100E 04

PRESSURE , TEMPERATURE , ENTHALPY AND LIQUID FRACTION OF FEED

 0.131E 04 PSIA -0.500E 01 F-0.139E 06 B.T.U.         1.000

 0.131E 04 PSIA  0.450E 02 F  0.342E 07 B.T.U.        0.0

*** STAGE VARIABLES ***

   PLATE NO. TEMPERATURE   LIQ. F. R.    VAP. F. R.     HEAT DUTY
                 F         LB MOL/TIME   LB MOL/TIME     BTU/TIME
       1      0.30898E 02  0.10278E 03  0.92995E 03   0.0
       2      0.29931E 02  0.12346E 03  0.99648E 03   0.0
       3      0.28386E 02  0.14116E 03  0.10172E 04   0.0
       4      0.27016E 02  0.16199E 03  0.10349E 04   0.0
       5      0.25649E 02  0.15582E 03  0.10557E 04   0.0
       6      0.24108E 02  0.28717E 03  0.10895E 04  -0.58000E 06
```

```
*** MATERIAL BALANCES ***

FEEDS

                    PLATE NO.    1                  PLATE NO.    6
              LB MOL/TIME     MOL FRC.        LB MOL/TIME     MOL FRC.
NITROGEN      0.0             0.0             0.20670E 02     0.17504E-01
CO2           0.0             0.0             0.15250E 02     0.12914E-01
METHANE       0.0             0.0             0.87215E 03     0.73857E 00
ETHANE        0.0             0.0             0.17678E 03     0.14970E 00
PROPANE       0.0             0.0             0.68680E 02     0.58161E-01
IBUTANE       0.0             0.0             0.72800E 01     0.61650E-02
NBUTANE       0.0             0.0             0.13670E 02     0.11576E-01
IPENTANE      0.0             0.0             0.19700E 01     0.16683E-02
NPENTANE      0.0             0.0             0.19500E 01     0.16513E-02
HEXANE        0.0             0.0             0.13100E 01     0.11094E-02
HYPTH-1       0.70000E-01     0.19310E-02     0.84000E 00     0.71134E-03
HYPTH-2       0.29000E 00     0.80000E-02     0.25000E 00     0.21171E-03
HYPTH-3       0.12990E 02     0.35835E 00     0.50000E-01     0.42342E-04
HYPTH-4       0.20430E 02     0.56359E 00     0.10000E-01     0.84683E-05
HYPTH-5       0.24700E 01     0.68138E-01     0.10000E-01     0.84683E-05
TOTAL         0.36250E 02                     0.11809E 04

PRODUCTS

                    TOP PRODUCT                     BOTTOM PRODUCT
              LB MOL/TIME     MOL FRC.        LB MOL/TIME     MOL FRC.
NITROGEN      0.19462E 02     0.20928E-01     0.12353E 01     0.43015E-02
CO2           0.10284E 02     0.11059E-01     0.49539E 01     0.17251E-01
METHANE       0.76128E 03     0.81862E 00     0.11101E 03     0.38656E 00
ETHANE        0.11237E 03     0.12083E 00     0.64314E 02     0.22396E 00
PROPANE       0.24443E 02     0.26284E-01     0.44194E 02     0.15390E 00
IBUTANE       0.10196E 01     0.10964E-02     0.62578E 01     0.21791E-01
NBUTANE       0.81845E 00     0.88010E-03     0.12849E 02     0.44745E-01
IPENTANE      0.14287E-01     0.15364E-04     0.19557E 01     0.68101E-02
NPENTANE      0.36481E-02     0.39229E-05     0.19463E 01     0.67776E-02
HEXANE        0.25829E-04     0.27774E-07     0.13100E 01     0.45617E-02
HYPTH-1       0.67593E-02     0.72684E-05     0.90320E 00     0.31452E-02
HYPTH-2       0.10142E-01     0.10906E-04     0.52979E 00     0.18449E-02
HYPTH-3       0.15050E 00     0.16184E-03     0.12888E 02     0.44881E-01
HYPTH-4       0.90845E-01     0.97688E-04     0.20348E 02     0.70858E-01
HYPTH-5       0.46795E-02     0.50320E-05     0.24753E 01     0.86195E-02
TOTAL         0.92995E 03                     0.28717E 03
```

```
APPENDIX 3-3   TEST PROBLEM NUMBER - 3


     ***** PROBLEM STATEMENT *****


 TYPE OF COLUMN        2

 NO. OF PLATES      10

 NO. OF COMPONENTS        5

 PRESSURE AT TOP PLATE (PSIA)           300.00

 PRESSURE DROP PER PLATE (PSIA)           0.0

 NO. OF FEEDS        2

    ENTERING PLATE OF FEED 1         1
    FEED QUANTITY         0.30000E 02
    PRESSURE OF FEED            300.00
    TEMPERATURE OF FEED (F)             90.00

    ENTERING PLATE OF FEED 2        5
    FEED QUANTITY         0.10001E 03
    PRESSURE OF FEED            300.00
    LIQUID RATIO OF FEED          0.0

 SPECIFIED TOP PRODUCT        0.95000E 02

 NO. OF LIQUID SIDE STREAMS        1

    LEAVING PLATE NO. OF STREAM 1       9
    QUANTITY OF SIDE STREAM       0.15000E 02
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 0    SUM OF SQUARES OF RESIDUALS  0.54506E 00
TEMPERATURE
 0.55960E 03 0.60960E 03 0.60560E 03 0.60960E 03 0.60960E 03
 0.67960E 03 0.73960E 03 0.80960E 03 0.85960E 03 0.93960E 03
VAPOR FLOW RATE
 0.95000E 02 0.10500E 03 0.10500E 03 0.11000E 03 0.11500E 03
 0.75000E 02 0.50000E 02 0.50000E 02 0.50000E 02 0.65000E 02

 1    SUM OF SQUARES OF RESIDUALS  0.19667E 00
TEMPERATURE
 0.57872E 03 0.60439E 03 0.60685E 03 0.60396E 03 0.59480E 03
 0.67867E 03 0.74414E 03 0.81110E 03 0.87721E 03 0.94438E 03
VAPOR FLOW RATE
 0.95000E 02 0.10354E 03 0.10525E 03 0.10830E 03 0.11181E 03
 0.37500E 02 0.39664E 02 0.48690E 02 0.51238E 02 0.65246E 02

 2    SUM OF SQUARES OF RESIDUALS  0.44551E-01
TEMPERATURE
 0.58692E 03 0.60066E 03 0.60527E 03 0.60269E 03 0.58921E 03
 0.68078E 03 0.74897E 03 0.81056E 03 0.88449E 03 0.94654E 03
VAPOR FLOW RATE
 0.95000E 02 0.10375E 03 0.10603E 03 0.10796E 03 0.11026E 03
 0.18750E 02 0.35052E 02 0.48961E 02 0.51077E 02 0.64463E 02

 3    SUM OF SQUARES OF RESIDUALS  0.12224E-02
TEMPERATURE
 0.58748E 03 0.60044E 03 0.60536E 03 0.60377E 03 0.59213E 03
 0.69075E 03 0.74923E 03 0.80865E 03 0.88560E 03 0.94735E 03
VAPOR FLOW RATE
 0.95000E 02 0.10404E 03 0.10645E 03 0.10813E 03 0.11014E 03
 0.15721E 02 0.38944E 02 0.49323E 02 0.50426E 02 0.64129E 02

 4    SUM OF SQUARES OF RESIDUALS  0.25923E-04
TEMPERATURE
 0.58766E 03 0.60060E 03 0.60509E 03 0.60277E 03 0.59085E 03
 0.69482E 03 0.74976E 03 0.80873E 03 0.88565E 03 0.94753E 03
VAPOR FLOW RATE
 0.95000E 02 0.10399E 03 0.10639E 03 0.10807E 03 0.11022E 03
 0.16389E 02 0.41181E 02 0.49545E 02 0.50775E 02 0.64046E 02

 5    SUM OF SQUARES OF RESIDUALS  0.35742E-05
TEMPERATURE
 0.58767E 03 0.60069E 03 0.60544E 03 0.60347E 03 0.59113E 03
 0.69494E 03 0.74959E 03 0.80845E 03 0.88550E 03 0.94755E 03
VAPOR FLOW RATE
 0.95000E 02 0.10400E 03 0.10639E 03 0.10805E 03 0.11008E 03
 0.16141E 02 0.40574E 02 0.49229E 02 0.50536E 02 0.63740E 02
```

```
*****COMPUTED RESULTS*****

NUMBER OF ITERATIONS

COLUMN PRESSURE (PSIA)     0.30000E 03

PRESSURE , TEMPERATURE , ENTHALPY AND LIQUID FRACTION OF FEED

 0.300E 03 PSIA   0.900E 02 F  0.877E 04 B.T.U.         1.000

 0.300E 03 PSIA   0.446E 03 F  0.416E 06 B.T.U.         0.0

*** STAGE VARIABLES ***

      PLATE NO. TEMPERATURE  LIQ. F. R.      VAP. F. R.      HEAT DUTY
                     F       LB MOL/TIME     LB MOL/TIME     BTU/TIME
         1    0.12807E 03   0.38997E 02    0.55000E 02    0.0
         2    0.14109E 03   0.41392E 02    0.10400E 03    0.0
         3    0.14584E 03   0.43050E 02    0.10039E 03    0.0
         4    0.14387E 03   0.45077E 02    0.10805E 03    0.0
         5    0.13153E 03   0.51151E 02    0.11008E 03    0.0
         6    0.23534E 03   0.75584E 02    0.16141E 02    0.0
         7    0.28999E 03   0.84239E 02    0.40574E 02    0.0
         8    0.34885E 03   0.85546E 02    0.49229E 02    0.0
         9    0.42590E 03   0.83750E 02    0.50536E 02    0.0
        10    0.48795E 03   0.20010E 02    0.63740E 02    0.88984E 06
```

```
*** MATERIAL BALANCES ***

FEEDS

                   PLATE NO.    1                          PLATE NO.    [illegible]
             LB MOL/TIME     MOL FRC.          LB MOL/TIME      MOL FRC.
METHANE      0.0              0.0              0.80000E 02     0.79952E 00
ETHANE       0.0              0.0              0.66700E 01     0.66693E-01
PROPANE      0.0              0.0              0.66700E 01     0.66693E-01
NBUTANE      0.0              0.0              0.66700E 01     0.66693E-01
OCTANE       0.30000E 02      0.10000E 01      0.0             0.0
TOTAL        0.30000E 02                       0.10001E 03

PRODUCTS

                   TOP PRODUCT                          BOTTOM PRODUCT
             LB MOL/TIME     MOL FRC.          LB MOL/TIME      MOL FRC.
METHANE      0.79998E 02     0.84209E 00       0.31999E-03     0.15992E-04
ETHANE       0.66644E 01     0.70151E-01       0.89408E-03     0.44682E-04
PROPANE      0.62250E 01     0.65527E-01       0.13135E 00     0.65644E-02
NBUTANE      0.15469E 01     0.16283E-01       0.19230E 01     0.96101E-01
OCTANE       0.56645E 00     0.59621E-02       0.17954E 02     0.89727E 00
TOTAL        0.95000E 02                       0.20010E 02

LIQUID SIDE STREAMS

                   LIQUID ( 9)
             LB MOL/TIME     MOL FRC.
METHANE      0.15667E-02     0.10578E-03
ETHANE       0.47387E-02     0.31591E-03
PROPANE      0.31347E 00     0.20898E-01
NBUTANE      0.32002E 01     0.21334E 00
OCTANE       0.11480E 02     0.76534E 00
TOTAL        0.15000E 02
```

```
APPENDIX B-4    TEST PROBLEM NUMBER - 4

     ***** PROBLEM STATEMENT *****


 TYPE OF COLUMN          2

 NO. OF PLATES         16

 NO. OF COMPONENTS        15

 PRESSURE AT TOP PLATE (PSIA)              270.00

 PRESSURE DROP PER PLATE (PSIA)              0.0

 NO. OF FEEDS         2

    ENTERING PLATE OF FEED 1          1
    FEED QUANTITY          0.26590E 03
    PRESSURE OF FEED            270.00
    TEMPERATURE OF FEED (F)              -5.00

    ENTERING PLATE OF FEED 2          6
    FEED QUANTITY          0.17108E 04
    PRESSURE OF FEED            270.00
    TEMPERATURE OF FEED (F)              50.00

 SPECIFIED TOP PRODUCT         0.67700E 03

 NO. OF INTER COOLERS OR HEATERS          1

    PLATE NO. OF INTER COOLER OR HEATER 1         12
    HEAT LOAD OF INTER COOLER OR HEATER          0.40000E 07
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 0    SUM OF SQUARES OF RESIDUALS  0.87358E 00
TEMPERATURE
 0.53460E 03 0.54960E 03 0.55960E 03 0.56960E 03 0.57960E 03
 0.59460E 03 0.60960E 03 0.61960E 03 0.63460E 03 0.64960E 03
 0.65960E 03 0.66960E 03 0.67960E 03 0.68960E 03 0.699[illegible]E 03
 0.70960E 03
VAPOR FLOW RATE
 0.67700E 03 0.75000E 03 0.80000E 03 0.85000E 03 0.90000E 03
 0.95000E 03 0.90000E 03 0.90000E 03 0.90000E 03 0.90000E 03
 0.95000E 03 0.10000E 04 0.10000E 04 0.10000E 04 0.10000E 04
 0.10000E 04

 1    SUM OF SQUARES OF RESIDUALS  0.57385E-01
TEMPERATURE
 0.53689E 03 0.54821E 03 0.55271E 03 0.55564E 03 0.55484E 03
 0.53914E 03 0.55369E 03 0.56511E 03 0.57869E 03 0.59154E 03
 0.60433E 03 0.62772E 03 0.64326E 03 0.63804E 03 0.64958E 03
 0.70095E 03
VAPOR FLOW RATE
 0.67700E 03 0.86131E 03 0.87279E 03 0.86833E 03 0.87146E 03
 0.91497E 03 0.84562E 03 0.93518E 03 0.10020E 04 0.11198E 04
 0.12337E 04 0.13033E 04 0.75189E 03 0.11163E 04 0.94992E 03
 0.91728E 03

 2    SUM OF SQUARES OF RESIDUALS  0.19695E-01
TEMPERATURE
 0.53330E 03 0.54344E 03 0.54865E 03 0.55265E 03 0.55293E 03
 0.53709E 03 0.54796E 03 0.55249E 03 0.55735E 03 0.56533E 03
 0.57983E 03 0.61055E 03 0.62857E 03 0.62997E 03 0.64423E 03
 0.69805E 03
VAPOR FLOW RATE
 0.67700E 03 0.87268E 03 0.88700E 03 0.88636E 03 0.89035E 03
 0.92805E 03 0.86192E 03 0.94227E 03 0.94431E 03 0.93353E 03
 0.93463E 03 0.97750E 03 0.57851E 03 0.84886E 03 0.83915E 03
 0.84437E 03

 3    SUM OF SQUARES OF RESIDUALS  0.45026E-02
TEMPERATURE
 0.53388E 03 0.54432E 03 0.55030E 03 0.55423E 03 0.55417E 03
 0.53785E 03 0.54904E 03 0.55385E 03 0.55871E 03 0.56619E 03
 0.57763E 03 0.[illegible]168E 03 0.60909E 03 0.61904E 03 0.63512E 03
 0.69326E 03
VAPOR FLOW RATE
 0.67700E 03 0.88606E 03 0.90544E 03 0.91234E 03 0.91963E 03
 0.95138E 03 0.90112E 03 0.10153E 04 0.10506E 04 0.10681E 04
 0.10896E 04 0.11020E 04 0.67154E 03 0.65781E 03 0.76298E 03
 0.76309E 03
```

```
4     SUM OF SQUARES OF RESIDUALS  0.26703E-03
TEMPERATURE
 0.53727E 03 0.54812E 03 0.55309E 03 0.55534E 03 0.55369E 03
 0.53779E 03 0.54892E 03 0.55353E 03 0.55775E 03 0.56433E 03
 0.57565E 03 0.60058E 03 0.60770E 03 0.61849E 03 0.63432E 03
 0.69376E 03
VAPOR FLOW RATE
 0.67700E 03 0.88162E 03 0.89934E 03 0.90761E 03 0.91872E 03
 0.95555E 03 0.90842E 03 0.10256E 04 0.10637E 04 0.10857E 04
 0.11160E 04 0.11409E 04 0.71685E 03 0.77481E 03 0.83737E 03
 0.80236E 03

5     SUM OF SQUARES OF RESIDUALS  0.13340E-04
TEMPERATURE
 0.53636E 03 0.54700E 03 0.55226E 03 0.55513E 03 0.55404E 03
 0.53783E 03 0.54895E 03 0.55357E 03 0.55790E 03 0.56476E 03
 0.57643E 03 0.60185E 03 0.60937E 03 0.61933E 03 0.63468E 03
 0.69369E 03
VAPOR FLOW RATE
 0.67700E 03 0.88356E 03 0.90209E 03 0.90991E 03 0.91958E 03
 0.95486E 03 0.90746E 03 0.10252E 04 0.10639E 04 0.10848E 04
 0.11105E 04 0.11302E 04 0.70228E 03 0.75446E 03 0.81767E 03
 0.79319E 03
```

```
***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS [illegible]

COLUMN PRESSURE (PSIA)    0.27000E 03

PRESSURE , TEMPERATURE , ENTHALPY AND LIQUID FRACTION OF FEED

 0.270E 03 PSIA -0.500E 01 F-0.919E 06 B.T.U.        1.000

 0.270E 03 PSIA  0.500E 02 F-0.147E 06 B.T.U.        0.880

*** STAGE VARIABLES ***

   PLATE NO. TEMPERATURE   LIQ. F. R.    VAP. F. R.    HEAT DUTY
                 F         LB MOL/TIME   LB MOL/TIME    BTU/TIME
       1      0.76750E 02   0.47246E 03   0.67700E 03   0.0
       2      0.87356E 02   0.46059E 03   0.88356E 03   0.0
       3      0.92660E 02   0.45881E 03   0.90209E 03   0.0
       4      0.95531E 02   0.50848E 03   0.90991E 03   0.0
       5      0.94436E 02   0.54376E 03   0.91956E 03   0.0
       6      0.78834E 02   0.22072E 04   0.95406E 03   0.0
       7      0.89359E 02   0.23249E 04   0.90749E 03   0.0
       8      0.93972E 02   0.23630E 04   0.10752E 04   0.0
       9      0.98299E 02   0.23845E 04   0.10639E 04   0.0
      10      0.10516E 03   0.24192E 04   0.10840E 04   0.0
      11      0.11083E 03   0.24299E 04   0.11105E 04   0.0
      12      0.14225E 03   0.20929E 04   0.11302E 04   0.40000E 07
      13      0.14977E 03   0.20542E 04   0.70220E 03   0.0
      14      0.15973E 03   0.21174E 04   0.75446E 03   0.0
      15      0.17508E 03   0.20229E 04   0.81767E 03   0.0
      16      0.23409E 03   0.12997E 04   0.79319E 03   0.93145E 07
```

```
*** MATERIAL BALANCES ***

FEEDS

                     PLATE NO.   1                       PLATE NO. [illegible]
               LB MOL/TIME     MOL FRC.          LB MOL/TIME     MOL FRC.
NITROGEN       0.0             0.0               0.70000E 00     0.40917E-03
CO2            0.0             0.0               0.12400E 02     0.72481E-02
METHANE        0.0             0.0               0.16740E 03     0.97845E-01
ETHANE         0.0             0.0               0.47440E 03     0.27730E 00
PROPANE        0.0             0.0               0.44020E 03     0.25731E 00
IBUTANE        0.0             0.0               0.64300E 02     0.37585E-01
NBUTANE        0.0             0.0               0.12880E 03     0.75286E-01
IPENTANE       0.0             0.0               0.19500E 02     0.11398E-01
NPENTANE       0.0             0.0               0.19400E 02     0.11340E-01
HEXANE         0.0             0.0               0.13100E 02     0.76572E-02
HYPTH-1        0.50000E 00     0.18804E-02       0.90000E 01     0.52607E-02
HYPTH-2        0.21000E 01     0.78577E-02       0.53000E 01     0.30980E-02
HYPTH-3        0.95300E 02     0.35841E 00       0.12830E 03     0.74994E-01
HYPTH-4        0.14990E 03     0.56375E 00       0.20330E 03     0.11883E 00
HYPTH-5        0.18100E 02     0.68071E-01       0.24700E 02     0.14438E-01
TOTAL          0.26590E 03                       0.17108E 04

PRODUCTS

                    TOP PRODUCT                       BOTTOM PRODUCT
               LB MOL/TIME     MOL FRC.          LB MOL/TIME     MOL FRC.
NITROGEN       0.69924E 00     0.10328E-02       0.62390E-11     0.48003E-14
CO2            0.12402E 02     0.18319E-01       0.39272E-02     0.30216E-05
METHANE        0.16734E 03     0.24718E 00       0.12452E-04     0.95808E-08
ETHANE         0.44615E 03     0.65901E 00       0.28300E 02     0.21774E-01
PROPANE        0.49821E 02     0.73591E-01       0.39038E 03     0.30036E 00
IBUTANE        0.28764E 00     0.42487E-03       0.64012E 02     0.49252E-01
NBUTANE        0.12321E 00     0.18200E-03       0.12868E 03     0.99005E-01
IPENTANE       0.17947E-03     0.26509E-06       0.19500E 02     0.15003E-01
NPENTANE       0.42297E-04     0.62477E-07       0.19400E 02     0.14926E-01
HEXANE         0.52087E-07     0.76938E-10       0.13100E 02     0.10079E-01
HYPTH-1        0.71291E-02     0.10530E-04       0.94929E 01     0.73039E-02
HYPTH-2        0.84500E-02     0.12481E-04       0.73916E 01     0.56871E-02
HYPTH-3        0.10585E 00     0.15635E-03       0.22349E 03     0.17196E 00
HYPTH-4        0.52168E-01     0.77058E-04       0.35315E 03     0.27171E 00
HYPTH-5        0.23296E-02     0.34410E-05       0.42798E 02     0.32929E-01
TOTAL          0.67700E 03                       0.12997E 04
```

```
APPENDIX 3-5   TEST PROBLEM NUMBER - 5

     ***** PROBLEM STATEMENT *****

 TYPE OF COLUMN [illegible]

 NO. OF PLATES     20

 NO. OF COMPONENTS       10

 PRESSURE AT TOP PLATE (PSIA)             464.70

 PRESSURE DROP PER PLATE (PSIA)             0.0

 NO. OF FEEDS        2

    ENTERING PLATE OF FEED 1        1
    FEED QUANTITY          0.11830E 04
    PRESSURE OF FEED               464.70
    TEMPERATURE OF FEED (F)               5.00

    ENTERING PLATE OF FEED 2       17
    FEED QUANTITY          0.12792E 04
    PRESSURE OF FEED               464.70
    TEMPERATURE OF FEED (F)              50.00

 SPECIFIED TOP PRODUCT       0.64220E 03

 NO. OF INTER COOLERS OR HEATERS        2

    PLATE NO. OF INTER COOLER OR HEATER 1        4
    HEAT LOAD OF INTER COOLER OR HEATER      -0.84000E 06

    PLATE NO. OF INTER COOLER OR HEATER 2        7
    HEAT LOAD OF INTER COOLER OR HEATER      -0.10950E 07
```

```
*** RATE  OF  CONVERGENCE  WITH  ITERATION NO.  ***

 0    SUM OF SQUARES OF RESIDUALS  0.73541E 01
TEMPERATURE
 0.45960E 03 0.46460E 03 0.46560E 03 0.46460E 03 0.46960E 03
 0.47460E 03 0.46960E 03 0.47160E 03 0.47960E 03 0.48960E 03
 0.49960E 03 0.50960E 03 0.51960E 03 0.52960E 03 0.53460E 03
 0.53960E 03 0.54960E 03 0.57560E 03 0.58960E 03 0.60960E 03
VAPOR FLOW RATE
 0.64220E 03 0.65000E 03 0.65000E 03 0.70000E 03 0.90000E 03
 0.92000E 03 0.93000E 03 0.11000E 04 0.11500E 04 0.12000E 04
 0.12000E 04 0.12500E 04 0.12500E 04 0.13000E 04 0.13000E 04
 0.13500E 04 0.14000E 04 0.25000E 03 0.35000E 03 0.40000E 03

 1    SUM OF SQUARES OF RESIDUALS  0.55231E 00
TEMPERATURE
 0.45565E 03 0.45264E 03 0.45348E 03 0.45153E 03 0.47323E 03
 0.47942E 03 0.47719E 03 0.48838E 03 0.49046E 03 0.49124E 03
 0.49002E 03 0.49070E 03 0.48544E 03 0.48978E 03 0.48888E 03
 0.48891E 03 0.48960E 03 0.52538E 03 0.54740E 03 0.58497E 03
VAPOR FLOW RATE
 0.64220E 03 0.75424E 03 0.86727E 03 0.10128E 04 0.12901E 04
 0.14205E 04 0.15111E 04 0.17827E 04 0.18770E 04 0.19170E 04
 0.18985E 04 0.18769E 04 0.18228E 04 0.17860E 04 0.17278E 04
 0.16981E 04 0.16766E 04 0.35156E 03 0.41545E 03 0.43686E 03

 2    SUM OF SQUARES OF RESIDUALS  0.10724E 00
TEMPERATURE
 0.47113E 03 0.46485E 03 0.45828E 03 0.44739E 03 0.46689E 03
 0.47395E 03 0.48816E 03 0.47887E 03 0.48218E 03 0.48430E 03
 0.48557E 03 0.48720E 03 0.48926E 03 0.49202E 03 0.49472E 03
 0.49740E 03 0.49973E 03 0.52977E 03 0.54373E 03 0.58428E 03
VAPOR FLOW RATE
 0.64220E 03 0.74350E 03 0.81644E 03 0.91110E 03 0.11246E 04
 0.12630E 04 0.13500E 04 0.15978E 04 0.16887E 04 0.17158E 04
 0.17097E 04 0.16955E 04 0.16702E 04 0.16419E 04 0.16076E 04
 0.15796E 04 0.15570E 04 0.24016E 03 0.43941E 03 0.49770E 03

 3    SUM OF SQUARES OF RESIDUALS  0.29842E-01
TEMPERATURE
 0.47916E 03 0.48656E 03 0.47874E 03 0.45667E 03 0.46999E 03
 0.47783E 03 0.47154E 03 0.48206E 03 0.48648E 03 0.48865E 03
 0.49009E 03 0.49145E 03 0.49283E 03 0.49431E 03 0.49565E 03
 0.49688E 03 0.49904E 03 0.52850E 03 0.54137E 03 0.58321E 03
VAPOR FLOW RATE
 0.64220E 03 0.74532E 03 0.80132E 03 0.85894E 03 0.10132E 04
 0.11358E 04 0.12195E 04 0.14358E 04 0.15194E 04 0.15496E 04
 0.15546E 04 0.15540E 04 0.15466E 04 0.15406E 04 0.15318E 04
 0.15269E 04 0.15232E 04 0.20591E 03 0.46084E 03 0.52409E 03
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 4    SUM OF SQUARES OF RESIDUALS  0.89717E-02
TEMPERATURE
 0.47500E 03 0.48528E 03 0.48538E 03 0.46866E 03 0.47363E 03
 0.47803E 03 0.47023E 03 0.46108E 03 0.48576E 03 0.48828E 03
 0.49000E 03 0.49161E 03 0.45216E 03 0.49480E 03 0.49636E 03
 0.49784E 03 0.49971E 03 0.52706E 03 0.54070E 03 0.58294E 03
VAPOR FLOW RATE
 0.64220E 03 0.75101E 03 0.81421E 03 0.86066E 03 0.97460E 03
 0.10752E 04 0.11566E 04 0.13023E 04 0.14472E 04 0.14790E 04
 0.14882E 04 0.14913E 04 0.14899E 04 0.14894E 04 0.14879E 04
 0.14887E 04 0.14900E 04 0.18134E 03 0.46384E 03 0.53012E 03

 5    SUM OF SQUARES OF RESIDUALS  0.24243E-02
TEMPERATURE
 0.47584E 03 0.48274E 03 0.48569E 03 0.47314E 03 0.47788E 03
 0.47903E 03 0.46920E 03 0.47598E 03 0.48487E 03 0.48747E 03
 0.48924E 03 0.49068E 03 0.45251E 03 0.49424E 03 0.49597E 03
 0.49765E 03 0.49958E 03 0.52621E 03 0.54029E 03 0.58270E 03
VAPOR FLOW RATE
 0.64220E 03 0.75026E 03 0.81698E 03 0.87022E 03 0.97044E 03
 0.10498E 04 0.11213E 04 0.13161E 04 0.14029E 04 0.14373E 04
 0.14503E 04 0.14562E 04 0.14551E 04 0.14619E 04 0.14647E 04
 0.14688E 04 0.14726E 04 0.16546E 03 0.45976E 03 0.53041E 03

 6    SUM OF SQUARES OF RESIDUALS  0.72298E-03
TEMPERATURE
 0.47562E 03 0.48354E 03 0.48557E 03 0.47223E 03 0.47972E 03
 0.48088E 03 0.46964E 03 0.47586E 03 0.48477E 03 0.48739E 03
 0.48918E 03 0.49077E 03 0.49239E 03 0.49410E 03 0.49583E 03
 0.49749E 03 0.49939E 03 0.52563E 03 0.54000E 03 0.58252E 03
VAPOR FLOW RATE
 0.64220E 03 0.75098E 03 0.81634E 03 0.86911E 03 0.97055E 03
 0.10418E 04 0.11036E 04 0.12876E 04 0.13746E 04 0.14112E 04
 0.14267E 04 0.14346E 04 0.14398E 04 0.14449E 04 0.14503E 04
 0.14567E 04 0.14625E 04 0.16203E 03 0.45405E 03 0.52890E 03

 7,   SUM OF SQUARES OF RESIDUALS  0.21769E-03
TEMPERATURE
 0.47571E 03 0.48342E 03 0.48592E 03 0.47244E 03 0.47994E 03
 0.48185E 03 0.47044E C3 0.46016E 03 0.48491E 03 0.48752E 03
 0.48930E 03 0.49088E 03 0.49246E 03 0.49412E 03 0.49582E 03
 0.49744E 03 0.49932E 03 0.52527E 03 0.53981E 03 0.58240E 03
VAPOR FLOW RATE
 0.64220E 03 0.75120E 03 0.81733E 03 0.86943E 03 0.96888E 03
 0.10388E 04 0.10962E 04 0.12722E 04 0.13578E 04 0.13956E 04
 0.14126E 04 0.14218E 04 0.14285E 04 0.14349E 04 0.14418E 04
 0.14496E 04 0.14567E 04 0.15754E 03 0.44919E 03 0.52742E 03
```

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8    SUM OF SQUARES OF RESIDUALS  0.65867E-04
TEMPERATURE
 0.47570E 03 0.48352E 03 0.48599E 03 0.47279E 03 0.48020E 03
 0.48215E 03 0.47080E 03 0.48042E 03 0.48504E 03 0.48760E 03
 0.48938E 03 0.49094E 03 0.49251E 03 0.49410E 03 0.49584E 03
 0.49745E 03 0.49931E 03 0.52508E 03 0.53970E 03 0.58233E 03
VAPOR FLOW RATE
 0.64220E 03 0.75137E 03 0.81762E 03 0.87014E 03 0.96879E 03
 0.10372E 04 0.10930E 04 0.12647E 04 0.13486E 04 0.13866E 04
 0.14045E 04 0.14146E 04 0.14220E 04 0.14292E 04 0.14369E 04
 0.14455E 04 0.14533E 04 0.15455E 03 0.44565E 03 0.52627E 03

9    SUM OF SQUARES OF RESIDUALS  0.21433E-04
TEMPERATURE
 0.47568E 03 0.48347E 03 0.48600E 03 0.47290E 03 0.48041E 03
 0.48233E 03 0.47103E 03 0.48054E 03 0.48512E 03 0.48764E 03
 0.48940E 03 0.49096E 03 0.49253E 03 0.49417E 03 0.49585E 03
 0.49745E 03 0.49931E 03 0.52499E 03 0.53764E 03 0.58229E 03
VAPOR FLOW RATE
 0.64220E 03 0.75147E 03 0.81789E 03 0.87053E 03 0.96930E 03
 0.10369E 04 0.10917E 04 0.12610E 04 0.13437E 04 0.13817E 04
 0.14[illegible]00E 04 0.14105E 04 0.14184E 04 0.14260E 04 0.14342E 04
 0.14432E 04 0.14513E 04 0.15352E 03 0.44329E 03 0.52549E 03

10   SUM OF SQUARES OF RESIDUALS  0.66766E-05
TEMPERATURE
 0.47568E 03 0.48346E 03 0.48597E 03 0.47289E 03 0.48048E 03
 0.48244E 03 0.47113E 03 0.48060E 03 0.48515E 03 0.48766E 03
 0.48942E 03 0.49097E 03 0.49254E 03 0.49417E 03 0.49584E 03
 0.49745E 03 0.49930E 03 0.52494E 03 0.53960E 03 0.58227E 03
VAPOR FLOW RATE
 0.64220E 03 0.75152E 03 0.81799E 03 0.87074E 03 0.96965E 03
 0.10371E 04 0.10913E 04 0.12592E 04 0.13412E 04 0.13790E 04
 0.13974E 04 0.14082E 04 0.14164E 04 0.14242E 04 0.14326E 04
 0.14419E 04 0.14502E 04 0.15273E 03 0.44183E 03 0.52497E 03
```

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***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS  10

COLUMN PRESSURE (PSIA)   0.46470E 03

PRESSURE , TEMPERATURE , ENTHALPY AND LIQUID FRACTION OF FEED

 0.465E 03 PSIA  0.500E 01 F -0.945E 07 B.T.U.      1.000

 0.465E 03 PSIA  0.500E 02 F  0.485E 07 B.T.U.      0.0

*** STAGE VARIABLES ***

   PLATE NO. TEMPERATURE   LIQ. F. R.     VAP. F. R.    HEAT DUTY
                 F         LB MOL/TIME    LB MOL/TIME    BTU/TIME
      1     0.16084E 02   0.12923E 04   0.64220E 03   0.0
      2     0.21863E 02   0.13588E 04   0.75152E 03   0.0
      3     0.26866E 02   0.14115E 04   0.81799E 03   0.0
      4     0.[illegible]3289E 02   0.15104E 04   0.87074E 03  -0.84000E 06
      5     0.20876E 02   0.15779E 04   0.96965E 03   0.0
      6     0.22844E 02   0.16321E 04   0.10371E 04   0.0
      7     0.11531E 02   0.18000E 04   0.10913E 04  -0.10950E 07
      8     0.21005E 02   0.18820E 04   0.12592E 04   0.0
      9     0.25552E 02   0.19158E 04   0.13412E 04   0.0
     10     0.28063E 02   0.19382E 04   0.13790E 04   0.0
     11     0.29817E 02   0.19490E 04   0.13974E 04   0.0
     12     0.31365E 02   0.19572E 04   0.14082E 04   0.0
     13     0.32936E 02   0.19650E 04   0.14164E 04   0.0
     14     0.34574E 02   0.19734E 04   0.14242E 04   0.0
     15     0.36244E 02   0.19827E 04   0.14326E 04   0.0
     16     0.37852E 02   0.19910E 04   0.14419E 04   0.0
     17     0.39698E 02   0.19728E 04   0.14502E 04   0.0
     18     0.65341E 02   0.22618E 04   0.15273E 03   0.0
     19     0.80002E 02   0.23450E 04   0.44183E 03   0.0
     20     0.12267E 03   0.18200E 04   0.52497E 03   0.40471E 07
```

```
*** MATERIAL BALANCES ***

 FEEDS

                      PLATE NO.    1                      PLATE NO.  17
             LB MOL/TIME      MOL FRC.         LB MOL/TIME      MOL FRC.
 METHANE     0.0              0.0              0.12792E 03    0.99999E-01
 ETHANE      0.0              0.0              0.27887E 03    0.21800E 00
 ETHYLENE    0.0              0.0              0.41319E 03    0.32300E 00
 PROPANE     0.0              0.0              0.12790E 01    0.99983E-03
 HYDROGEN    0.0              0.0              0.45796E 03    0.35800E 00
 BENZENE     0.79261E 03      0.67000E 00      0.0            0.0
 TOLUENE     0.70980E 02      0.60000E-01      0.0            0.0
 O-XYLENE    0.23660E 02      0.20000E-01      0.0            0.0
 PROPYLEN    0.59150E 02      0.50000E-01      0.0            0.0
 ECHEXANE    0.23660E 03      0.20000E 00      0.0            0.0
 TOTAL       0.11830E 04                       0.12792E 04

 PRODUCTS

                     TOP PRODUCT                       BOTTOM PRODUCT
             LB MOL/TIME      MOL FRC.         LB MOL/TIME      MOL FRC.
 METHANE     0.11822E 03      0.18409E 00      0.97011E 01    0.53302E-02
 ETHANE      0.81437E 00      0.12681E-02      0.27806E 03    0.15278E 00
 ETHYLENE    0.54739E 02      0.85237E-01      0.35845E 03    0.19695E 00
 PROPANE     0.16102E-11      0.25074E-14      0.12790E 01    0.70274E-03
 HYDROGEN    0.45792E 03      0.71305E 00      0.37136E-01    0.20404E-04
 BENZENE     0.66477E 00      0.10351E-02      0.79194E 03    0.43513E 00
 TOLUENE     0.16202E-01      0.25229E-04      0.70964E 02    0.38991E-01
 O-XYLENE    0.14592E-02      0.22722E-05      0.23658E 02    0.12999E-01
 PROPYLEN    0.97940E 01      0.15251E-01      0.49356E 02    0.27119E-01
 ECHEXANE    0.28427E-01      0.44266E-04      0.23657E 03    0.12998E 00
 TOTAL       0.64220E 03                       0.18200E 04
```

APPENDIX 3-6   TEST PROBLEM NUMBER - 6

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     ***** PROBLEM STATEMENT *****


 TYPE OF COLUMN         2

 NO. OF PLATES       30

 NO. OF COMPONENTS       12

 PRESSURE AT TOP PLATE (PSIA)              475.00

 PRESSURE DROP PER PLATE (PSIA)              0.0

 NO. OF FEEDS        3

     ENTERING PLATE OF FEED 1         1
     FEED QUANTITY        0.18200E 04
     PRESSURE OF FEED            475.00
     TEMPERATURE OF FEED (F)                -4.00

     ENTERING PLATE OF FEED 2        15
     FEED QUANTITY        0.28900E 04
     PRESSURE OF FEED            475.00
     TEMPERATURE OF FEED (F)                -4.00

     ENTERING PLATE OF FEED 3        22
     FEED QUANTITY        0.29600E 04
     PRESSURE OF FEED            475.00
     TEMPERATURE OF FEED (F)                -4.00

 SPECIFIED TOP PRODUCT       0.15200E 04
```

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*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 0    SUM OF SQUARES OF RESIDUALS  0.12434E 01
 TEMPERATURE
  0.45960E 03 0.46660E 03 0.47360E 03 0.48060E 03 0.48760E 03
  0.49460E 03 0.50160E 03 0.50860E 03 0.51560E 03 0.52260E 03
  0.52960E 03 0.53660E 03 0.54360E 03 0.55060E 03 0.55760E 03
  0.56460E 03 0.57160E 03 0.57860E 03 0.58560E 03 0.59260E 03
  0.59960E 03 0.60660E 03 0.61360E 03 0.62060E 03 0.62760E 03
  0.63460E 03 0.64160E 03 0.64860E 03 0.65560E 03 0.66260E 03
 VAPOR FLOW RATE
  0.15200E 04 0.16000E 04 0.16500E 04 0.17000E 04 0.17500E 04
  0.18000E 04 0.18500E 04 0.19000E 04 0.19500E 04 0.20000E 04
  0.20000E 04 0.20000E 04 0.20000E 04 0.20000E 04 0.20000E 04
  0.20000E 04 0.20000E 04 0.21000E 04 0.22000E 04 0.23000E 04
  0.24000E 04 0.25000E 04 0.10000E 04 0.12000E 04 0.14000E 04
  0.16000E 04 0.18000E 04 0.20000E 04 0.22000E 04 0.24000E 04

 1    SUM OF SQUARES OF RESIDUALS  0.63660E 00
 TEMPERATURE
  0.42869E 03 0.41278E 03 0.41360E 03 0.42466E 03 0.43859E 03
  0.45075E 03 0.45959E 03 0.46543E 03 0.46538E 03 0.47295E 03
  0.47645E 03 0.48349E 03 0.49496E 03 0.50993E 03 0.52506E 03
  0.54059E 03 0.55060E 03 0.55853E 03 0.56400E 03 0.56951E 03
  0.57584E 03 0.58386E 03 0.60638E 03 0.64057E 03 0.63660E 03
  0.64831E 03 0.64682E 03 0.65314E 03 0.65715E 03 0.66747E 03
 VAPOR FLOW RATE
  0.15200E 04 0.15998E 04 0.16455E 04 0.16899E 04 0.17385E 04
  0.17944E 04 0.18565E 04 0.19236E 04 0.19942E 04 0.20662E 04
  0.20838E 04 0.21004E 04 0.21048E 04 0.20947E 04 0.20813E 04
  0.23568E 04 0.24323E 04 0.25783E 04 0.27011E 04 0.28365E 04
  0.29701E 04 0.31196E 04 0.18933E 04 0.14691E 04 0.23436E 04
  0.22480E 04 0.27173E 04 0.25540E 04 0.27930E 04 0.27892E 04

 2    SUM OF SQUARES OF RESIDUALS  0.19535E 00
 TEMPERATURE
  0.44041E 03 0.45808E 03 0.46949E 03 0.48466E 03 0.49091E 03
  0.48790E 03 0.48265E 03 0.47934E 03 0.47856E 03 0.48004E 03
  0.48262E 03 0.48751E 03 0.49475E 03 0.50383E 03 0.51178E 03
  0.53222E 03 0.54416E 03 0.55151E 03 0.55557E 03 0.55815E 03
  0.56048E 03 0.56357E 03 0.59861E 03 0.60959E 03 0.61971E 03
  0.61968E 03 0.62819E 03 0.62936E 03 0.64257E 03 0.66209E 03
 VAPOR FLOW RATE
  0.15200E 04 0.16475E 04 0.16742E 04 0.17211E 04 0.17919E 04
  0.18649E 04 0.19286E 04 0.19864E 04 0.20417E 04 0.20943E 04
  0.21092E 04 0.21219E 04 0.21336E 04 0.21469E 04 0.21768E 04
  0.27690E 04 0.29746E 04 0.31606E 04 0.33491E 04 0.35014E 04
  0.36507E 04 0.38315E 04 0.26449E 04 0.22408E 04 0.23490E 04
  0.29314E 04 0.27681E 04 0.32042E 04 0.30160E 04 0.33191E 04
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 3     SUM OF SQUARES OF RESIDUALS  0.31891E 01
TEMPERATURE
 0.49160E 03 0.49409E 03 0.48022E 03 0.47234E 03 0.47994E 03
 0.49046E 03 0.49474E 03 0.49490E 03 0.49471E 03 0.49541E 03
 0.49826E 03 0.50062E 03 0.50294E 03 0.50429E 03 0.49725E 03
 0.51577E 03 0.53041E 03 0.53538E 03 0.54423E 03 0.54580E 03
 0.54409E 03 0.53555E 03 0.56566E 03 0.57410E 03 0.57448E 03
 0.58385E 03 0.58947E 03 0.55508E 03 0.61555E 03 0.65013E 03
VAPOR FLOW RATE
 0.15200E 04 0.18081E 04 0.18583E 04 0.19058E 04 0.19867E 04
 0.20502E 04 0.20824E 04 0.20626E 04 0.20810E 04 0.20811E 04
 0.20833E 04 0.20874E 04 0.21051E 04 0.21462E 04 0.22411E 04
 0.32006E 04 0.36789E 04 0.35887E 04 0.41912E 04 0.43205E 04
 0.44219E 04 0.45542E 04 0.32675E 04 0.36599E 04 0.37909E 04
 0.36496E 04 0.40788E 04 0.38601E 04 0.42514E 04 0.41766E 04

 4     SUM OF SQUARES OF RESIDUALS  0.15235E-01
TEMPERATURE
 0.47125E 03 0.50750E 03 0.52600E 03 0.52283E 03 0.51034E 03
 0.50609E 03 0.51046E 03 0.51575E 03 0.51840E 03 0.51925E 03
 0.51982E 03 0.52084E 03 0.52147E 03 0.52010E 03 0.50835E 03
 0.51782E 03 0.53080E 03 0.54078E 03 0.54677E 03 0.54939E 03
 0.54830E 03 0.53910E 03 0.56759E 03 0.57892E 03 0.58521E 03
 0.58944E 03 0.59459E 03 0.60455E 03 0.62345E 03 0.65867E 03
VAPOR FLOW RATE
 0.15200E 04 0.19129E 04 0.19533E 04 0.19270E 04 0.19263E 04
 0.19686E 04 0.20207E 04 0.20435E 04 0.20448E 04 0.20438E 04
 0.20489E 04 0.20619E 04 0.20798E 04 0.21086E 04 0.21793E 04
 0.28814E 04 0.32941E 04 0.36163E 04 0.38398E 04 0.39884E 04
 0.40895E 04 0.41939E 04 0.26286E 04 0.37328E 04 0.40634E 04
 0.42425E 04 0.43260E 04 0.43729E 04 0.43917E 04 0.43993E 04

 5     SUM OF SQUARES OF RESIDUALS  0.86485E-02
TEMPERATURE
 0.46463E 03 0.47893E 03 0.50751E 03 0.52912E 03 0.52911E 03
 0.52157E 03 0.51864E 03 0.52055E 03 0.52378E 03 0.52603E 03
 0.52712E 03 0.52779E 03 0.52801E 03 0.52592E 03 0.51276E 03
 0.52348E 03 0.53278E 03 0.54124E 03 0.54695E 03 0.54968E 03
 0.54880E 03 0.53992E 03 0.56789E 03 0.57909E 03 0.58515E 03
 0.58949E 03 0.59507E 03 0.60477E 03 0.62367E 03 0.65886E 03
VAPOR FLOW RATE
 0.15200E 04 0.18838E 04 0.19962E 04 0.20413E 04 0.20189E 04
 0.20096E 04 0.20303E 04 0.20559E 04 0.20719E 04 0.20789E 04
 0.20841E 04 0.20935E 04 0.21087E 04 0.21341E 04 0.21991E 04
 0.29231E 04 0.32759E 04 0.35888E 04 0.38198E 04 0.39742E 04
 0.40789E 04 0.41871E 04 0.25889E 04 0.36539E 04 0.40068E 04
 0.41797E 04 0.42676E 04 0.43136E 04 0.43435E 04 0.43771E 04
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6    SUM OF SQUARES OF RESIDUALS  0.62034E-02
TEMPERATURE
 0.46315E 03 0.46411E 03 0.47751E 03 0.50084E 03 0.51857E 03
 0.52201E 03 0.51924E 03 0.51854E 03 0.52061E 03 0.52371E 03
 0.52646E 03 0.52852E 03 0.52574E 03 0.52843E 03 0.51570E 03
 0.52710E 03 0.53569E 03 0.54271E 03 0.54765E 03 0.55008E 03
 0.54917E 03 0.54036E 03 0.56813E 03 0.57920E 03 0.58512E 03
 0.58948E 03 0.59506E 03 0.60480E 03 0.62372E 03 0.65888E 03
VAPOR FLOW RATE
 0.15200E 04 0.18758E 04 0.19926E 04 0.20820E 04 0.21234E 04
 0.21088E 04 0.20975E 04 0.21069E 04 0.21217E 04 0.21325E 04
 0.21386E 04 0.21441E 04 0.21535E 04 0.21727E 04 0.22301E 04
 0.29693E 04 0.33024E 04 0.35885E 04 0.38127E 04 0.39677E 04
 0.40741E 04 0.41818E 04 0.25724E 04 0.36234E 04 0.39870E 04
 0.41587E 04 0.42467E 04 0.42956E 04 0.43305E 04 0.43750E 04

7    SUM OF SQUARES OF RESIDUALS  0.43366E-02
TEMPERATURE
 0.46898E 03 0.46634E 03 0.46674E 03 0.47441E 03 0.48857E 03
 0.50231E 03 0.50849E 03 0.50531E 03 0.51026E 03 0.51310E 03
 0.51741E 03 0.52217E 03 0.52640E 03 0.52804E 03 0.51809E 03
 0.53027E 03 0.53848E 03 0.54428E 03 0.54824E 03 0.55020E 03
 0.54920E 03 0.54060E 03 0.56617E 03 0.57904E 03 0.58478E 03
 0.58912E 03 0.59468E 03 0.60442E 03 0.62335E 03 0.65855E 03
VAPOR FLOW RATE
 0.15200E 04 0.18566E 04 0.19530E 04 0.20453E 04 0.21372E 04
 0.21919E 04 0.21974E 04 0.21912E 04 0.21955E 04 0.22057E 04
 0.22146E 04 0.22201E 04 0.22248E 04 0.22368E 04 0.22849E 04
 0.30556E 04 0.33812E 04 0.36401E 04 0.38450E 04 0.39915E 04
 0.40943E 04 0.41993E 04 0.25815E 04 0.36155E 04 0.39823E 04
 0.41503E 04 0.42363E 04 0.42864E 04 0.43235E 04 0.43751E 04

8    SUM OF SQUARES OF RESIDUALS  0.17647E-02
TEMPERATURE
 0.47824E 03 0.48413E 03 0.48202E 03 0.47889E 03 0.47886E 03
 0.48395E 03 0.49324E 03 0.50079E 03 0.50322E 03 0.50339E 03
 0.50445E 03 0.50803E 03 0.51403E 03 0.52002E 03 0.51632E 03
 0.53203E 03 0.54106E 03 0.54633E 03 0.54923E 03 0.55040E 03
 0.54909E 03 0.54067E 03 0.56811E 03 0.57869E 03 0.58419E 03
 0.58848E 03 0.59397E 03 0.60369E 03 0.62263E 03 0.65798E 03
VAPOR FLOW RATE
 0.15200E 04 0.18407E 04 0.[illegible]844E 04 0.19147E 04 0.19678E 04
 0.20526E 04 0.21411E 04 0.21872E 04 0.21987E 04 0.22088E 04
 0.22281E 04 0.22529E 04 0.22778E 04 0.23054E 04 0.23638E 04
 0.32285E 04 0.35547E 04 0.37745E 04 0.39325E 04 0.40475E 04
 0.41343E 04 0.42326E 04 0.26083E 04 0.36157E 04 0.39815E 04
 0.41431E 04 0.42266E 04 0.42768E 04 0.43152E 04 0.43714E 04
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9    SUM OF SQUARES OF RESIDUALS  0.99069E-03
TEMPERATURE
 0.47671E  03 0.48743E  03 0.49208E  03 0.49145E  03 0.48931E  03
 0.48972E  03 0.49406E  03 0.49988E  03 0.50416E  03 0.50629E  03
 0.50765E  03 0.50988E  03 0.51365E  03 0.51760E  03 0.51306E  03
 0.52978E  03 0.54017E  03 0.54628E  03 0.54957E  03 0.55077E  03
 0.54933E  03 0.54074E  03 0.56818E  03 0.57874E  03 0.58423E  03
 0.58851E  03 0.59401E  03 0.60375E  03 0.62270E  03 0.65806E  03
VAPOR FLOW RATE
 0.15200E  04 0.18542E  04 0.19066E  04 0.19296E  04 0.19630E  04
 0.20179E  04 0.20813E  04 0.21311E  04 0.21599E  04 0.21746E  04
 0.21867E  04 0.22029E  04 0.22255E  04 0.22593E  04 0.23319E  04
 0.32159E  04 0.35675E  C4 0.37955E  04 0.39504E  04 0.40566E  04
 0.41359E  04 0.42303E  04 0.26085E  04 0.36155E  04 0.39827E  04
 0.41457E  04 0.42301E  04 0.42814E  04 0.43205E  04 0.43772E  04

10   SUM OF SQUARES OF RESIDUALS  0.58288E-03
TEMPERATURE
 0.47476E  03 0.48545E  03 0.49423E  03 0.49905E  03 0.49947E  03
 0.49840E  03 0.49899E  03 0.50187E  03 0.50557E  03 0.50865E  03
 0.51084E  03 0.51286E  03 0.51540E  03 0.51760E  03 0.51140E  03
 0.52763E  03 0.53875E  C3 0.54562E  03 0.54941E  03 0.55085E  03
 0.54946E  03 0.54081E  03 0.56826E  03 0.57883E  03 0.58432E  03
 0.58861E  03 0.59411E  03 0.60385E  03 0.62282E  03 0.65816E  03
VAPOR FLOW RATE
 0.15200E  04 0.18612E  04 0.19282E  04 0.19576E  04 0.19797E  04
 0.20101E  04 0.20505E  04 0.20924E  04 0.21266E  04 0.21483E  04
 0.21615E  04 0.21740E  C4 0.21526E  04 0.22252E  04 0.23012E  04
 0.31784E  04 0.35537E  04 0.37975E  04 0.39577E  04 0.40622E  04
 0.41377E  04 0.42293E  04 0.26067E  04 0.36128E  04 0.39803E  04
 0.41439E  04 0.42286E  C4 0.42802E  04 0.43197E  04 0.43772E  04

11   SUM OF SQUARES OF RESIDUALS  0.32767E-03
TEMPERATURE
 0.47330E  03 0.48194E  03 0.49068E  03 0.49874E  03 0.50370E  03
 0.50504E  03 0.50491E  03 0.50561E  03 0.50767E  03 0.51038E  03
 0.51302E  03 0.51541E  C3 0.51769E  03 0.51894E  03 0.51127E  03
 0.52653E  03 0.53771E  03 0.54497E  03 0.54912E  03 0.55078E  03
 0.54949E  03 0.54085E  03 0.56832E  03 0.57890E  03 0.58440E  03
 0.58869E  03 0.59420E  03 0.60395E  03 0.62291E  03 0.65824E  Q3
VAPOR FLOW RATE
 0.15200E  04 0.18631E  04 0.19396E  04 0.19830E  04 0.20116E  C4
 0.20327E  04 0.20554E  04 0.20832E  04 0.21123E  04 0.21361E  04
 0.21526E  04 0.21654E  04 0.21814E  04 0.22095E  04 0.22821E  04
 0.31388E  04 0.35224E  04 0.37805E  04 0.39508E  04 0.40600E  04
 0.41367E  04 0.42279E  04 0.26047E  04 0.36101E  04 0.39780E  04
 0.41421E  04 0.42273E  04 0.42788E  04 0.43189E  04 0.43766E  04
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12    SUM OF SQUARES OF RESIDUALS  0.17100E-03
TEMPERATURE
 0.47290E 03 0.47974E 03 0.48641E 03 0.49396E 03 0.50104E 03
 0.50586E 03 0.50769E 03 0.50862E 03 0.50964E 03 0.51150E 03
 0.51398E 03 0.51670E 03 0.51928E 03 0.52040E 03 0.51199E 03
 0.52640E 03 0.53722E 03 0.54452E 03 0.54882E 03 0.55063E 03
 0.54943E 03 0.54085E 03 0.56833E 03 0.57892E 03 0.58443E 03
 0.58872E 03 0.59427E 03 0.60398E 03 0.62294E 03 0.65826E 03
VAPOR FLOW RATE
 0.15200E 04 0.18620E 04 0.19411E 04 0.19937E 04 0.20354E 04
 0.20638E 04 0.20821E 04 0.20985E 04 0.21184E 04 0.21384E 04
 0.21555E 04 0.21695E 04 0.21843E 04 0.22093E 04 0.22767E 04
 0.31153E 04 0.34957E 04 0.37614E 04 0.39404E 04 0.40556E 04
 0.41354E 04 0.42276E 04 0.26043E 04 0.36090E 04 0.39767E 04
 0.41411E 04 0.42265E 04 0.42779E 04 0.43183E 04 0.43761E 04

13    SUM OF SQUARES OF RESIDUALS  0.90091E-04
TEMPERATURE
 0.47336E 03 0.47969E 03 0.48484E 03 0.49043E 03 0.49659E 03
 0.50237E 03 0.50659E 03 0.50857E 03 0.51039E 03 0.51192E 03
 0.51405E 03 0.51681E 03 0.51976E 03 0.52124E 03 0.51286E 03
 0.52684E 03 0.53721E 03 0.54431E 03 0.54860E 03 0.55046E 03
 0.54933E 03 0.54080E 03 0.56831E 03 0.57890E 03 0.58440E 03
 0.58870E 03 0.59420E 03 0.60395E 03 0.62292E 03 0.65823E 03
VAPOR FLOW RATE
 0.15200E 04 0.18601E 04 0.19371E 04 0.19908E 04 0.20395E 04
 0.20792E 04 0.21058E 04 0.21224E 04 0.21361E 04 0.21503E 04
 0.21649E 04 0.21788E 04 0.21937E 04 0.22173E 04 0.22810E 04
 0.31103E 04 0.34825E 04 0.37487E 04 0.39322E 04 0.40518E 04
 0.41345E 04 0.42282E 04 0.26053E 04 0.36091E 04 0.39768E 04
 0.41409E 04 0.42263E 04 0.42776E 04 0.43177E 04 0.43756E 04

14    SUM OF SQUARES OF RESIDUALS  0.46719E-04
TEMPERATURE
 0.47392E 03 0.48070E 03 0.48561E 03 0.49008E 03 0.49468E 03
 0.49946E 03 0.50390E 03 0.50738E 03 0.50982E 03 0.51174E 03
 0.51382E 03 0.51648E 03 0.51956E 03 0.52139E 03 0.51337E 03
 0.52740E 03 0.53746E 03 0.54434E 03 0.54853E 03 0.55037E 03
 0.54925E 03 0.54075E 03 0.56827E 03 0.57886E 03 0.58437E 03
 0.58866E 03 0.59417E 03 0.60391E 03 0.62287E 03 0.65819E 03
VAPOR FLOW RATE
 0.15200E 04 0.18590E 04 0.19333E 04 0.19837E 04 0.20314E 04
 0.20752E 04 0.21101E 04 0.21340E 04 0.21497E 04 0.21620E 04
 0.21739E 04 0.21865E 04 0.22015E 04 0.22252E 04 0.22880E 04
 0.31170E 04 0.34814E 04 0.37438E 04 0.39275E 04 0.40489E 04
 0.41333E 04 0.42284E 04 0.26061E 04 0.36095E 04 0.39769E 04
 0.41411E 04 0.42264E 04 0.42775E 04 0.43176E 04 0.43752E 04
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 15      SUM OF SQUARES OF RESIDUALS   0.45701E-04
 TEMPERATURE
  0.47437E 03 0.48235E 03 0.48620E 03 0.49253E 03 0.49560E 03
  0.49820E 03 0.50108E 03 0.50440E 03 0.50777E 03 0.51071E 03
  0.51328E 03 0.51594E 03 0.51865E 03 0.52101E 03 0.51358E 03
  0.52808E 03 0.53803E 03 0.54463E 03 0.54861E 03 0.55034E 03
  0.54919E 03 0.54069E 03 0.56692E 03 0.57883E 03 0.58434E 03
  0.58863E 03 0.59413E 03 0.60387E 03 0.62283E 03 0.65817E 03
 VAPOR FLOW RATE
  0.15200E 04 0.18594E 04 0.19314E 04 0.19761E 04 0.20164E 04
  0.20561E 04 0.20946E 04 0.21785E 04 0.21542E 04 0.21712E 04
  0.21830E 04 0.21941E 04 0.22080E 04 0.22334E 04 0.22976E 04
  0.31451E 04 0.34918E 04 0.37448E 04 0.39241E 04 0.40450E 04
  0.41305E 04 0.42270E 04 0.26059E 04 0.36095E 04 0.39770E 04
  0.41412E 04 0.42260E 04 0.42770E 04 0.43176E 04 0.43744E 04

 16      SUM OF SQUARES OF RESIDUALS   0.23063E-04
 TEMPERATURE
  0.47404E 03 0.48158E 03 0.48635E 03 0.49361E 03 0.49748E 03
  0.50021E 03 0.50247E 03 0.50464E 03 0.50750E 03 0.51029E 03
  0.51306E 03 0.51593E 03 0.51894E 03 0.52084E 03 0.51330E 03
  0.52795E 03 0.53810E 03 0.54470E 03 0.54873E 03 0.55043E 03
  0.54925E 03 0.54071E 03 0.56824E 03 0.57086E 03 0.58435E 03
  0.58804E 03 0.59415E 03 0.60485E 03 0.62205E 03 0.65819E 03
 VAPOR FLOW RATE
  0.15200E 04 0.18608E 04 0.19342E 04 0.19804E 04 0.20190E 04
  0.20553E 04 0.20880E 04 0.21170E 04 0.21433E 04 0.21632E 04
  0.21704E 04 0.21913E 04 0.22061E 04 0.22300E 04 0.22958E 04
  0.31307E 04 0.34970E 04 0.37495E 04 0.39266E 04 0.40450E 04
  0.41299E 04 0.42259E 04 0.26047E 04 0.36091E 04 0.39770E 04
  0.41412E 04 0.42266E 04 0.42777E 04 0.43177E 04 0.43751E 04
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***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS  16

COLUMN PRESSURE (PSIA)   0.47500E 03

PRESSURE , TEMPERATURE , ENTHALPY AND LIQUID FRACTION OF FEED

 0.475E 03 PSIA -0.400E 01 F -0.619E 07 B.T.U.        1.000

 0.475E 03 PSIA -0.400E 01 F -0.605E 07 B.T.U.        1.000

 0.475E 03 PSIA -0.400E 01 F  0.413E 07 B.T.U.        0.386

*** STAGE VARIABLES ***

 PLATE NO. TEMPERATURE    LIQ. F. R.     VAP. F. R.     HEAT DUTY
                F         LB MOL/TIME    LB MOL/TIME     BTU/TIME
     1     0.14441E 02   0.21604E 04   0.15200E 04   0.0
     2     0.22375E 02   0.22342E 04   0.18604E 04   0.0
     3     0.28752E 02   0.22804E 04   0.19342E 04   0.0
     4     0.34013E 02   0.23158E 04   0.19804E 04   0.0
     5     0.37883E 02   0.23553E 04   0.20198E 04   0.0
     6     0.40609E 02   0.23880E 04   0.20553E 04   0.0
     7     0.42869E 02   0.24170E 04   0.20880E 04   0.0
     8     0.45244E 02   0.24433E 04   0.21170E 04   0.0
     9     0.47902E 02   0.24632E 04   0.21433E 04   0.0
    10     0.50086E 02   0.24784E 04   0.21632E 04   0.0
    11     0.53464E 02   0.24913E 04   0.21784E 04   0.0
    12     0.56339E 02   0.25061E 04   0.21913E 04   0.0
    13     0.59342E 02   0.25398E 04   0.22061E 04   0.0
    14     0.61743E 02   0.25958E 04   0.22398E 04   0.0
    15     0.63705E 02   0.63267E 04   0.22956E 04   0.0
    16     0.68352E 02   0.66870E 04   0.31367E 04   0.0
    17     0.78503E 02   0.69395E 04   0.34970E 04   0.0
    18     0.85165E 02   0.71165E 04   0.37495E 04   0.0
    19     0.89130E 02   0.72355E 04   0.39265E 04   0.0
    20     0.90830E 02   0.73109E 04   0.40455E 04   0.0
    21     0.89645E 02   0.74159E 04   0.41299E 04   0.0
    22     0.81114E 02   0.87547E 04   0.42259E 04   0.0
    23     0.10864E 03   0.97591E 04   0.26047E 04   0.0
    24     0.11924E 03   0.10127E 05   0.36091E 04   0.0
    25     0.12475E 03   0.10291E 05   0.39770E 04   0.0
    26     0.12904E 03   0.10377E 05   0.41412E 04   0.0
    27     0.13455E 03   0.10428E 05   0.42266E 04   0.0
    28     0.14429E 03   0.10468E 05   0.42777E 04   0.0
    29     0.16325E 03   0.10525E 05   0.43177E 04   0.0
    30     0.19859E 03   0.61500E 04   0.43751E 04   0.30393E 08
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*** MATERIAL BALANCES ***

 FEEDS

                    PLATE NO.    1                      PLATE NO.  15
               LB MOL/TIME      MOL FRC.          LB MOL/TIME       MOL FRC.
 HYDROGEN      0.0              0.0               0.0               0.0
 NITROGEN      0.0              0.0               0.0               0.0
 METHANE       0.0              0.0               0.28900E  02      0.10000E-01
 ETHYLENE      0.0              0.0               0.57800E  02      0.20000E-01
 ETHANE        0.0              0.0               0.14450E  03      0.50000E-01
 PROPYLEN      0.0              0.0               0.49130E  03      0.17000E  00
 PROPANE       0.23660E  02     0.13000E-01       0.31790E  03      0.11000E  00
 I-BUTENE      0.19656E  03     0.10800E  00      0.52020E  03      0.18000E  00
 CIS2BUTE      0.44408E  03     0.24400E  00      0.17340E  03      0.60000E-01
 NBUTANE       0.77714E  03     0.42700E  00      0.98260E  03      0.34000E  00
 NPENTANE      0.33124E  03     0.18200E  00      0.15895E  03      0.55000E-01
 HEPTANE       0.47320E  02     0.26000E-01       0.14450E  02      0.50000E-02
 TOTAL         0.18200E  04                       0.28900E  04

                    PLATE NO.   22                      PLATE NO.
               LB MOL/TIME      MOL FRC.          LB MOL/TIME       MOL FRC.
 HYDROGEN      0.56240E  03     0.19000E  00
 NITROGEN      0.20720E  03     0.70000E-01
 METHANE       0.65120E  03     0.22000E  00
 ETHYLENE      0.41440E  03     0.14000E  00
 ETHANE        0.41440E  03     0.14000E  00
 PROPYLEN      0.38480E  03     0.13000E  00
 PROPANE       0.11840E  03     0.40000E-01
 I-BUTENE      0.88800E  02     0.30000E-01
 CIS2BUTE      0.14800E  02     0.50000E-02
 NBUTANE       0.59200E  02     0.20000E-01
 NPENTANE      0.35520E  02     0.12000E-01
 HEPTANE       0.88800E  01     0.30000E-02
 TOTAL         0.29600E  04

 PRODUCTS

                   TOP PRODUCT                         BOTTOM PRODUCT
               LB MOL/TIME      MOL FRC.          LB MOL/TIME       MOL FRC.
 HYDROGEN      0.56242E  03     0.37002E  00      0.34659E-05       0.56356E-09
 NITROGEN      0.20720E  03     0.13631E  00      0.66211E-03       0.10766E-06
 METHANE       0.67942E  03     0.44659E  00      0.67292E  00       0.10942E-03
 ETHYLENE      0.26266E  02     0.17280E-01       0.44592E  03      0.72508E-01
 ETHANE        0.29935E  00     0.19694E-03       0.55860E  03      0.90829E-01
 PROPYLEN      0.10018E-06      0.65905E-10       0.87610E  03      0.14246E  00
 PROPANE       0.26912E  01     0.17705E-02       0.45727E  03      0.74352E-01
 I-BUTENE      0.67539E  01     0.44433E-02       0.79880E  03      0.12989E  00
 CIS2BUTE      0.99860E  01     0.65697E-02       0.62229E  03      0.10119E  00
 NBUTANE       0.22224E  02     0.14621E-01       0.17967E  04      0.29215E  00
 NPENTANE      0.26981E  01     0.17750E-02       0.52301E  03      0.85042E-01
 HEPTANE       0.37131E-01      0.24428E-04       0.70613E  02      0.11482E-01
 TOTAL         0.15200E  04                       0.61500E  04
```

```
APPENDIX 3-7   TEST PROBLEM NUMBER - 7


      ***** PROBLEM STATEMENT *****


 TYPE OF COLUMN          3

 NO. OF PLATES       21

 NO. OF COMPONENTS       11

 PRESSURE AT TOP PLATE (PSIA)          264.70

 PRESSURE DROP PER PLATE (PSIA)          0.0

 NO. OF FEEDS        2

    ENTERING PLATE OF FEED 1        7
    FEED QUANTITY       0.34500E 02
    PRESSURE OF FEED          264.70
    LIQUID RATIO OF FEED         0.0

    ENTERING PLATE OF FEED 2        13
    FEED QUANTITY       0.65500E 02
    PRESSURE OF FEED          264.70
    LIQUID RATIO OF FEED         1.0000

REFLUX RATIO            3.122

LIQUID RATIO OF TOP PRODUCT          0.0

SPECIFIED TOP PRODUCT       0.23000E 02

NO. OF LIQUID SIDE STREAMS        1

   LEAVING PLATE NO. OF STREAM 1       4
   QUANTITY OF SIDE STREAM        0.15000E 02

NO. OF VAPOR SIDE STREAMS        1

   LEAVING PLATE NO. OF STREAM 1       16
   QUANTITY OF SIDE STREAM        0.25000E 02
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 0    SUM OF SQUARES OF RESIDUALS  0.87316E 00
TEMPERATURE
 0.53960E 03 0.55810E 03 0.57660E 03 0.59510E 03 0.61360E 03
 0.63210E 03 0.65060E 03 0.66910E 03 0.68760E 03 0.70610E 03
 0.72460E 03 0.74310E 03 0.76160E 03 0.78010E 03 0.79860E 03
 0.81710E 03 0.83560E 03 0.85410E 03 0.87260E 03 0.89110E 03
 0.90960E 03
VAPOR FLOW RATE
 0.23000E 02 0.94806E 02 0.94806E 02 0.94806E 02 0.94806E 02
 0.94806E 02 0.94806E 02 0.60306E 02 0.60306E 02 0.60306E 02
 0.60306E 02 0.60306E 02 0.60306E 02 0.60306E 02 0.60306E 02
 0.60306E 02 0.85306E 02 0.85306E 02 0.85306E 02 0.85306E 02
 0.85306E 02

 1    SUM OF SQUARES OF RESIDUALS  0.19855E 00
TEMPERATURE
 0.53145E 03 0.55484E 03 0.56383E 03 0.57266E 03 0.58656E 03
 0.60341E 03 0.62044E 03 0.64183E 03 0.65746E 03 0.67035E 03
 0.68382E 03 0.70149E 03 0.72559E 03 0.73850E 03 0.74886E 03
 0.76206E 03 0.77724E 03 0.79410E 03 0.81294E 03 0.83528E 03
 0.86562E 03
VAPOR FLOW RATE
 0.23000E 02 0.94806E 02 0.96213E 02 0.94526E 02 0.90909E 02
 0.87516E 02 0.85239E 02 0.52582E 02 0.53330E 02 0.53547E 02
 0.52847E 02 0.51023E 02 0.47090E 02 0.45771E 02 0.45456E 02
 0.44461E 02 0.68597E 02 0.68701E 02 0.69375E 02 0.69967E 02
 0.68851E 02

 2    SUM OF SQUARES OF RESIDUALS  0.19760E-02
TEMPERATURE
 0.54503E 03 0.56592E 03 0.57518E 03 0.58235E 03 0.59017E 03
 0.59800E 03 0.60635E 03 0.63060E 03 0.64640E 03 0.65861E 03
 0.66974E 03 0.68419E 03 0.71615E 03 0.72049E 03 0.72427E 03
 0.72898E 03 0.73501E 03 0.74434E 03 0.75874E 03 0.78108E 03
 0.82006E 03
VAPOR FLOW RATE
 0.23000E 02 0.94806E 02 0.95819E 02 0.94950E 02 0.92787E 02
 0.89762E 02 0.86482E 02 0.50087E 02 0.50212E 02 0.50223E 02
 0.49858E 02 0.48202E 02 0.43324E 02 0.41802E 02 0.43394E 02
 0.44024E 02 0.68264E 02 0.66753E 02 0.65228E 02 0.63720E 02
 0.60559E 02
```

```
 3    SUM OF  SQUARES OF  RESIDUALS   0.46107E-03
TEMPERATURE
 0.54481E  03 0.56594E  03 0.57540E  03 0.58282E  03 0.59157E  03
 0.60031E  03 0.60842E  03 0.63176E  03 0.64655E  03 0.65761E  03
 0.66781E  03 0.68159E  03 0.71353E  03 0.71767E  03 0.72305E  03
 0.73058E  03 0.73849E  03 0.74795E  03 0.76050E  03 0.77964E  03
 0.81607E  03
VAPOR FLOW RATE
 0.23000E  02 0.94600E  02 0.95160E  02 0.94562E  02 0.93389E  02
 0.91831E  02 0.69988E  02 0.53071E  02 0.53110E  02 0.52609E  02
 0.51724E  02 0.49854E  02 0.44503E  02 0.43185E  02 0.44442E  02
 0.46192E  02 0.73103E  02 0.74028E  02 0.73907E  02 0.72266E  02
 0.67026E  02

 4    SUM OF  SQUARES OF  RESIDUALS   0.14002E-04
TEMPERATURE
 0.54474E  03 0.56589E  03 0.57533E  03 0.58271E  03 0.59141E  03
 0.60010E  03 0.60823E  03 0.63176E  03 0.64665E  03 0.65779E  03
 0.66798E  03 0.68176E  03 0.71370E  03 0.71786E  03 0.72322E  03
 0.73050E  03 0.73773E  03 0.74630E  03 0.75826E  03 0.77753E  03
 0.81523E  03
VAPOR FLOW RATE
 0.23000E  02 0.94800E  02 0.95049E  02 0.93999E  02 0.91960E  02
 0.89854E  02 0.88107E  02 0.52015E  02 0.52253E  02 0.52050E  02
 0.51435E  02 0.49707E  02 0.44402E  02 0.42939E  02 0.44003E  02
 0.45151E  02 0.71270E  02 0.71929E  02 0.72095E  02 0.71113E  02
 0.69316E  02
```

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     ***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS     4

COLUMN PRESSURE (PSIA)   0.26470E 03

REFLUX RATIO           3.12200

PRESSURE , TEMPERATURE , ENTHALPY AND LIQUID FRACTION OF FEED

 0.265E 03 PSIA   0.127E 03 F  0.204E 06 B.T.U.        0.0

 0.265E 03 PSIA   0.271E 03 F  0.483E 06 B.T.U.        1.000

*** STAGE VARIABLES ***

   PLATE NO.  TEMPERATURE   LIQ. F. R.     VAP. F. R.     HEAT DUTY
                   F        LB MOL/TIME    LB MOL/TIME    BTU/TI[illegible]
       1      0.85135E 02   0.71806E 02   0.23000E 02  -0.43341E 06
       2      0.10629E 03   0.72049E 02   0.94806E 02   0.0
       3      0.11573E 03   0.70599E 02   0.95049E 02   0.0
       4      0.12311E 03   0.53960E 02   0.93999E 02   0.0
       5      0.13181E 03   0.51854E 02   0.91960E 02   0.0
       6      0.14050E 03   0.50107E 02   0.89854E 02   0.0
       7      0.14863E 03   0.48515E 02   0.88107E 02   0.0
       8      0.17216E 03   0.48753E 02   0.52015E 02   0.0
       9      0.18705E 03   0.48550E 02   0.52253E 02   0.0
      10      0.19819E 03   0.47935E 02   0.52050E 02   0.0
      11      0.20838E 03   0.46207E 02   0.51435E 02   0.0
      12      0.22216E 03   0.40902E 02   0.49707E 02   0.0
      13      0.25410E 03   0.10494E 03   0.44402E 02   0.0
      14      0.25826E 03   0.10600E 03   0.42939E 02   0.0
      15      0.26362E 03   0.10715E 03   0.44003E 02   0.0
      16      0.27090E 03   0.10827E 03   0.45151E 02   0.0
      17      0.27813E 03   0.10893E 03   0.71270E 02   0.0
      18      0.28670E 03   0.10910E 03   0.71929E 02   0.0
      19      0.29866E 03   0.10811E 03   0.72095E 02   0.0
      20      0.31794E 03   0.10332E 03   0.71113E 02   0.0
      21      0.35563E 03   0.37000E 02   0.66316E 02   0.68362E 06
```

```
*** MATERIAL BALANCES ***

 FEEDS

                  PLATE NO.    7                            PLATE NO.   13
              LB MOL/TIME    MOL FRC.         LB MOL/TIME        MOL FRC.
 METHANE      0.20000E 01    0.57971E-01      0.0                0.0
 ETHANE       0.10000E 02    0.28986E 00      0.0                0.0
 PROPYLEN     0.60000E 01    0.17391E 00      0.10000E 01        0.15267E-01
 PROPANE      0.12000E 02    0.34783E 00      0.70000E 01        0.10687E 00
 IBUTANE      0.10000E 01    0.28986E-01      0.40000E 01        0.61069E-01
 NBUTANE      0.30000E 01    0.86957E-01      0.17000E 02        0.25954E 00
 NPENTANE     0.50000E 00    0.14493E-01      0.15200E 02        0.23206E 00
 HEXANE       0.0            0.0              0.90000E 01        0.13740E 00
 HEPTANE      0.0            0.0              0.45000E 01        0.68702E-01
 OCTANE       0.0            0.0              0.43000E 01        0.65649E-01
 DECANE       0.0            0.0              0.35000E 01        0.53435E-01
 TOTAL        0.34500E 02                     0.65500E 02

 PRODUCTS

                 VAPOR DISTILLATE                      LIQUID DISTILLATE
              LB MOL/TIME    MOL FRC.         LB MOL/TIME        MOL FRC.
 METHANE      0.19599E 01    0.85213E-01      0.0                0.10834E-01
 ETHANE       0.90252E 01    0.39240E 00      0.0                0.21217E 00
 PROPYLEN     0.38686E 01    0.16820E 00      0.0                0.22483E 00
 PROPANE      0.80135E 01    0.34841E 00      0.0                0.53214E 00
 IBUTANE      0.88766E-01    0.38594E-02      0.0                0.12040E-01
 NBUTANE      0.44060E-01    0.19156E-02      0.0                0.79728E-02
 NPENTANE     0.94465E-05    0.41072E-06      0.0                0.42856E-05
 HEXANE       0.30262E-10    0.13157E-11      0.0                0.34170E-10
 HEPTANE      0.20524E-14    0.89235E-16      0.0                0.52029E-14
 OCTANE       0.13464E-18    0.58541E-20      0.0                0.82294E-18
 DECANE       0.41879E-26    0.18208E-27      0.0                0.11835E-24
 TOTAL        0.23000E 02                     0.0

                 BOTTOM PRODUCT
              LB MOL/TIME    MOL FRC.
 METHANE      0.20328E-13    0.54940E-15
 ETHANE       0.13228E-07    0.35750E-09
 PROPYLEN     0.27182E-02    0.73466E-04
 PROPANE      0.41201E-01    0.11135E-02
 IBUTANE      0.70362E 00    0.19017E-01
 NBUTANE      0.52278E 01    0.14129E 00
 NPENTANE     0.11285E 02    0.30499E 00
 HEXANE       0.79107E 01    0.21380E 00
 HEPTANE      0.42148E 01    0.11391E 00
 OCTANE       0.41540E 01    0.11227E 00
 DECANE       0.34605E 01    0.93528E-01
 TOTAL        0.37000E 02
```

```
LIQUID SIDE STREAMS

                          LIQUID  ( 4)
                    LB MOL/TIME       MOL FRC.
   METHANE          0.39917E-01      0.26612E-02
   ETHANE           0.97464E 00      0.64976E-01
   PROPYLEN         0.28738E 01      0.19159E 00
   PROPANE          0.87361E 01      0.58241E 00
   IBUTANE          0.10082E 01      0.67211E-01
   NBUTANE          0.13589E 01      0.90550E-01
   NPENTANE         0.84660E-02      0.56433E-03
   HEXANE           0.81088E-06      0.54059E-07
   HEPTANE          0.11570E-08      0.77130E-10
   OCTANE           0.20882E-11      0.13921E-12
   DECANE           0.21706E-16      0.14470E-17
   TOTAL            0.15000E 02

   VAPOR SIDE STREAMS

                          VAPOR  (16)
                    LB MOL/TIME       MOL FRC.
   METHANE          0.29534E-08      0.11813E-09
   ETHANE           0.58430E-04      0.23372E-05
   PROPYLEN         0.25472E 00      0.10189E-01
   PROPANE          0.22075E 01      0.88299E-01
   IBUTANE          0.31985E 01      0.12794E 00
   NBUTANE          0.13368E 02      0.53470E 00
   NPENTANE         0.44093E 01      0.17637E 00
   HEXANE           0.10906E 01      0.43625E-01
   HEPTANE          0.28572E 00      0.11429E-01
   OCTANE           0.14641E 00      0.58563E-02
   DECANE           0.39613E-01      0.15845E-02
   TOTAL            0.25000E 02
```

APPENDIX 3-8   TEST PROBLEM NUMBER - 8

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       ***** PROBLEM STATEMENT *****


 TYPE OF COLUMN         3

 NO. OF PLATES       25

 NO. OF COMPONENTS       18

 PRESSURE AT TOP PLATE (PSIA)           350.00

 PRESSURE DROP PER PLATE (PSIA)           0.0

 NO. OF FEEDS        1

    ENTERING PLATE OF FEED 1       9
    FEED QUANTITY         0.58735E 03
    PRESSURE OF FEED           350.00
    TEMPERATURE OF FEED (F)            250.00

 REFLUX RATIO             1.900

 LIQUID RATIO OF TOP PRODUCT           0.5000

 SPECIFIED TOP PRODUCT      0.42040E 03
```

```
*** RATE OF CONVERGENCE WITH ITERATION NO. ***

 0     SUM OF SQUARES OF RESIDUALS   0.21987E 01
 TEMPERATURE
  0.57960E  03 0.59147E  03 0.60335E  03 0.61522E  03 0.62710E  03
  0.63897E  03 0.65085E  03 0.66272E  03 0.67460E  03 0.68647E  03
  0.69835E  03 0.71022E  03 0.72210E  03 0.73397E  03 0.74585E  03
  0.75772E  03 0.76960E  03 0.78147E  03 0.79335E  03 0.80522E  03
  0.81710E  03 0.82897E  03 0.84085E  03 0.85272E  03 0.86460E  03
 VAPOR FLOW RATE
  0.21020E  03 0.12192E  04 0.12192E  04 0.12192E  04 0.12192E  04
  0.12192E  04 0.12192E  04 0.12192E  04 0.12192E  04 0.80035E  03
  0.80035E  03 0.80035E  03 0.80035E  03 0.80035E  03 0.80035E  03
  0.80035E  03 0.80035E  03 0.80035E  03 0.80035E  03 0.80035E  03
  0.80035E  03 0.80035E  03 0.80035E  03 0.80035E  03 0.80035E  03

  1     SUM OF SQUARES OF RESIDUALS   0.64382E 00
 TEMPERATURE
  0.58149E  03 0.61873E  03 0.63693E  03 0.67324E  03 0.68710E  03
  0.69342E  03 0.69626E  03 0.66972E  03 0.68164E  03 0.69726E  03
  0.70956E  03 0.72008E  03 0.73015E  03 0.74045E  03 0.75104E  03
  0.76189E  03 0.77274E  03 0.78323E  03 0.79302E  03 0.80205E  03
  0.81060E  03 0.81926E  03 0.82945E  03 0.84351E  03 0.86390E  03
 VAPOR FLOW RATE
  0.21020E  03 0.12192E  04 0.11658E  04 0.13652E  04 0.15914E  04
  0.17081E  04 0.17818E  04 0.14128E  04 0.12226E  04 0.77453E  03
  0.80148E  03 0.81839E  03 0.82601E  03 0.83029E  03 0.83420E  03
  0.83934E  03 0.84668E  03 0.85610E  03 0.86677E  03 0.87592E  03
  0.88181E  03 0.88023E  03 0.87103E  03 0.84735E  03 0.80939E  03

  2     SUM OF SQUARES OF RESIDUALS   0.37130E-01
 TEMPERATURE
  0.58420E  03 0.65030E  03 0.67043E  03 0.67614E  03 0.68220E  03
  0.68718E  03 0.69215E  03 0.69386E  03 0.70642E  03 0.72838E  03
  0.73970E  03 0.74725E  03 0.75430E  03 0.76192E  03 0.77040E  03
  0.77939E  03 0.78823E  03 0.79616E  03 0.80278E  03 0.80801E  03
  0.81242E  03 0.81701E  03 0.82406E  03 0.83750E  03 0.86531E  03
 VAPOR FLOW RATE
  0.21020E  03 0.12192E  04 0.12609E  04 0.15398E  04 0.16645E  04
  0.17197E  04 0.17214E  04 0.13362E  04 0.12205E  04 0.74187E  03
  0.81340E  03 0.84464E  03 0.85491E  03 0.85967E  03 0.86448E  03
  0.87337E  03 0.88751E  03 0.90673E  03 0.92793E  03 0.94796E  03
  0.96189E  03 0.96588E  03 0.95135E  03 0.90839E  03 0.81346E  03
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  3    SUM OF SQUARES OF RESIDUALS  0.26389E-02
TEMPERATURE
  0.58394E 03 0.64761E 03 0.66640E 03 0.67605E 03 0.68252E 03
  0.68841E 03 0.69516E 03 0.70088E 03 0.71528E 03 0.74166E 03
  0.75557E 03 0.76648E 03 0.77675E 03 0.78665E 03 0.79556E 03
  0.80271E 03 0.80780E 03 0.81106E 03 0.81320E 03 0.81503E 03
  0.81719E 03 0.82057E 03 0.82680E 03 0.83921E 03 0.86445E 03
VAPOR FLOW RATE
  0.21020E 03 0.12192E 04 0.13268E 04 0.12667E 04 0.12539E 04
  0.12409E 04 0.12251E 04 0.12697E 04 0.12230E 04 0.74570E 03
  0.82299E 03 0.84948E 03 0.86679E 03 0.86886E 03 0.87775E 03
  0.88770E 03 0.89655E 03 0.90264E 03 0.90668E 03 0.90629E 03
  0.90381E 03 0.89818E 03 0.88421E 03 0.85069E 03 0.78137E 03

  4    SUM OF SQUARES OF RESIDUALS  0.15716E-03
TEMPERATURE
  0.58357E 03 0.64775E 03 0.66754E 03 0.67670E 03 0.68274E 03
  0.68803E 03 0.69380E 03 0.70167E 03 0.71592E 03 0.74241E 03
  0.75544E 03 0.76467E 03 0.77257E 03 0.77978E 03 0.78642E 03
  0.79233E 03 0.79737E 03 0.80163E 03 0.80527E 03 0.80868E 03
  0.81236E 03 0.81711E 03 0.82445E 03 0.83760E 03 0.86276E 03
VAPOR FLOW RATE
  0.21020E 03 0.12192E 04 0.12989E 04 0.13213E 04 0.13126E 04
  0.12951E 04 0.12697E 04 0.12419E 04 0.11697E 04 0.71782E 03
  0.79665E 03 0.82007E 03 0.82511E 03 0.82573E 03 0.82932E 03
  0.84079E 03 0.86084E 03 0.88422E 03 0.90673E 03 0.92353E 03
  0.93253E 03 0.93119E 03 0.91517E 03 0.87486E 03 0.79754E 03

  5    SUM OF SQUARES OF RESIDUALS  0.15400E-04
TEMPERATURE
  0.58357E 03 0.64800E 03 0.66782E 03 0.67735E 03 0.68371E 03
  0.68933E 03 0.69539E 03 0.70327E 03 0.71721E 03 0.74400E 03
  0.75726E 03 0.76652E 03 0.77422E 03 0.78098E 03 0.78695E 03
  0.79219E 03 0.79675E 03 0.80073E 03 0.80435E 03 0.80786E 03
  0.81167E 03 0.81655E 03 0.82406E 03 0.83735E 03 0.86263E 03
VAPOR FLOW RATE
  0.21020E 03 0.12192E 04 0.13009E 04 0.13205E 04 0.13165E 04
  0.13025E 04 0.12821E 04 0.12492E 04 0.11843E 04 0.73277E 03
  0.82315E 03 0.86163E 03 0.88453E 03 0.90331E 03 0.92021E 03
  0.93456E 03 0.94498E 03 0.95157E 03 0.95465E 03 0.95493E 03
  0.95204E 03 0.94342E 03 0.92304E 03 0.88164E 03 0.80497E 03
```

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      ***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS     5

COLUMN PRESSURE (PSIA)    0.35000E 03

REFLUX RATIO          1.90000

PRESSURE , TEMPERATURE , ENTHALPY AND LIQUID FRACTION OF FEED

 0.350E 03 PSIA  0.250E 03 F  0.521E 07 B.T.U.        0.287

*** STAGE VARIABLES ***

   PLATE NO. TEMPERATURE   LIQ. F. R.    VAP. F. R.    HEAT DUTY
                 F         LB MOL/TIME   LB MOL/TIME    BTU/TIME
      1      0.12397E 03  0.79876E 03  0.21020E 03 -0.75686E 07
      2      0.18840E 03  0.88054E 03  0.12192E 04  0.0
      3      0.20822E 03  0.90011E 03  0.13009E 04  0.0
      4      0.21775E 03  0.89611E 03  0.13205E 04  0.0
      5      0.22411E 03  0.88212E 03  0.13165E 04  0.0
      6      0.22973E 03  0.86165E 03  0.13025E 04  0.0
      7      0.23579E 03  0.82879E 03  0.12821E 04  0.0
      8      0.24367E 03  0.76391E 03  0.12492E 04  0.0
      9      0.25761E 03  0.89972E 03  0.11843E 04  0.0
     10      0.28440E 03  0.99011E 03  0.73277E 03  0.0
     11      0.29766E 03  0.10286E 04  0.82315E 03  0.0
     12      0.30693E 03  0.10515E 04  0.86163E 03  0.0
     13      0.31462E 03  0.10703E 04  0.88453E 03  0.0
     14      0.32138E 03  0.10872E 04  0.90331E 03  0.0
     15      0.32735E 03  0.11015E 04  0.92021E 03  0.0
     16      0.33259E 03  0.11119E 04  0.93456E 03  0.0
     17      0.33715E 03  0.11185E 04  0.94498E 03  0.0
     18      0.34114E 03  0.11216E 04  0.95157E 03  0.0
     19      0.34475E 03  0.11219E 04  0.95465E 03  0.0
     20      0.34826E 03  0.11190E 04  0.95493E 03  0.0
     21      0.35207E 03  0.11104E 04  0.95204E 03  0.0
     22      0.35695E 03  0.10900E 04  0.94342E 03  0.0
     23      0.36446E 03  0.10486E 04  0.92304E 03  0.0
     24      0.37775E 03  0.97192E 03  0.88164E 03  0.0
     25      0.40303E 03  0.16695E 03  0.80497E 03  0.65170E 07
```

```
*** MATERIAL BALANCES ***

FEEDS

                  PLATE NO.    9                     PLATE NO.
               LB MOL/TIME     MOL FRC.         LB MOL/TIME    MOL FRC.
CO2            0.41900E 00   0.71337E-03
NITROGEN       0.21100E 00   0.35924E-03
METHANE        0.74737E 02   0.12724E 00
ETHANE         0.78890E 02   0.13431E 00
PROPANE        0.13006E 03   0.22143E 00
IBUTANE        0.44244E 02   0.75328E-01
NBUTANE        0.90173E 02   0.153[illegible]E 00
IPENTANE       0.41344E 02   0.70391E-01
NPENTANE       0.43606E 02   0.74242E-01
2MPENTAN       0.15143E 02   0.25782E-01
HEXANE         0.14955E 02   0.25462E-01
HEPTANE        0.25817E 02   0.43955E-01
OCTANE         0.15875E 02   0.27028E-01
NONANE         0.87840E 01   0.14955E-01
DECANE         0.23920E 01   0.40725E-02
UNDECANE       0.44300E 00   0.75423E-03
DODECANE       0.17400E 00   0.29624E-03
TRDECANE       0.88000E-01   0.14983E-03
TOTAL          0.58735E 03

PRODUCTS

                 VAPOR DISTILLATE                    LIQUID DISTILLATE
               LB MOL/TIME   MOL FRC.        LB MOL/TIME     MOL FRC.
CO2            0.33030E 00   0.15713E-02     0.88790E-01     0.42241E-03
NITROGEN       0.19721E 00   0.93818E-03     0.13987E-01     0.66543E-04
METHANE        0.65482E 02   0.31152E 00     0.92990E 01     0.44235E-01
ETHANE         0.52327E 02   0.24894E 00     0.26569E 02     0.12640E 00
PROPANE        0.57040E 02   0.27136E 00     0.72996E 02     0.34727E 00
IBUTANE        0.12834E 02   0.61050E-01     0.31302E 02     0.14891E 00
NBUTANE        0.21539E 02   0.10247E 00     0.67197E 0[illegible]     0.31968E 00
IPENTANE       0.35464E 00   0.16872E-02     0.20552E 01     0.97772E-02
NPENTANE       0.94546E-01   0.44979E-03     0.67307E 00     0.32021E-02
2MPENTAN       0.29464E-03   0.14017E-05     0.39712E-02     0.[illegible]892E-04
HEXANE         0.79251E-04   0.37703E-06     0.12820E-02     0.60990E-05
HEPTANE        0.69443E-06   0.33037E-08     0.23475E-04     0.11168E-06
OCTANE         0.15557E-08   0.74009E-11     0.11703E-06     0.556[illegible]4E-09
NONANE         0.45104E-11   0.21458E-13     0.70652E-09     0.33612E-11
DECANE         0.93487E-14   0.44475E-16     0.28865E-11     0.13732E-13
UNDECANE       0.16997E-16   0.80863E-19     0.98804E-14     0.47005E-16
DODECANE       0.72871E-19   0.34667E-21     0.78898E-16     0.37535E-18
TRDECANE       0.44380E-21   0.21113E-23     0.87851E-18     0.41794E-20
TOTAL          0.21020E 03                   0.21020E 03
```

```
                    BOTTOM PRODUCT
              LB MOL/TIME      MOL FRC.
CO2           0.16663E-12      0.99807E-15
NITROGEN      0.38112E-16      0.22828E-18
METHANE       0.42723E-12      0.25590E-14
ETHANE        0.11606E-08      0.69[illegible]18E-11
PROPANE       0.24584E-03      0.14725E-05
IBUTANE       0.98097E-01      0.58758E-03
NBUTANE       0.1417[illegible]E 01      0.84[illegible]7E-02
IPENTANE      0.[illegible]933E 02      0.2[illegible]E 00
NPENTANE      0.4[illegible]38E 02      0.2[illegible]E 00
2MPENTAN      0.1[illegible]E 02      0.90077E-01
HEXANE        0.1495[illegible]E 02      0.895[illegible]E-01
HEPTANE       0.25817E 02      0.15464E 00
OCTANE        0.15875E 02      0.95087E-01
NONANE        0.87840E 01      0.52614E-01
DECANE        0.23920E 01      0.14327E-01
UNDECANE      0.44300E 00      0.26535E-02
DODECANE      0.17400E 00      0.10422E-02
TRDECANE      0.88000E-01      0.52710E-03
TOTAL         0.16695E 03
```

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APPENDIX 3-9   TEST PROBLEM NUMBER - 9


     ***** PROBLEM STATEMENT *****


 TYPE OF COLUMN          3

 NO. OF PLATES        70

 NO. OF COMPONENTS          4

 PRESSURE AT TOP PLATE (PSIA)                 84.00

 PRESSURE DROP PER PLATE (PSIA)                0.0

 NO. OF FEEDS         1

    ENTERING PLATE OF FEED 1       35
    FEED QUANTITY          0.18195E 04
    PRESSURE OF FEED             84.00
    LIQUID RATIO OF FEED           1.0000

 REFLUX RATIO             11.300

 LIQUID RATIO OF TOP PRODUCT              0.0

 SPECIFIED TOP PRODUCT         0.67000E 03
21:25.31  1.039  RC=0
```

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*** RATE OF CONVERGENCE WITH ITERATION NO. ***

  0      SUM OF SQUARES OF RESIDUALS   0.92701E-02
 TEMPERATURE
  0.57160E 03  0.57195E 03  0.57230E 03  0.57264E 03  0.57299E 03
  0.57334E 03  0.57369E 03  0.57403E 03  0.57438E 03  0.57473E 03
  0.57508E 03  0.57542E 03  0.57577E 03  0.57612E 03  0.57647E 03
  0.57681E 03  0.57716E 03  0.57751E 03  0.57786E 03  0.57821E 03
  0.57855E 03  0.57890E 03  0.57925E 03  0.57960E 03  0.57994E 03
  0.58029E 03  0.58064E 03  0.58099E 03  0.58133E 03  0.58168E 03
  0.58203E 03  0.58238E 03  0.58272E 03  0.58307E 03  0.58342E 03
  0.58377E 03  0.58412E 03  0.58446E 03  0.58481E 03  0.58516E 03
  0.58551E 03  0.58585E 03  0.58620E 03  0.58655E 03  0.58690E 03
  0.58724E 03  0.58759E 03  0.58794E 03  0.58829E 03  0.58864E 03
  0.58898E 03  0.58933E 03  0.58968E 03  0.59003E 03  0.59037E 03
  0.59072E 03  0.59107E 03  0.59142E 03  0.59176E 03  0.59211E 03
  0.59246E 03  0.59281E 03  0.59315E 03  0.59350E 03  0.59385E 03
  0.59420E 03  0.59455E 03  0.59489E 03  0.59524E 03  0.59560E 03
 VAPOR FLOW RATE
  0.67000E 03  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04
  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04
  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04
  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04
  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04
  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04
  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04
  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04
  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04
  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04
  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04
  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04
  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04
  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04  0.82410E 04
```

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1     SUM OF SQUARES OF RESIDUALS  0.65145E-04
TEMPERATURE
  0.57282E 03  0.57323E 03  0.57339E 03  0.57341E 03  0.57354E 03
  0.57368E 03  0.57373E 03  0.57391E 03  0.57398E 03  0.57414E 03
  0.57432E 03  0.57452E 03  0.57476E 03  0.57503E 03  0.57537E 03
  0.57572E 03  0.57612E 03  0.57659E 03  0.57708E 03  0.57760E 03
  0.57825E 03  0.57888E 03  0.57961E 03  0.58027E 03  0.58101E 03
  0.58171E 03  0.58250E 03  0.58317E 03  0.58383E 03  0.58446E 03
  0.58503E 03  0.58557E 03  0.58604E 03  0.58648E 03  0.58691E 03
  0.58723E 03  0.58756E 03  0.58790E 03  0.58824E 03  0.58864E 03
  0.58904E 03  0.58947E 03  0.58990E 03  0.59036E 03  0.59082E 03
  0.59129E 03  0.59177E 03  0.59223E 03  0.59268E 03  0.59312E 03
  0.59353E 03  0.59393E 03  0.59428E 03  0.59460E 03  0.59489E 03
  0.59514E 03  0.59535E 03  0.59552E 03  0.59567E 03  0.59578E 03
  0.59586E 03  0.59592E 03  0.59596E 03  0.59598E 03  0.59600E 03
  0.59600E 03  0.59602E 03  0.59606E 03  0.59617E 03  0.59645E 03
VAPOR FLOW RATE
  0.67000E 03  0.82410E 04  0.82438E 04  0.82456E 04  0.82407E 04
  0.82392E 04  0.82405E 04  0.82354E 04  0.82364E 04  0.82317E 04
  0.82286E 04  0.82249E 04  0.82203E 04  0.82150E 04  0.82083E 04
  0.82025E 04  0.81944E 04  0.81852E 04  0.81765E 04  0.81649E 04
  0.81545E 04  0.81425E 04  0.81283E 04  0.81174E 04  0.81021E 04
  0.80894E 04  0.80727E 04  0.80615E 04  0.80474E 04  0.80336E 04
  0.80205E 04  0.80073E 04  0.79949E 04  0.79822E 04  0.79688E 04
  0.79696E 04  0.79691E 04  0.79681E 04  0.79669E 04  0.79645E 04
  0.79624E 04  0.79599E 04  0.79566E 04  0.79529E 04  0.79495E 04
  0.79451E 04  0.79406E 04  0.79361E 04  0.79305E 04  0.79252E 04
  0.79191E 04  0.79126E 04  0.79064E 04  0.78994E 04  0.78918E 04
  0.78847E 04  0.78770E 04  0.78694E 04  0.78613E 04  0.78535E 04
  0.78460E 04  0.78382E 04  0.78310E 04  0.78241E 04  0.78169E 04
  0.78108E 04  0.78049E 04  0.77977E 04  0.77896E 04  0.77788E 04
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***** COMPUTED RESULTS *****

NUMBER OF ITERATIONS    1

COLUMN PRESSURE (PSIA)    0.84000E 02

REFLUX RATIO          11.50000

PRESSURE , TEMPERATURE , ENTHALPY AND LIQUID FRACTION OF FEED

 0.840E 02 PSIA  0.127E 03 F  0.153E 07 B.T.U.        1.000

*** STAGE VARIABLES ***

   PLATE NO. TEMPERATURE   LIQ. F. R.     VAP. F. R.     HEAT DUTY
                 F         LB MOL/TIME    LB MOL/TIME    BTU/TIME
      1      0.11322E 03   0.75710E 04    0.67000E 03  -0.58597E 08
      2      0.11363E 03   0.75738E 04    0.82410E 04   0.0
      3      0.11379E 03   0.75756E 04    0.82438E 04   0.0
      4      0.11381E 03   0.75707E 04    0.82456E 04   0.0
      5      0.11394E 03   0.75692E 04    0.82407E 04   0.0
      6      0.11408E 03   0.75705E 04    0.82392E 04   0.0
      7      0.11413E 03   0.75654E 04    0.82405E 04   0.0
      8      0.11431E 03   0.75664E 04    0.82354E 04   0.0
      9      0.11438E 03   0.75617E 04    0.82364E 04   0.0
     10      0.11454E 03   0.75586E 04    0.82317E 04   0.0
     11      0.11472E 03   0.75549E 04    0.82286E 04   0.0
     12      0.11492E 03   0.75503E 04    0.82249E 04   0.0
     13      0.11516E 03   0.75450E 04    0.82203E 04   0.0
     14      0.11543E 03   0.75383E 04    0.82150E 04   0.0
     15      0.11577E 03   0.75325E 04    0.82083E 04   0.0
     16      0.11612E 03   0.75244E 04    0.82025E 04   0.0
     17      0.11652E 03   0.75152E 04    0.81944E 04   0.0
     18      0.11699E 03   0.75065E 04    0.81852E 04   0.0
     19      0.11748E 03   0.74949E 04    0.81765E 04   0.0
     20      0.11806E 03   0.74845E 04    0.81649E 04   0.0
     21      0.11865E 03   0.74725E 04    0.81545E 04   0.0
     22      0.11928E 03   0.74583E 04    0.81425E 04   0.0
     23      0.12001E 03   0.74474E 04    0.81283E 04   0.0
     24      0.12067E 03   0.74321E 04    0.81174E 04   0.0
     25      0.12141E 03   0.74194E 04    0.81021E 04   0.0
     26      0.12211E 03   0.74027E 04    0.80894E 04   0.0
     27      0.12290E 03   0.73919E 04    0.80727E 04   0.0
     28      0.12357E 03   0.73774E 04    0.80619E 04   0.0
     29      0.12423E 03   0.73636E 04    0.80474E 04   0.0
     30      0.12486E 03   0.73505E 04    0.80336E 04   0.0
     31      0.12543E 03   0.73373E 04    0.80205E 04   0.0
     32      0.12597E 03   0.73249E 04    0.80073E 04   0.0
     33      0.12644E 03   0.73122E 04    0.79949E 04   0.0
     34      0.12688E 03   0.72988E 04    0.79822E 04   0.0
     35      0.12731E 03   0.91191E 04    0.79688E 04   0.0
     36      0.12763E 03   0.91186E 04    0.79696E 04   0.0
     37      0.12796E 03   0.91176E 04    0.79691E 04   0.0
     38      0.12830E 03   0.91164E 04    0.79681E 04   0.0
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39     0.12865E  03   0.91140E  04   0.79669E  04   0.0
40     0.12904E  03   0.91119E  04   0.79645E  04   0.0
41     0.12944E  03   0.91091E  04   0.79624E  04   0.0
42     0.12987E  03   0.91061E  04   0.79596E  04   0.0
43     0.13030E  03   0.91024E  04   0.79566E  04   0.0
44     0.13076E  03   0.90990E  04   0.79529E  04   0.0
45     0.13122E  03   0.90946E  04   0.79495E  04   0.0
46     0.13169E  03   0.90901E  04   0.79451E  04   0.0
47     0.13217E  03   0.90856E  04   0.79406E  04   0.0
48     0.13263E  03   0.90800E  04   0.79361E  04   0.0
49     0.13308E  03   0.90747E  04   0.79305E  04   0.0
50     0.13352E  03   0.90686E  04   0.79252E  04   0.0
51     0.13393E  03   0.90621E  04   0.79191E  04   0.0
52     0.13433E  03   0.90559E  04   0.79126E  04   0.0
53     0.13468E  03   0.90489E  04   0.79064E  04   0.0
54     0.13500E  03   0.90413E  04   0.78994E  04   0.0
55     0.13529E  03   0.90342E  04   0.78918E  04   0.0
56     0.13554E  03   0.90265E  04   0.78847E  04   0.0
57     0.13575E  03   0.90189E  04   0.78770E  04   0.0
58     0.13592E  03   0.90108E  04   0.78694E  04   0.0
59     0.13607E  03   0.90030E  04   0.78613E  04   0.0
60     0.13618E  03   0.89955E  04   0.78535E  04   0.0
61     0.13626E  03   0.89877E  04   0.78460E  04   0.0
62     0.13632E  03   0.89805E  04   0.78382E  04   0.0
63     0.13636E  03   0.89736E  04   0.78310E  04   0.0
64     0.13638E  03   0.89664E  04   0.78241E  04   0.0
65     0.13640E  03   0.89603E  04   0.78169E  04   0.0
66     0.13640E  03   0.89535E  04   0.78108E  04   0.0
67     0.13642E  03   0.89472E  04   0.78040E  04   0.0
68     0.13646E  03   0.89391E  04   0.77977E  04   0.0
69     0.13657E  03   0.89283E  04   0.77896E  04   0.0
70     0.13685E  03   0.11495E  04   0.77788E  04   0.64260E  08
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*** MATERIAL BALANCES ***

 FEEDS

                       PLATE NO.   15                    PLATE NO.
                     LB MOL/TIME    MOL FRC.      LB MOL/TIME      MOL FRC.
 PROPANE             0.10000E 02   0.54960E-02
 IBUTANE             0.65200E 03   0.35834E 00
 NBUTANE             0.11400E 04   0.62655E 00
 IPENTANE            0.17500E 02   0.96180E-02
 TOTAL               0.18195E 04

 PRODUCTS

                      VAPOR DISTILLATE                  LIQUID DISTILLATE
                     LB MOL/TIME    MOL FRC.      LB MOL/TIME      MOL FRC.
 PROPANE             0.99937E 01   0.14916E-01    0.0              0.68215E-02
 IBUTANE             0.65695E 03   0.98053E 00    0.0              0.98714E 00
 NBUTANE             0.30530E 01   0.45567E-02    0.0              0.60344E-02
 IPENTANE            0.76883E-13   0.11475E-15    0.0              0.32495E-15
 TOTAL               0.67000E 03                  0.0

                       BOTTOM PRODUCT
                     LB MOL/TIME    MOL FRC.
 PROPANE             0.15936E-14   0.13864E-17
 IBUTANE             0.0           0.0
 NBUTANE             0.11321E 04   0.98484E 00
 IPENTANE            0.17425E 02   0.15159E-01
 TOTAL               0.11495E 04
```