5-31-1973

Sidestream tower fractionation : a short-cut calculation method

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SIDESTREAM TOWER FRACTIONATION -

A SHORT-CUT CALCULATION METHOD

By

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A THESIS

PRESENTED IN PARTIAL FULFILLMENT OF

THE REQUIREMENTS FOR THE DEGREE

OF

MASTER OF SCIENCE IN CHEMICAL ENGINEERING

AT

NEWARK COLLEGE OF ENGINEERING

Newark, New Jersey 1973

ABSTRACT

A short-cut procedure has been developed for making calculations on a complex fractionation tower. A Simplification of the Thiele-Geddes plate-to-plate procedure provided the basis for the short-cut procedure. The application discussed in this paper is for a tower with a liquid sidestream drawoff in the rectifying section.

The tower was broken at the feed point and sidestream drawoff locations into three calculation sections. The fractionation in each tower section can then be represented by a rigorous series solution expressed in terms of absorption or stripping factors. These rigorous equations can then be simplified by the use of average absorption or stripping factors.

The short-cut procedure has two methods of determining the average stripping or absorption factors for each tower section. The one method uses the assumption of a linear profile of absorption or stripping factors based on end values in each section and is called the Stand-Alone Simplified Thiele-Geddes Method. The other method determines average absorption or stripping factor for each tower section from a force-fit to a rigorous plate-to-plate solution. This method is called the Force-Fit Thiele-Geddes Method and is suitable for accurate parametric studies around a base case rigorous solution.

Computer programs were prepared for the Thiele-Geddes plate-to-plate method and the stand-alone short-cut procedure. In addition, a computer program was written to obtain the force-fit fractions required for the Force-Fit Thiele-Geddes Method. Parametric cases were then run for a five-component debutanizer column, and the results of the short-cut method were compared with the rigorous solution for each case.

The results of these comparisons show the Stand-Alone Simplified Thiele-Geddes Method to be of suitable accuracy for preliminary design calculations. The Force-Fit Thiele-Geddes Method results in a higher degree of accuracy in most cases and is suitable for parametric studies on a final design. The degree of accuracy obtained from the Force-Fit Method is believed to be the highest available from a short-cut procedure.

APPROVAL OF THESIS

SIDESTREAM TOWER FRACTIONATION -

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PREFACE

The procedure for simplifying the Rigorous Thiele-Geddes equations and applying them to short-cut, fractionation calculations was developed by Dr. Ralph Cecchetti while teaching stage equilibrium processes at Newark College of Engineering.

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INTRODUCTION

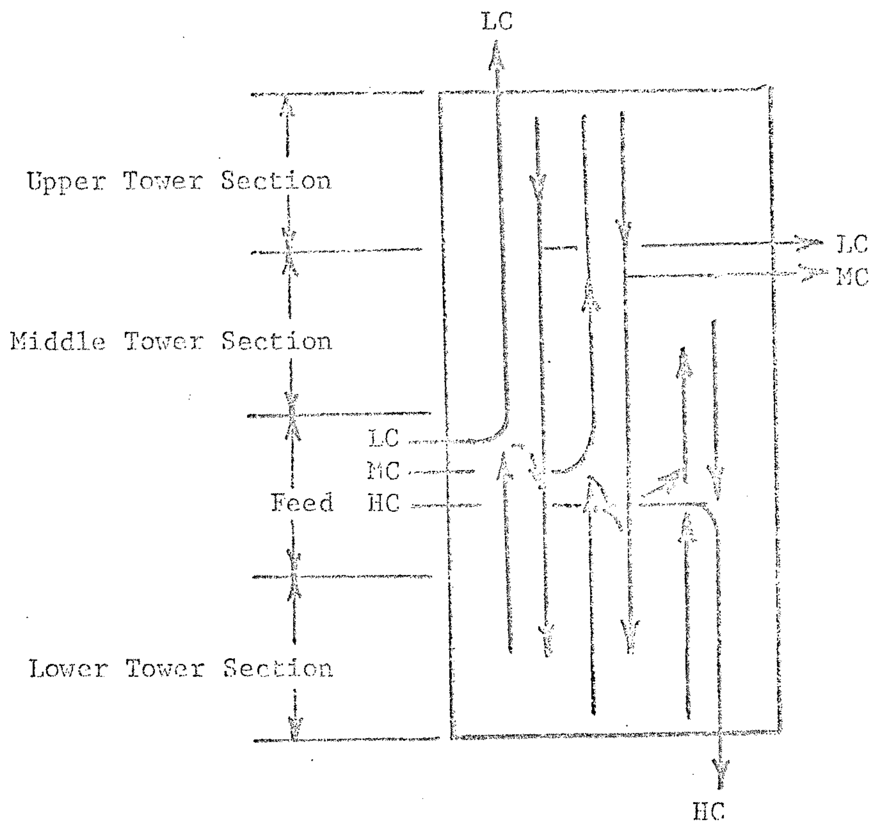
This section will first discuss the purpose of a fractionation tower with a liquid sidestream drawoff in the rectifying section. This will be followed by a discussion concerning the degrees of freedom and variables involved in developing a fractionation calculation procedure. The reasons as to why the Thiele-Geddes Method[2] was selected as a bases for a short-cut fractionation procedure will then be enumerated.

Three products can be produced in a single tower by taking advantage of a sidestream drawoff. The conventional practice, for reasons of control and equipment costs, is to have a liquid sidestream drawoff in the rectifying section. The component distribution profiles that result from a sidestream tower can be exemplified by considering three components: LC = Light, MC = Middle, and HC = Heavy. These are to be separated into three streams, each enriched in one of the components.

For a liquid sidestream drawoff in the rectifying section, it is possible to provide sufficient reflux and stages in the top section of the tower to fractionate to any specification of MC in LC in the overhead. It is also possible to meet any specification on HC in the sidestream drawoff by the combination of reflux and stages in the middle tower section. The specification of MC in the bottoms can also be controlled by stages and stripping in the lower section. Figure 1 illustrates the splits that take place.

FIGURE 1

COMPONENT DISTRIBUTION FOR A
FRACTIONATION TOWER WITH A LIQUID
SIDESTREAM DRAWOFF IN THE RECTIFYING SECTION



It is only the concentration of light components, LC, that are primarily leaving the tower in the distillate, that cannot be controlled. Their concentration depends on the relative equilibrium constant values of LC and MC, and the concentration of LC in the rising vapors. However, these rising vapors must include all the moles of LC coming in with the feed and whatever is in the liquid reflux below the sidestream drawoff. (It is assumed that no LC goes out the bottoms with HC.) Therefore, a sidestream product rich in MC and very low in HC can be produced. However, pure MC cannot be produced as this system is designed. A sidestream stripper tower can be used to control the concentration of LC in the sidestream product, but this option was not considered.

Sidestream towers are difficult to control accurately. They are usually used when rough product cuts are desired.

Figure 2 illustrates the particular sidestream tower on which the fractionation calculations in this study were performed. The tower has one feed, liquid sidestream drawoff in the rectifying section, a total condenser, and a partial reboiler. The degrees of freedom or variables to be specified are expressed by the following equation:

$$DDF = NC + NTT + 10$$

where:

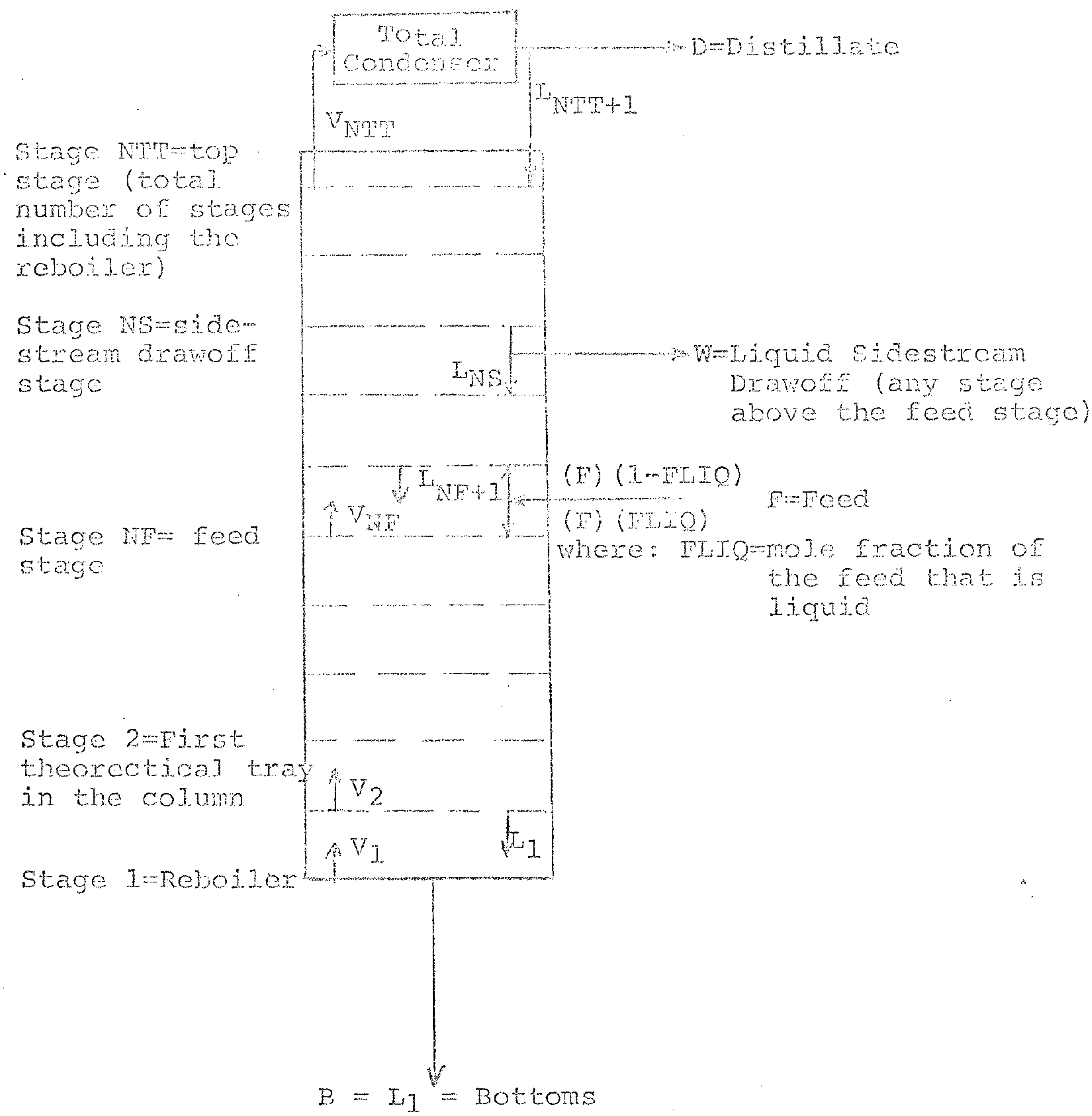
DDF = Design degrees of freedom

NC = Number of components

NTT = Number of stages

Figure 2

A Fractionation Tower
with a
Liquid Sidestream Drawoff
in the
Rectifying Section



The above equation assumes adiabatic operation except for the condenser and reboiler. The variables specified in the rigorous Thiele-Geddes program are:

Feed composition and rate	NC
Feed temperature and pressure	2
*Pressure drop per stage	NTT
Feed stage location	1
Sidestream location	1
*Condenser pressure	1
Reflux temperature (Bubble point of distillate)	1
Sidestream rate	1
Distillate rate	1
Total number of stages	1
Reflux rate	1

The program therefore only handles the "design performance" case.

The difficulty of rigorous calculation for multicomponent mixtures is that the number of variables that can be specified is very small relative to the total number of variables in the system. The number that can be specified is dictated by the design degrees of freedom for the proposed system, as shown on page 3. The number of specified variables can neither exceed nor be less than the design degrees of freedom. Once these design specifications are set, then all remaining variables are established by the restrictions of equilibrium, enthalpy, and material balance.

* The pressure drops are specified as zero in the calculation program, therefore, resulting in a constant pressure operation.

The problem is to determine the complete set of all system variables which satisfy the above restrictions and which leave the specified variables unchanged. Then with a knowledge of the values for all the variables, the ability of the proposed unit to meet all the desired specification can be reviewed by the engineer. If all specifications are not met, the values of the design variables are adjusted in the direction of the desired change in performance. If acceptable, the unit can be designed and built; or if the unit is an existing tower, the proposed operation can be reviewed to see if it is an acceptable performance.

Whenever we have a calculation in which the design variables allowed to be specified are far less in number than the total possibilities, there are two general techniques that can be used for solution:

1. Sequential Iterative Methods - Make assumptions on sufficient additional variables so that calculations can be made to determine the remaining variables. The assumed variables are then calculated from this solution and, by means of a convergence procedure, a new set of assumptions is made in an effort to bring assumed and calculated variables together. The procedure is repeated until convergence of assumed and calculated variables is obtained.
2. Matrix Methods - A complete set of equations is written to satisfy all restrictions in the system, and these equations are solved simultaneously.

Rigorous methods for all complex stage separation systems fall into either of these techniques. However, the nonlinear form of the equilibrium, heat, and material balance equations precludes a direct matrix analytical solution for fractionation systems unless some simplifications are made which convert the equations to linear form.

The Thiele-Geddes Method is of the Sequential Iterative type and it was selected as the method on which to base a short-cut procedure. The criteria for selecting the Thiele-Geddes Method were that it converges easily, it is a well established method and meets the following requirements which are necessary for a good reliable short-cut procedure:

1. A broad flexibility to solve for a variety of process models and design parameters.
2. A sound theoretical foundation - no empirical correlations.
3. Lends itself to simplification.
4. Allows itself to become "educated" by a plate-to-plate solution so that accurate parametric studies can be determined.
5. Reduces the cost of fractionation studies by permitting fast manual or computer solution.
6. Improves the engineers' understanding of the effect of key tower design variables.

The proposed short-cut procedure can be used for either an initial short-cut design, with the usual inaccuracies of trying to estimate average stripping factors, or alternatively, a force-fit can be made to a solution from a plate-to-plate calculation in order to obtain more accurate absorption or stripping factors for subsequent parametric studies on reflux, stages, etc. The simplified procedure, like the Rigorous Thiele-Geddes, is a design performance calculation.

Computer programs were developed for the Thiele-Geddes plate-to-plate method and the short-cut procedure. In addition, a computer program was written to obtain force-fit fractions required from a plate-to-plate solution to "educate" the short-cut procedure. Parametric cases were run for a five-component debutanizer column, and the accuracies of the methods were compared.

The following chapters show the equations used in the Rigorous Thiele-Geddes Method and how they can be simplified for the short-cut procedure.

THE RIGOROUS THIELE-GEDDES METHOD

The Thiele-Geddes Method for a column with a liquid side-stream in the rectifying section is based on calculating the following ratios:

$$\left(\frac{\ell}{d}\right)_{n,i} \quad \text{in the rectifying section NTT} \geq n \geq \text{NF}$$

$$\left(\frac{v}{b}\right)_{n,i} \quad \text{in the stripping section NF} \geq n \geq 1$$

where:

ℓ = Liquid flow rate of component i off stage n

v = Vapor flow rate of component i off stage n

d = Distillate flow rate of component i

b = Bottoms flow rate of component i

n = Any stage (stage 1 is the reboiler)

NF = Feed stage (Stage 1 is the reboiler)

NTT = Total number of stages including the reboiler but not the condenser.

These ratios are calculated from equations based on component balances around the stage in question and the top or bottom of the column. The top and bottom component ratios can then be solved simultaneously to give individual component rates of the distillate and bottoms.

A material balance around a total condenser (ref. Figure 1) gives the following equations:

$$v_{NTT,i} = \ell_{NTT+1,i} + d_i \tag{1}$$

$$\left(\frac{v_{NTT}}{d}\right)_i = \left(\frac{\ell_{NTT+1}}{d}\right)_i + 1 \tag{2}$$

by definition the absorption factor is:

$$A_{n,i} = \frac{L_n}{V_n K_{n,i}} \tag{3}$$

$A_{n,i}$ = Absorption factor for component i on stage n

L_n = Total liquid rate off stage n

V_n = Total vapor rate off stage n

$K_{n,i}$ = The equilibrium ratio value of component i on stage n

Multiplying both sides of equation (2) by $A_{NTT,i}$ and noting that $\left(\frac{\ell_{NTT+1}}{d}\right)_i$ is equal to the external reflux ratio (R):

$$\left(\frac{\ell}{d}\right)_{NTT,i} = A_{NTT,i}\ (R + 1) \tag{4}$$

A material balance around any stage n below the top stage (NTT) and above the sidestream drawoff stage (NS) results in the following equation:

$$v_{n,i} = \ell_{n+1,i} + d_i \tag{5}$$

Multiplying both sides of equation (5) by $A_{n,i}$ and dividing by d's:

$$\left(\frac{\ell}{d}\right)_{n,i} = A_{n,i}\left(\left(\frac{\ell}{d}\right)_{n+1,i} + 1\right) \tag{6}$$

where:

$n < NTT$

$n > NS$

NS = Sidestream drawoff stage

A material balance around the top of the column and any stage between the sidestream drawoff stage and the feed stage results in the following equation:

$$v_{n,i} = \ell_{n+1,i} + d_i + w_i \tag{7}$$

where:

w_i = Flow rate of component i in sidestream drawoff

Multiplying both sides of equation (7) by $A_{n,i}$ and dividing by d_i:

$$\left(\frac{\ell}{d}\right)_{n,i} = A_{n,i}\left(\left(\frac{\ell}{d}\right)_{n+1,i} + \left(\frac{w}{d}\right)_i + 1\right) \tag{8}$$

where:

$n \leq NS-1$ (see equation 10 for $n = NS-1$)

$N > NF$

The $\left(\frac{w}{d}\right)_i$ ratios are obtained from the following equation:

$$\left(\frac{w}{d}\right)_i = \underbrace{\left(\frac{\ell}{d}\right)_{NS,i}}_{\text{obtained from equation (6)}}\left(\frac{W}{L_{NS}}\right) \tag{9}$$

where:

W = Sidestream drawoff rate

L_{NS} = Liquid rate off the sidestream stage before the sidestream is drawn off

For the stage below the sidestream (NS-1) equation (8) is used with $\left(\frac{\ell}{d}\right)_{NS,i}$ representing the ratio after the sidestream has been drawn off to calculate $\left(\frac{\ell}{d}\right)_{NS-1,i}$. This is calculated by:

$$\underbrace{\left(\frac{\ell}{d}\right)_{NS,i}}_{\text{to be used in equation (8)}} = \underbrace{\left(\frac{\ell}{d}\right)_{NS,i}}_{\text{from equation (6)}} \left(\frac{L_{NS-W}}{L_{NS}}\right) \tag{10}$$

The stripping section is represented by a material balance around the stage in question and the bottom of the column.

$$v_{n,i} + b_i = \ell_{n+1,i} \tag{11}$$

Multiply both sides of equation (11) by $S_{n+1} = \left(\frac{VK}{L}\right)_{n+1,i}$ and dividing by b_i results in the following equation:

$$\left(\frac{v}{b}\right)_{n+1,i} = S_{n+1,i}\left(\left(\frac{v}{b}\right)_{n,i} + 1\right) \tag{12}$$

where:

$n > 1$

$n \leq NF$

The $\left(\frac{v}{b}\right)_{1,i}$ is represented by the equilibrium relationship:

$$\left(\frac{v}{b}\right)_{1,i} = \frac{V_1 y_{1,i}}{B\ X_{1,i}} = \frac{K_{1,i} V_1}{B} = S_{1,i} \tag{13}$$

Using the assumed values of stage temperatures, total liquid and total vapor rates on each stage the $\left(\frac{\ell}{d}\right)_{n,i}$ ratios in the rectifying section and the $\left(\frac{v}{b}\right)_{n,i}$ ratios in the stripping section can be calculated from the previous equations. The directions of calculations are from the bottom of the column to the feed plate and the top of the column to the feed plate.

Rearrangement of an overall material balance around the column results in the following equation:

$$d_i = \frac{(F)(z_{F,i})}{1 + \left(\frac{b}{d}\right)_i + \left(\frac{w}{d}\right)_i} \tag{14}$$

The $\left(\frac{b}{d}\right)_i$ ratio in equation (14) is obtained from the following equation which is derived from an overall material balance, and a material balance equation around the top of the column and the tray above the feed plate. A material balance around the top of the column and the tray above the feed plate (see Figure 2) results in the following equation:

$$v_{F,i} + v_{f,i} = \ell_{f+1,i} + d_i + w_i \tag{15}$$

Dividing by d_i:

$$\left(\frac{v_F}{d}\right)_i + \left(\frac{v_f}{d}\right)_i = \left(\frac{\ell_{f+1}}{d}\right)_i + 1 + \left(\frac{w}{d}\right)_i \tag{16}$$

By manipulation:

$$\left(\frac{v_F}{(F)(z_F)}\right)_i \left(\frac{(F)(z_F)}{d}\right)_i + \left(\frac{v_f}{b}\right)_i \left(\frac{b}{d}\right)_i = \left(\frac{\ell_{f+1}}{d}\right)_i + 1 + \left(\frac{w}{d}\right)_i \tag{17}$$

Rearrangement of the overall tower material balance equation gives:

$$\left(\frac{(F)(z_F)}{d}\right)_i = 1 + \left(\frac{b}{d}\right)_i + \left(\frac{w}{d}\right)_i \tag{18}$$

Substituting equation (18) into equation (17) and solving for $\left(\frac{b}{d}\right)_i$:

$$\left(\frac{b}{d}\right)_i = \frac{\left(\frac{\ell}{d}\right)_{NF+1,i} + 1 + \left(\frac{w}{d}\right)_i - \left(\frac{v_f}{(F)(X_F)}\right)_i - \left(\frac{v_F}{(F)(x_F)}\right)_i \left(\frac{w}{d}\right)_i}{\left(\frac{v_F}{(F)(X_F)}\right)_i + \left(\frac{v_f}{b}\right)} \tag{19}$$

Rearrangement of the feed balance equation gives:

$$\left(\frac{v_F}{(F)(x_F)}\right)_i + \left(\frac{\ell_F}{(F)(x_F)}\right)_i = 1 \tag{20}$$

Substituting equation (20) into (19) and simplifying results in the following equations:

$$\left(\frac{b}{d}\right)_i = \frac{\left(\frac{\ell}{d}\right)_{NF+1,i} + \left(\frac{\ell_F}{(F)(x_F)}\right)_i \left(1 + \left(\frac{w}{d}\right)_i\right)}{\left(\frac{v_F}{(F)(x_F)}\right)_i + \left(\frac{v}{b}\right)_{f,i}} \tag{21}$$

The Thiele-Geddes Method combines the restrictions of heat, equilibrium and material balance. The summation of the distillate component rates and sidestream component rates does not equal the specified distillate rate or the sidestream rate until the solution has converged. The theta convergence method is used to facilitate convergence. The theta method of convergence selects a set of d's and w's such that their sum will equal the specified distillate and sidestream rates, respectively. There are two Θ's required which are defined by the following equations:

$$d_{i'} = \frac{(F)(z_{NF,i})}{1+\left(\frac{b}{d}\right)_i \theta_d + \left(\frac{w}{d}\right)_i \theta_w} \tag{22}$$

where:

$$\sum_{i=1}^{NC} d_{i'} = D \text{ specified} \tag{23}$$

$$\sum_{i=1}^{nc} \left(\frac{w}{d}\right)_i \theta_w\, d_{i'} = \sum_{i=1}^{NC} w_{i'} = W \text{ specified} \tag{24}$$

The thetas (θ_d and θ_w) are determined by the Newton-Raphson Method. Equation 22 can be differentiated analytically for use in the Newton-Raphson Method.[1]

The component rates of the bottoms and sidestream which are normalized to the specified summations, are now found from the following equations:

$$b_{i'} = \theta_d \left(\frac{b}{d}\right)_i d_{i'} \tag{25}$$

$$w_{i'} = \theta_w \left(\frac{w}{d}\right)_i d_{i'} \tag{26}$$

Round off error is minimized by using the above equations instead of differences. The solution has converged when the thetas equal unity.

The compositions for each stage are determined by taking the (ℓ/d)'s or (v/b)'s, determined from equations (4), (6), (8), (12), and (13), and multiplying them by the respective d_i' or b_i'. The temperature profile for the next trial is determined by either dew or bubble points. The method of convergence used for bubble and dew points is the Newton Method. The liquid and vapor rates for the next trial are now determined by enthalpy balance calculated by the Constant Composition Method.[1] The enthalpy balance is calculated from the condenser down to the reboiler.

SIMPLIFYING THE THIELE-GEDDES METHOD

The Simplified Thiele-Geddes Method is based on the Thiele-Geddes plate-to-plate method. The equations developed in the next paragraph are completely rigorous.

Equations (14) and (21) are still to be used, therefore series equations are developed to obtain $\left(\frac{w}{d}\right)_i$, $\left(\frac{\ell}{d}\right)_{NF+1,i}$ and $\left(\frac{v}{b}\right)_i$. Successive substitution of equations (4) and (6) results in the following equation in terms of the component absorption factors:

$$\left(\frac{\ell}{d}\right)_{NS,i} = (R)(A_{NTT,i}) \cdot \cdot \cdot (A_{NS,i}) + (A_{NTT,i}) \cdot \cdot \cdot (A_{NS,i}) + \cdot \cdot \cdot + A_{NS} \tag{27}$$

where:

R = External reflux ratio, L_{NTT+1}/D

and:

$$\left(\frac{w}{d}\right)_i = \left(\frac{\ell}{d}\right)_{NS,i}\left(\frac{W}{L_{NS}}\right) \tag{28}$$

With successive substitution of equation (8), and remembering the restriction of equation (10) the following equation results:

$$\left(\frac{\ell}{d}\right)_{NF+1,i} = \Big((A_{NS-1,i}) \cdot \cdot \cdot (A_{NF+1,i})\Big)\underbrace{\left(\frac{\ell}{d}\right)_{NS,i}}_{\text{obtained from equation (27)}} - \left(\frac{w}{d}\right)_i + \left(1 + \left(\frac{w}{d}\right)_i\right)\Big((A_{NS-1,i})(A_{NS-2,i}) \cdot \cdot \cdot (A_{NF+1,i}) + \cdot \cdot + A_{NF+1,i}\Big) \tag{29}$$

Successive substitution of equations (13) and (12) results in the following series equation:

$$\left(\frac{v}{b}\right)_{NF,i} = (S_{NF,i})(S_{NF-1,i}) \ . \ . \ . \ (S_1) + (S_{NF}) \ . \ . \ . \ (S_2) + \ . \ . \ . + (S_{NF,i})\cdot(S_{NF-1}) + S_{NF} \qquad (30)$$

The simplified approach to the Thiele-Geddes Method divides the column into three sections defined by equations (27), (29), and (30). The first step in the simplification of the Rigorous Thiele-Geddes Method involves the elimination of bubble or dew point calculations for each tray. Only the solutions of the end temperatures of the three tower sections are considered. The problem then becomes one of finding the representative stripping or absorption factors for each tower section.

Five temperatures are calculated for each trial. These temperatures are assumed for the initial trial. These temperatures and their methods of determination are:

1. Top tray temperature (TT) - dew point of the overhead vapor (same composition as the distillate).
2. Sidestream tray temperature (TS) - bubble point of the side-stream product.
3. Bottom tray temperature (T1) - bubble point of the bottoms.
4. Second stage temperature (T2) - T_1, V_1, B, and L_2 are known along with their compositions. The composition of L_2 is obtained by material balance. The bubble point of L_2 is therefore T2.

5. Feed plate temperature (TF) - this is the "slack" temperature used to converge the solution.

The reasons why these temperatures are calculated will become evident in the following paragraphs. The end temperatures for the middle tower section should be the tray temperature below the sidestream tray temperature, and the tray temperature above the feed tray. It was first attempted to estimate their values by linear interpolation between TS and TF. The increase in accuracy did not seem to justify pursuing this method further. Therefore TS and TF are used as the end temperatures for the middle section.

Constant molal overflow was used to set internal liquid and vapor flow rates. Absorption or stripping factors for the ends of each tower section are determined by combining the equilibrium constant values with the respective liquid and vapor rates. The reboiler stripping and condenser absorption factors are solved for separately, since these are quite different from the values in the adjacent tower section. The absorption factor for the total condenser is the external reflux ratio.

The core of this simplified fractionation procedure is, therefore, the calculation of only five temperatures, the assumption of constant molal overflow in calculating absorption or stripping factors, and the solution of forms of equations (27), (28), (29), and (30).

One method for solving equations (27), (28), (29), and (30) is to assume a linear profile of absorption or stripping factors between the calculated end values. This constitutes the stand-alone version of the calculation. With this approach the calculation procedure is as follows:

1. $A_{NTT,i} = \dfrac{(L3)}{(V3)(K_{TT,i})}$

where:

$L3 = (R)(D)$

$V3 = (R)(D) + D$

2. $A_{NS,i} = \dfrac{(L3)}{(V3)(K_{TS,i})}$

3. Solve equation (27) for $\left(\dfrac{\ell}{d}\right)_{NS,i}$ using a linear interpolation for the A's between $A_{NTT,i}$ and $A_{NS,i}$.

4. $\left(\dfrac{w}{d}\right)_i = \left(\dfrac{\ell}{d}\right)_{NS,i}\left(\dfrac{W}{L_{NS}}\right)$

where:

$L_{NS} = (R)(D) + D$

5. $A_{NS-1,i} = \dfrac{L2}{(V2)(K_{TS,i})}$

where:

$L2 = (R)(D) - W$

$V2 = V3 = (R)(D) + D$

6. $A_{NF+1,i} = \dfrac{L2}{(V2)(K_{TF,i})}$

7. Linearly interpolate for the intermediate A's for the middle tower section and solve equation (29) for $\left(\frac{\ell}{d}\right)_{NF + 1,i}$

8. $S_{1,i} = \frac{(K_{T1,i})(V1) - (F)(1 - FLIQ)}{B}$

where:

FLIQ = mole fraction of the feed that is liquid

$V1 = (R)(D) + D-(F)(1 - FLIQ)$

where:

$L1 = V1 + B$

9. $S_{2,i} = \frac{(K_{T2})(V1)}{L1}$

10. $S_{NF,i} = \frac{(K_{NF,i})(V1)}{L1}$

11. Linearly interpolate for intermediate S's and solve equation (3) for $\left(\frac{v}{b}\right)_{NF,i}$

12. Solve equation (21) for $\left(\frac{b}{d}\right)_i$.

13. Solve a modified form of equation (14) for d_i using Θ_W which is initially unity.

$$d_i = \frac{(F)(z_i)}{1 + \left(\frac{b}{d}\right) + \left(\frac{w}{d}\right)_i \Theta_w} \tag{31}$$

where:

Θ_w is a forcing factor which is required to have the calculated sidestream rate equal the specified sidestream rate.

14. Solve for θ_w

$$\theta_w = \frac{\sum_{i=1}^{NC} w_i}{W} = \frac{\sum_{i=1}^{NC} \left(\frac{w}{d}\right)_i d_i}{W}$$

15. Solve equation (31) using the calculated value of θ_w.

16. Determine the compositions on the four key locations by multiplying the appropriate $(\ell/d)_i$ by d_i or $(v/b)_i$ by b_i.

17. Solve for the four equilibrium temperatures T1, T2, TS, and TT, using the appropriate location compositions.

18. Go back to step 1 and repeat until the assumed temperatures (T1, T2, TS, and TT) equal the calculated temperatures for a given trial.

19. If $\sum_{i=1}^{NC} d_i$ from step 13 equal the calculated distillate rate the solution has converged. If they are not equal assume a new TF and return to step 1. Standard linear interpolation procedure on distillate rate and TF is used to converge TF.

Another method of solving equations (27), (29), and (30) is to define an average absorption or stripping factor for each equation. Equation (27) becomes:

$$\left(\frac{\ell}{d}\right)_{NS,i} = \left(\frac{A3_{ave,i}^{(NTT-NS)} - A3_{ave,i}}{A3_{ave,i} - 1} + (R)\left(A3_{ave,i}^{(NTT-NS-1)}\right)\right) \qquad (32)$$

where:

$A3_{ave,i}$ . . . "average" absorption factor of component i in the upper tower section.

Equation (29) becomes:

$$\left(\frac{\ell}{d}\right)_{NF+1,i} = \left(A2_{ave,i}^{(NS-NF+1)}\right)\left(\left(\frac{\ell}{d}\right)_{NS,i} - \left(\frac{v}{d}\right)_i\right) + \frac{\left(1 + \left(\frac{w}{d}\right)_i\right)\left(A2_{ave,i}^{(NS-NF)} - A2_{ave,i}\right)}{\left(A2_{ave,i} - 1\right)} \qquad (33)$$

where:

$A2_{ave,i}$ . . . "average" absorption factor of component i in the middle tower section.

Equation (30) becomes:

$$\left(\frac{v}{b}\right)_{NF,i} = \frac{\left(S1_{ave,i}^{(NF)} - S1_{ave,i}\right)}{\left(S1_{ave,i} - 1\right)} + \left(S_{1,i}\right)\left(S1_{ave,i}^{(NF-1)}\right) \qquad (34)$$

where:

$S1_{ave,i}$ . . . "average" stripping factor of component i in the stripping section.

Since constant molal overflow is used in the simplified calculation procedure equation (32) equates to:

$$\left(\frac{w}{d}\right)_{NS,i} = \left(\frac{W}{(R)(D)}\right)\left(\frac{A3_{ave,i}^{(NTT-NS)} - A3_{ave,i}}{A3_{ave,i} - 1} + (R)\left(A3_{ave,i}^{(NTT-NS-1)}\right)\right) \qquad (35)$$

and:

$$\left(\frac{\ell}{d}\right)_{NS,i} = \left(\frac{w}{d}\right)_{NS,i} \frac{(R)(D)}{(W)} \qquad (36)$$

One method of finding $A3_{ave,i}$, $A2_{ave,i}$, and $S1_{ave,i}$ would be to take the arithmetic average of the respective tower section end values of absorption or stripping factors. It has been shown in the earlier unpublished work by Dr. Cecchetti on simple towers that the accuracy obtained by using arithmetic average values for stripping or absorption factors is less than if a linear profile were assumed between the end absorption or stripping factors.

The best way to determine the "average" absorption or stripping factors is to obtain definitive "average" fractions for each component that reproduce the rigorous plate-to-plate solution exactly for a "base" case. These fractions can then be used to make parametric studies at other tower conditions. First, the fractions describing where the "average" absorption or stripping factors lie need to be defined.

Upper tower section:

$$FRAC3_i = \frac{A3_{ave,i}}{\frac{(L3)}{(V3)(K_{TT,i})} - \frac{(L3)}{(K_{TS,i})(V3)}} \tag{37}$$

Middle tower section:

$$FRAC2_i = \frac{A2_{ave,i} - \frac{(L2)}{(K_{TF,i})(V2)}}{\frac{(L2)}{(V2)(K_{TS,i})} - \frac{(L2)}{(K_{TF,i})(V2)}} \tag{38}$$

Lower tower section:

$$FRAC1_i = \frac{S1_{ave,i} - \frac{(K_{TF,i})(V1)}{(L1)}}{\frac{(K_{T2,i})(V1)}{(L1)} - \frac{(K_{TF,i})(V1)}{(L1)}} \tag{39}$$

The $\left(\frac{w}{d}\right)_i$, $\left(\frac{\ell}{d}\right)_{NF+1,i}$, and $\left(\frac{v}{b}\right)_{NF,i}$ ratios from the Rigorous Thiele-Geddes solution are inserted into the appropriate equations to solve for $A3_{ave,i}$, $A2_{ave,i}$, and $S1_{ave,i}$. Equations (33), (34), and (35) are solved by a trial and error procedure for $A3_{ave,i}$, $A2_{ave,i}$, and $S1_{ave,i}$, respectively. The half-interval method of convergence is used, with the rigorous absorption or stripping factors as limits for the respective tower section end values.

The fractions are next determined using equations (37), (38), and (39). These fractions usually lie between zero and unity, but they can be negative due to the fact that the end values of the absorption or stripping factors used in equations (33), (34), and (35) are based on constant molal overflow. These fractions when used in the simplified Thiele-Geddes Method reproduce the rigorous solution within any desired tolerance convergence on $\left(\frac{w}{d}\right)_i$, $\left(\frac{\ell}{d}\right)_{NF+1,i}$, and $\left(\frac{V}{b}\right)_{NF,i}$.

The real benefit of using force-fit fractions ($FRAC3_i$, $FRAC2_i$, $FRAC1_i$) is that parametric cases can then be run with a high degree of accuracy. The calculation procedure for the parametric cases, obtains the $A3_{ave,i}$, $A2_{ave,i}$, and $S1_{ave,i}$ from the following equations:

$$A3_{ave,i} = (FRAC3_i)\ \frac{(L3)}{(V3)(K_{TT,i})} - \frac{(L3)}{(V3)(K_{TS,i})} + \frac{(L3)}{(V3)(K_{TS,i})} \qquad (40)$$

$$A2_{ave,i} = (FRAC2_i)\ \frac{(L2)}{(V2)(K_{TS,i})} - \frac{(L2)}{(V2)(K_{TF,i})} + \frac{(L2)}{(V2)(K_{TF,i})} \qquad (41)$$

$$S1_{ave,i} = (FRAC1_i)\ \frac{(V1)(K_{T2,i})}{(L1)} - \frac{(K_{TF,i})(V1)}{(L1)} + \frac{(K_{TF,i})(V1)}{(L1)} \qquad (42)$$

The calculation procedure for the Force-Fit Thiele-Geddes Method is essentially the same as that for the Stand-Alone Simplified Thiele-Geddes shown on pages 20 to 23. The difference between the two methods are the equations used for the component ratios $\left(\frac{\ell}{d}\right)_{NF+1,i}$, $\left(\frac{w}{d}\right)_i$ and $\left(\frac{v}{b}\right)_i$. The equations to be used for the Force-Fit Thiele-Geddes Method are (33), (34), (35), (36), (37), (38), and (39).

DISCUSSION OF RESULTS

Table 1 on the following page summarizes the cases that were investigated using three calculation methods. The three calculation methods are: (1) Rigorous Thiele-Geddes Method, (2) Stand-Alone Simplified Thiele-Geddes Method, (3) Force-Fit Thiele-Geddes Method. Computer programs were written to carry out these investigations. A total of six debutanizer column cases was studied. Case 1 was selected as the base case from which the force-fit fractions were extracted for use with the Force-Fit Thiele-Geddes Method for the other five cases.

Tables 3 through 8 tabulate the results for these six cases using the three calculation methods. The force-fit fractions which would be required to duplicate the rigorous base case solution may be found in Table 2. The accuracy of the Force-Fit Thiele-Geddes Method is considerably better than the Stand-Alone Simplified Thiele-Geddes Method, with the exception of case number three, which has a reflux ratio considerably higher than that used in the base case. It is apparent that in this instance the force-fit fractions extended into a region which is beyond the accuracy of the method.

Temperatures calculated for the distillate, bottoms, and sidestreams were within 2° or better of the rigorous solution values for the Stand-Alone Simplified Thiele-Geddes Method and within 0.5° for the Force-Fit Thiele-Geddes Method (except case 3). Compositions were within 0.3 moles for the Stand-Alone and 0.1 moles for the Force-Fit.

Table 1

Tower Case Studies

Fixed Variables

Feed, Mole %

C_3	5	
iC_4	15	
nC_4	25	- Light Key
iC_5	20	- Heavy Key
nC_5	35	

Liquid Feed at its bubble point of 181.6°F
Fixed Feed Rate of 100 moles/hr.
Fixed Tower Pressure (120 psia)
Total Condenser
Side Stream Drawoff Rate = 10 moles/hr.

Case #	Parametric Variables	Reflux Ratio	Distillate Rate (moles/hr)	Number of Stages*	Feed Stage*	Side Stream Drawoff Stage*
1	Base	2.0	30	10	5	8
2	High Reflux	2.5	30	10	5	8
3	High Reflux	3.0	30	10	5	8
4	Low Distill-ate	2.0	25	10	5	8
5	High Stages	2.0	30	11	6	9
6	Low Feed Stage	2.0	30	10	8	4

*Stage 1 is the reboiler

Table 2

Case 1

Parametric Variable:

Reflux Rate:-------------------- 2
Distillate Rate:----------------30
Number of Stages----------------10
Feed Stages:-------------------- 5
Side Stream Drawoff Stage:------ 8

Force Fit Fraction From Rigorous Solution

Component Number	Top Tower Section	Middle Tower Section	Bottom Tower Section
1	.2850	-0.4872	.1037
2	.3038	-0.3804	.1322
3	.3160	-0.3371	.1311
4	.3551	-0.2907	.0397

Table 3

Case 1

Parametric Varialbe:
Reflux Rate:------------------- 2
Distillate Rate:---------------30
Number of Stages:--------------10
Feed Stage:-------------------- 5
Side Stream Drawoff Stage:---- 8

Com-po-nent No.	Distillate Mole Fraction	Distillate Moles/Hour	Temp °F	Bottoms Mole Fraction	Bottoms Moles/Hour	Temp °F	Side Streams Mole Fraction	Side Streams Moles/Hour	Temp °F	Calculation Method Used
1	.1530	4.59		.0017	.10		.0307	.31		
2	.3370	10.11	153.1	.0501	3.01	213.3	.1885	1.89	174.2	Rigorous
3	.4254	12.76		.1436	8.61		.3623	3.62		Thiele-
4	.0485	1.46		.2777	16.67		.1880	1.88		Geddes
5	.0361	1.08		.5269	31.61		.2305	2.30		
	1.0000	30.00		1.0000	60.00		1.0000	10.00		
1	.1534	4.60		.0016	.09		.0302	.30		Stand-Alone
2	.3405	10.21	152.2	.0478	2.87	213.9	.1918	1.92	173.4	Simplified
3	.4286	12.86		.1403	8.42		.3724	3.72		Thiele-
4	.0451	1.35		.2800	16.80		.1846	1.85		Geddes
5	.0324	.97		.5303	31.82		.2210	2.21		
	1.0000	30.00		1.0000	60.00		1.0000	10.00		
1	.1530	4.59	153.1	.0017	.10	213.3	.0307	.31	174.2	Force-Fit
2	.3370	10.11		.0501	3.01		.1885	1.89		Thiele-
3	.4254	12.76		.1436	8.61		.3623	3.62		Geddes
4	.0485	1.46		.2777	16.67		.1880	1.88		
5	.0361	1.08		.5269	31.61		.2305	2.30		
	1.0000	30.00		1.0000	60.00		1.0000	10.00		

Table 4

Case 2

Parametric Variable:
- Reflux Rate:------------------2.5
- Distillate Rate-----------------30
- Number of Stages----------------10
- Feed Stage-----------------------5
- Side Stream Drawoff Stage--------8

Com- po- nent No.	Distillate Mole Fraction	Distillate Moles/ Hour	Distillate Temp °F	Bottoms Mole Fraction	Bottoms Moles/ Hour	Bottoms Temp °F	Side Streams Mole Fraction	Side Streams Moles/ Hour	Side Streams Temp °F	Calculation Method Used
1	.1544	4.63	149.9	.0012	.07	215.3	.0294	.29	170.3	
2	.3476	10.43		.0425	2.55		.2018	2.02		Rigorous
3	.4358	13.08		.1320	7.92		.4005	4.01		Thiele-
4	.0373	1.12		.2859	17.15		.1732	1.73		Geddes
5	.0248	.74		.5384	32.31		.1951	1.95		
	1.0000	30.00		1.0000	60.00		1.0000	10.00		
1	.1547	4.64	149.0	.0011	.07	215.9	.0290	.29	169.5	Stand-Alone
2	.3509	10.53		.0401	2.41		.2066	2.07		Simplified
3	.4380	13.16		.1284	7.70		.4140	4.14		Thiele-
4	.0340	1.02		.2885	17.31		.1673	1.67		Geddes
5	.0218	.65		.5419	32.52		.1831	1.83		
	1.0000	30.00		1.0000	60.00		1.000	10.00		
1	.1544	4.63	150.1	.0012	.07	215.2	.0296	.30	171.0	Force-Fit
2	.3473	10.42		.0420	2.57		.2012	2.01		Thiele-
3	.4349	13.05		.1330	7.98		.3975	3.97		Geddes
4	.0379	1.14		.2853	17.12		.1741	1.74		(Based on Case 1)
5	.0255	.76		.5376	32.26		.1976	1.98		
	1.0000	30.00		1.0000	60.00		1.0000	10.00		

Table 5

Case 3

Parametric Variable:

Reflux Rate:--------------------3
Distillate Rate-----------------30
Number of Stages----------------10
Feed Stage----------------------5
Side Stream Drawoff Stage-------8

Com-po-nent No.	Distillate Mole Fraction	Distillate Moles/Hour	Distillate Temp °F	Bottoms Mole Fraction	Bottoms Moles/Hour	Bottoms Temp °F	Side Streams Mole Fraction	Side Streams Moles/Hour	Side Streams Temp °F	Calculation Method Used
1	.1554	4.66	147.2	.0008	.05	217.3	.0287	.24	166.6	
2	.3571	10.71		.0350	2.10		.2187	2.19		Rigorous
3	.4439	13.32		.1204	7.22		.4460	4.46		Thiele-
4	.0274	.82		.2945	17.67		.1511	1.51		Geddes
5	.0162	.49		.5493	32.96		.1555	1.55		
	1.0000	30.00		1.0000	60.00		1.0000	10.00		
1	.1556	4.67	147.1	.0008	.05	217.5	.0282	.28	166.6	Stand-Alone
2	.3578	10.73		.0347	2.08		.2186	2.19		Simplified
3	.4442	13.33		.1198	7.19		.4482	4.48		Thiele-
4	.0267	.80		.2949	17.69		.1507	1.51		Geddes
5	.0157	.47		.5498	32.99		.1543	1.54		
	1.0000	30.00		1.0000	60.00		1.0000	10.00		
1	.1554	4.66	148.1	.0009	.05	216.7	.0287	.29	168.3	Force-Fit
2	.3544	10.63		.0375	2.25		.2119	2.12		Thiele-
3	.4407	13.22		.1250	7.50		.4280	4.28		Geddes
4	.0305	.92		.2913	17.48		.1602	1.60		(Based on Case 1)
5	.0190	.57		.5453	32.72		.1714	1.71		
	1.0000	30.00		1.0000	60.00		1.0000	10.00		

Table 6

Case 4

Parametric Variable:
- Reflux Rate:----------------------2
- Distillate Rate-----------------25
- Number of Stages---------------10
- Feed Stage-----------------------5
- Side Stream Drawoff Stage------8

Component No.	Distillate Mole Fraction	Distillate Moles/Hour	Temp °F	Bottoms Mole Fraction	Bottoms Moles/Hour	Temp °F	Side Streams Mole Fraction	Side Streams Moles/Hour	Temp °F	Calculation Method Used
1	.1774	4.43	150.2	.0031	.20	208.2	.0365	.37	171.7	
2	.3429	8.57		.0680	4.42		.2004	2.00		Rigorous
3	.4058	10.15		.1725	11.21		.3645	3.65		Thiele-
4	.0424	1.06		.2640	17.16		.1781	1.78		Geddes
5	.0315	.79		.4924	32.01		.2205	2.20		
	1.0000	25.00		1.0000	65.00		1.0000	10.00		
1	.1806	4.51	148.4	.0018	.12	209.3	.0369	.37	169.7	Stand-Alone
2	.3520	8.80		.0629	4.09		.2114	2.11		Simplified
3	.4046	10.11		.1706	11.09		.3799	3.80		Thiele-
4	.0366	.92		.2676	17.39		.1685	1.69		Geddes
5	.0262	.66		.4971	32.31		.2033	2.03		
	1.0000	25.00		1.0000	65.00		1.0000	10.00		
1	.1799	4.50	150.3	.0020	.13	208.3	.0370	.37	172.2	Force-Fit
2	.3459	8.65		.0668	4.34		.2010	2.01		Thiele-
3	.3988	9.97		.1765	11.47		.3559	3.56		Geddes
4	.0419	1.05		.2647	17.21		.1745	1.74		(Based on Case 1)
5	.0335	.84		.4900	31.85		.2316	2.32		
	1.0000	25.00		1.0000	65.00		1.0000	10.00		

Table 7

Case 5

Parametric Variable:
- Reflux Rate:-------------------------2.0
- Distillate Rate---------------------30
- Number of Stages-------------------11
- Feed Stage--------------------------6
- Side Stream Drawoff Stage-----------9

Component No.	Distillate Mole Fraction	Distillate Moles/Hour	Distillate Temp °F	Bottoms Mole Fraction	Bottoms Moles/Hour	Bottoms Temp °F	Side Streams Mole Fraction	Side Streams Moles/Hour	Side Streams Temp °F	Calculation Method Used
1	.1543	4.63	152.1	.0010	.06	214.1	.0314	.31	172.8	
2	.3426	10.28		.0461	2.77		.1958	1.96		Rigorous
3	.4252	12.7		.1421	8.53		.3716	3.72		Thiele-
4	.0449	1.35		.2807	16.84		.1810	1.81		Geddes
5	.0330	.99		.5301	31.81		.2202	2.20		
	1.0000	30.00		1.0000	60.00		1.0000	10.00		
1	.1545	4.63	151.0	.0009	.06	214.7	.0309	.31	171.7	Stand-Alone
2	.3464	10.39		.0434	2.60		.2001	2.00		Simplified
3	.4287	12.86		.1383	8.30		.3839	3.84		Thiele-
4	.0412	1.24		.2834	17.00		.1763	1.76		Geddes
5	.0292	.88		.5340	32.04		.2088	2.09		
	1.0000	30.00		1.0000	60.00		1.0000	10.00		
1	.1543	4.63	152.2	.0010	.06	214.0	.0313	.31	173.0	Force-Fit
2	.3419	10.26		.0466	2.80		.1948	1.95		Thiele-
3	.4248	12.74		.1427	8.56		.3698	3.70		Geddes
4	.0455	1.36		.2803	16.81		.1822	1.82		Method
5	.0335	1.01		.5295	31.77		.2219	2.21		(Based on Case 1)
	1.0000	30.00		1.0000	60.00		1.0000	10.00		

Table 8

Case 6

Parametric Variable:

- Reflux Rate--------------------2
- Distillate Rate---------------30
- Number of Stages-------------10
- Feed Stage----------------------3
- Side Stream Drawoff Stage-----4

Component No.	Distillate Mole Fraction	Distillate Moles/Hour	Distillate Temp °F	Bottoms Mole Fraction	Bottoms Moles/Hour	Bottoms Temp °F	Side Streams Mole Fraction	Side Streams Moles/Hour	Side Streams Temp °F	Calculation Method Used
1	.1508	4.53	154.1	.0029	.13	212.4	.0299	.30	175.5	
2	.3304	9.91		.0546	3.27		.1812	1.81		Rigorous
3	.4273	12.82		.1438	8.63		.3552	3.55		Thiele-
4	.0533	1.60		.2734	16.40		.1996	2.00		Geddes
5	.0382	1.14		.5253	31.52		.2341	2.34		
	1.0000	30.00		1.0000	60.00		1.0000	10.00		
1	.1515	4.54	152.8	.0027	.16	213.2	.0295	.29	174.2	Stand-Alone
2	.3346	10.04		.0517	3.10		.1858	1.86		Simplified
3	.4317	12.95		.1394	8.37		.3686	3.69		Thiele-
4	.0489	1.47		.2763	16.53		.1954	1.95		Geddes
5	.0333	1.00		.5299	31.79		.2207	2.21		
	1.0000	30.00		1.0000	60.00		1.0000	10.00		
1	.1509	4.53	153.9	.0029	.17	212.5	.0300	.30	175.3	Force-Fit
2	.3310	9.93		.0542	3.25		.1819	1.82		Thiele-
3	.4275	12.83		.1435	8.61		.3565	3.56		Geddes
4	.0529	1.58		.2737	16.43		.1999	1.99		(Based on Case 1)
5	.0377	1.13		.5257	31.54		.2327	2.33		
	1.0000	30.00		1.0000	60.00		1.0000	10.00		

CONCLUSIONS

The Simplified Thiele-Geddes Methods make possible rapid, accurate screening calculations. The Force-Fit Thiele-Geddes Method is well suited for parametric studies around a rigorous solution. The degree of accuracy that can be obtained from the Force-Fit Thiele-Geddes Method is believed to be the highest available from a short-cut procedure. Reduced costs for fractionation studies and a better engineering understanding of the effort of key tower design variables, are the principle assets of these methods.

It should be emphasized that the Force-Fit Thiele-Geddes Method is not limited by the constant molar overflow assumption used in the development of the simplified equations. The force-fit fractions take into account deviations from constant molar overflow by force fitting the rigorous solution. The force-fit also takes into consideration any composition effects which were used in the basic data for the plate-to-plate procedure.

RECOMMENDATIONS

The simplified fractionation procedure based on the Thiele-Geddes Method can be adapted for any type of tower with a two-phase system. This can be accomplished by developing modular calculation blocks for each type of tower section.

An improved convergence procedure using the theta method for complex towers could facilitate convergence. This short-cut fractionation procedure requires investigation for towers with very nonideal systems such as extraction, extractive distillation, and azeotropic distillation.

The equations used in the simplified fractionation procedure are fundamentally sound, and improvements can be made only for methods for estimating the average absorption or stripping factors. It may be possible to develop a method for adjusting force-fit fractions to give more accurate answers for parametric cases. The distribution curve of the average absorption or stripping fraction as a function of the absorption or stripping factor at the respective tower end values could provide a basis for improving the force-fit method.

Graphical methods can be developed for each type of tower section thus permitting easy hand calculations. Work using graphical methods has been done by Dr. Ralph Cecchetti an adjunct professor at Newark College of Engineering. His work has not yet been published.

NOMENCLATURE

$A_{n,i}$	Absorption factor on stage n for component i $A_{n,i} = \frac{L_n}{V_n L_{n,i}}$
$A3_{ave,i}$	"Average" absorption factor of component i in the upper tower section
$A2_{ave,i}$	"Average" absorption factor of component i in the upper tower section
B	Bottom molar flow rate
b_i	Molar flow rate of component i in the bottoms
D	Molar distillate flow rate
d_i	Molar flow rate of component in in the distillate
di'	Molar flow rate of component in in the distillate calculated by use of the theta convergence method
DDF	Design degrees of freedom
F	Molar feed flow rate
FLIQ	Mole fraction of the feed that is liquid
$FRAC3_i$	Fraction describing $A3_{ave,i}$
$FRAC2_i$	Fraction describing $A2_{ave,i}$
$FRAC1_1$	Fraction describing $S1_{ave,i}$
$H_{t,i}$	Vapor enthalpy at temperature t of component i
HC	Heavy component
$h_{t,i}$	Liquid enthalpy of temperature t of component i
i	Subscript designating component i
$K_{n,i}$	Equilibrium constant on stage n for component i $K_{n,i} = \frac{Y_{n,i}}{x_{n,i}}$

$K_{t,i}$	Equilibrium constant of temperatures t for component i
L_n	Total molar liquid rate off stage n
L_{NS}	Liquid molar rate off the sidestream stage before the sidestream is drawn off
L1	Liquid molar flow rate in the lower tower section based on constant molal overflow
L2	Liquid molar flow rate in the middle tower section based on constant molal overflow
L3	Liquid molar flow rate in the upper tower section based on constant molal overflow
$\ell_{F,i}$	Liquid molar flow rate of component i in the feed
$\ell_{n,i}$	Liquid molar flow rate off stage n of component i
LC	Light component
NTT	Number of stages including the reboiler but not the condenser
NF	Feed stage
NS	Sidestream drawoff stage
R	External reflux ratio ($L_{NTT} + 1/D$)
$S_{n,i}$	Stripping factor on stage n for component i $S_{n,i} = \frac{V_n K_{n,i}}{L_n}$
$S1_{ave,i}$	"Average" stripping factor of component i in the stripping section
T1	Bottom (reboiler) tray temperature
T2	Second stage (tray above the reboiler) temperature
TF	Feed tray temperature
TS	Sidestream tray temperature
TT	Top tray temperature
V	Total molar vapor rate off stage n

V1	Vapor molar flow rate in the lower tower section based on constant molal overflow
V2	Vapor molar flow rate in the middle tower section based on constant molal overflow
V3	Vapor molar flow rate in the upper tower section based on constant molal overflow
$v_{F,i}$	Molar vapor flow rate of component i in the feed
$v_{n,i}$	Molar vapor flow rate off stage n of component i
W	Molar sidestream flow rate
w_i	Molar flow rate of component i in the sidestream
wi'	Molar flow rate of component i in the sidestream calculated by the theta convergence method
$x_{n,i}$	Liquid mole fraction on stage n of component i
$x_{F,i}$	Mole fraction of component i in the feed (regardless of vapor or liquid)
$y_{n,i}$	Vapor mole fraction on stage n of component i
$z_{n,i}$	Mole fraction of component i in composite feed.

APPENDIX

APPENDIX A

Main Program for the Rigorous Thiele-Geddes Method

```
      DIMENSION A(5),B(5),C(5),D(5),E(5),X(5),XL(5),XV(5)
     1,VOB(5)       ,WOD(5),T(16),AAL(16),VV(16),RAT(5,16),BOD(5),ALB(5)
      COMMON A,B,C,D,E    ,
     1      A1(5),B1(5),C1(5),D1(5),E1(5),A2(5),B2(5),C2(5),D2(5),E2(5)
      AK(AA,BB,CC,DD,EE,TT)=AA+TT*(BB+TT*(CC+TT*(DD+TT*EE)))
   76 READ(2,100)  NC,NTT,NS,NF
      READ(2,101) (A(I),B(I),C(I),D(I),E(I),I=1,NC)
      WRITE(3,700)
  700 FORMAT (///,20X,'K DATA CONSTANTS(K=A+BT+CTT+DTTT+ETTT)', /3X,
     1'COMPONENT NUMBER(I)', 4X,'A(I)')
      WRITE(3,301)
  301 FORMAT(1H1,8X,'**DISTILLATION PROGRAM**',/8X,'**THIELE-GEDDES METHO
     1D**',///,3X,'**NOTE**TRAYS ARE NUMBERED FROM THE BOTTOM WITH THE R
     1EBOILER BEING TRAY NUMBER 1')
  302 FORMAT(6X,'DISTILLATE RATE(MOLES/HR)=',F11.5,/6X,'SIDE STREAM RATE
     1(MOLES/HR)=',F11.5,/6X,'REFLUX RATIO=',F11.5,/6X,'FEED RATE(MOLES/
     1HR)=',F11.5)
      WRITE(3,701) (I,A(I),B(I),C(I),D(I),E(I),I=1,NC)
  701 FORMAT(3X,I3,5E18.8)
      READ(2,102) (X(I) ,XL(I),XV(I), I=1,NC)
      READ(2,102) F,DDD,R,S,FLIQ,TF
      WRITE(3,302) DDD,S,R,F
      NN=NTT+1
      READ(2,102) (T(I),I=1,NN )
      WRITE(3,300)  NC,NTT,NS,NF
  300 FORMAT(1H1,12X,'INPUT SPECIFICATIONS',/3X,'***NOTE TRAY 1 IS THE R
     1EBOILER***',/6X,'NUMBER OF COMPONENTS=',  10X,I3,/6X,'NUMBER OF TR
     2AYS (INCLUDING THE REBOILER)=',2X,I3,/6X,'SIDE STREAM PLATE NUMBER
     3=',8X   ,I3,/6X,'FEED TRAY NUMBER=',8X,I3)
  100 FORMAT(4I5)
  101 FORMAT(5E15.9)
  102 FORMAT(8F10.0)
      THETD=.5
      THETW=.5
      ITN=0
      KEY=0
      AAL(1)=F-DDD-S
      AAL(NTT+1)=R*DDD
      VV(NTT)=DDD+AAL(NTT+1)
      J=NF-1
      DO 30 I=1,J
      VV(I)=VV(NTT)-F*(1.-FLIQ)
   30 AAL(I+1)=AAL(NTT+1)-S+F*FLIQ
      J=NS-2
      DO 31 I=NF,J
      VV(I)=VV(NTT)
```

```
   31 AAL(I+1)=AAL(NTT+1)-S
      J=NTT-1
      NN=NS-1
      DO 32 I=NN,J
      VV(I)=VV(NTT)
   32 AAL(I+1)=AAL(NTT+1)
   72 DO 1 I=1,NC
    1 RAT(I,NTT+1)=R
      NN=NTT-NS+1
      DO 2 J=1,NN
      N=NTT+1-J
      DO 2 I=1,NC
      AK1=AK( A(I),B(I),C(I),D(I),E(I),T(N) )
    2 RAT(I,N)=AAL(N)*(RAT(I,N+1)+1.)/(VV(N)*AK1)
      DO 4 I=1,NC
      WOD(I)=RAT(I,NS)*S/AAL(NS)
    4 RAT(I,NS)=RAT(I,NS)-WOD(I)
      NN=NS-NF-1
      DO 3 J=1,NN
      N=NS-J
      DO 3 I=1,NC
      AK1=AK( A(I),B(I),C(I),D(I),E(I),T(N))
    3 RAT(I,N)=AAL(N)*(RAT(I,N+1)+WOD(I)+1.)/(VV(N)*AK1)
      DO 6 I=1,NC
      AK1=AK(A(I),B(I),C(I),D(I),E(I),T(1))
    6 RAT(I,1)=AK1*VV(1)/AAL(1)
      DO 5 J=2,NF
      DO 5 I=1,NC
      AK1=AK(A(I),B(I),C(I),D(I),E(I),T(J))
    5 RAT(I,J)=AK1*VV(J)*(RAT(I,J-1)+1)/AAL(J)
C     CALCULATE B/D'S
      DO 7 I=1,NC
    7 BOD(I)=(RAT(I,NF+1)+XL(I)/(F*X(I))   *(1.+WOD(I)))/
     1(RAT(I,NF)+XV(I)/(F*X(I)))
   45 SUM=0.
      SUM1=0.
      SUM2=0.
      SUM3=0.
      SUM4=0.
      SUM5=0.
      DO 13 I=1,NC
      SS=F*X(I)/(1.+THETD*BOD(I)+THETW*WOD(I))
      SUM=SUM+SS
      SUM3=SS*THETW*WOD(I)+SUM3
      SS=          F*X(I)/(1.+(THETD+.001)*BOD(I)+THETW*WOD(I))
      SUM1=SUM1+SS
      SUM4=SS*THETW*WOD(I)+SUM4
      SS=          F*X(I)/(1.+THETD*BOD(I)+(THETW+.001)*WOD(I))
      SUM5=SS*(THETW+.001)*WOD(I)+SUM5
   13 SUM2=SUM2+SS
      IF(ABS(SUM-DDD)/DDD-.00001   ) 49,49,48
   49 IF(ABS(S-SUM3)/S-.00001) 47,47,48
   48 F1X=(SUM1-SUM)/.001
      F1Y=(SUM2-SUM)/.001
      F2X=(SUM4-SUM3)/.001
      F2Y=(SUM5-SUM3)/.001
      THE=         (F2X*(SUM-DDD)-F1X*(SUM3-S))/(F2Y*F1X-F2X*F1Y)
      THETW=THE+THETW
```

```
      THETD=THETD-((SUM-DDD)+F1Y*THE )/F1X
      WRITE(3,969) THETD,THETW,SUM,SUM4
      GO TO 45
  969 FORMAT (6X,'THETD=',E15.8,/6X,'THETW=',E15.8,/5X,'DISTILLATE=',
     1 E15.8,/5X,'SIDE STREAM=', E15.8)
   47 DO 46 I=1,NC
      RAT(I,NTT+1)=F*X(I)/(1.+THETD*BOD(I)+THETW*WOD(I))
      VOB(I)=RAT(I,NF)
      ALD(I)=RAT(I,NF+1)
   46 RAT(I,1)=BOD(I)*THETD*RAT(I,NTT+1)
C CALCULATE THE MOLE FRACTIONS ON EACH TRAY
      NN=1
      DO 55 J=2,NTT
      SUM=0.
      DO 51 I=1,NC
      IF(J-NF) 51,51,52
   52 NN=NTT+1
   51 SUM=SUM + RAT(I,J)*RAT(I,NN)
      DO 55 I=1,NC
   55 RAT(I,J)=RAT(I,J)*RAT(I,NN)/SUM
      DO 56 I=1,NC
      RAT(I,NTT+1)=RAT(I,NTT+1)/DDD
   56 RAT(I,1)=RAT(I,1)/(F-DDD-S)
      K=0
      NN=NTT+1
      DO 58 J=1,NN
      DO 59 I=1,NC
   59 BOD(I)=RAT(I,J)
      IF(J-NF) 78,78,86
   78 IF(J-1) 79,58,79
   79 K=1
      GO TO 58
   86 K=0
   58 CALL BUBBA (A,B,C,D,E,BOD, T(J),NC,K)
      DO 96 J=2,NF
      DO 96 I=1,NC
      AK1=AK(A(I),B(I),C(I),D(I),E(I),T(J))
   96 RAT(I,J)=RAT(I,J)/AK1
      IF(ITH) 62,61,62
   62 IF(ABS(THETD -1.)-.00001) 64,64,63
   63 ITH=0
      GO TO 69
   61 IF(ABS(THETD -1.)-.00001)66,66,69
   66 ITH=1
   69 CALL DATSW(10,IDSW)
      GO TO (70,71), IDSW
   70 CALL OUT  (NTT,AAL,VV,T,DDD,F,NF,NS,NC,TF,A,B,C,D,E,RAT,X,HNF
     1,QR,QDD,QBB,QCC,HNS)
   71 CALL HEAT (RAT,AAL,VV,X,NTT,NF,NS,NC,DDD,     TF,T,F,KEY,HNF,QR,
     1 QDD,QBB,QCC,S,HNS)
      GO TO 72
   64 WRITE(3,107)
      WRITE(3,969) THETD,THETW,SUM,SUM3
      CALL OUT  (NTT,AAL,VV,T,DDD,F,NF,NS,NC,TF,A,B,C,D,E,RAT,X,HNF
     1,QR,QDD,QBB,QCC,HNS)
      TSM1=T(NS-1)
      CALL FIT(T(1),T(2),T(NF),T(NF+1),TSM1    ,T(NS),T(NTT),R,DDD,F,S
     1,NC,NS,NF,NTT,FLIQ,WOD,ALD,VOB,      VV,AAL)
  107 FORMAT(/6X,'***SOLUTION CONVERGED***')
      STOP
      END
```

Enthalpy Subroutine Using the Constant Composition Method

```
      SUBROUTINE HEAT (XX,AL,V,X,NTT,NF,NS,NC,DDD,TF,T,F,KEY,HNF,QR,QDD
     1,QBB,QCC,S,HNS)
C     ENTHALPY BALANCE USING THE CONSTANT-COMPOSITION METHOD
      DIMENSION A1(5),A2(5),B1(5),B2(5),C1(5),C2(5),D1(5),D2(5),E1(5),E2
     1(5),XX(5,16),AL(16),V(16),X(5),T(16),XD(5)
      COMMON A(5),B3(5),C(5),D3(5),E(5),A1,B1,C1,D1,E1,A2,B2,C2,D2,E2
C****READ IN ENTHALPY DATA
  101 FORMAT(5E15.9)
      IF(KEY) 12,11,12
   11 KEY=1
      READ(2,101)(A1(I),B1(I),C1(I),D1(I)        ,E1(I),I=1,NC)
      READ(2,101)(A2(I),B2(I),C2(I),D2(I)        ,E2(I),I=1,NC)
   12 QD=0.
      D=DDD
      QDV=0.
      K=(-1)
      DO 10 I=1,NC
   10 XD(I)=XX(I,NTT+1)
      DB=DDD
      NT=NS-1
      DO 1 I=1,NC
      QDV=QDV+XX(I,NTT+1)*(A2(I)+T(NTT)*(B2(I)+T(NTT)*(C2(I)+T(NTT)*(D2(
     1I)+T(NTT)*E2(I)))))
    1 QD=QD+XX(I,NTT+1)*(A1(I)+T(NTT+1)*(B1(I)+T(NTT+1)*(C1(I)+T(NTT+1)*
     1(D1(I)+T(NTT+1)*E1(I)))))
      QDD=QD*DDD
      QD=QDV*V(NTT)-AL(NTT+1)*QD
      QCC=(QD-QDD )*.001
      N=NTT
    2 N=N-1
      IF(N-NT) 3,4,4
    4 HNVD=0.
      HNV=0.
      HPL=0.
      DO 5 I=1,NC
      Q=             (A2(I)+T(N)*(B2(I)+T(N)*(C2(I)+T(N)*(D2(I)+T(N)*
     1E2(I)))))
      HNVD=HNVD+XD(I)*Q
      HNV=HNV+Q*XX(I,N+1 )
    5 HPL=HPL+XX(I,N+1)*(A1(I)+T(N+1)*(B1(I)+T(N+1)*(C1(I)+T(N+1)*(D1(I)
     1+T(N+1)*E1(I)))))
```

```
      AL(N   +1)=(QD-DB*HNVD)/(HNV-HPL)
      V(N)=AL(N+1)+DB
      GO TO 2
    3 IF(K) 17,23,7
   17 NT=NF
      DB=DDD+S
      K=0
      HNF=0.
      DO 16 I=1,NC
      XD(I)=(XX(I,NTT+1)*DDD+S*XX(I,NS))/DB
   16 HNF=HNF+XX(I,NS)*(A1(I)+T(NS)*(B1(I)+T(NS)*(C1(I)+T(NS)*(D1(I)+
     1T(NS)*E1(I)))))
      HNF=HNF*S
      HNS=HNF
      QD=QD+HNF
      N=N+1
      GO TO 2
   23 NT=1
      DB=DB-F
      K=1
      HNF=0.
      DO 6 I=1,NC
      XD(I)=(XX(I,NTT+1)*D-F*X(I)+S*XX(I,NS))/DB
    6 HNF=HNF+X(I)*(A1(I)+TF*(B1(I)+TF*(C1(I)+TF*(D1(I)+TF*E1(I)))))
      HNF=HNF*F
      QD=QD-HNF
      N=N+1
      GO TO 2
    7 QBB=0.0
      AL2=0.0
      V1=0.0
      DO 69 I=1,NC
      QBB=QBB+XX(I,1)*(A1(I)+T(1)*(B1(I)+T(1)*(C1(I)+T(1)*(D1(I)+T(1)*E
     1(I)))))
      AL2=AL2+XX(I,2)*(A1(I)+T(2)*(B1(I)+T(2)*(C1(I)+T(2)*(D1(I)+T(2)*E1
     2(I)))))
      AK=A(I)+T(1)*(B3(I)+T(1)*(C(I)+T(1)*(D3(I)+T(1)*E(I))))
   69 V1=V1+XX(I,1)*AK*(A2(I)+T(1)*(B2(I)+T(1)*(C2(I)+T(1)*(D2(I)+T(1)*E
     22(I)))))
      HNS=HNS*.001
      QDD=QDD*0.001
      HNF=HNF*0.001
      QBB=QBB*.001*(F-DDD-S)
      QR=(V1*V(1)-AL2*AL(2))*0.001+QBB
      RETURN
      END
```

Output Subroutine for the Rigorous Thiele-Geddes Program

```
      SUBROUTINE OUT  (NTT,AL,V,TT,DDD,F,NF,NS,NC,TF,A,B,C,D,E,XX,X,HNF,
     1QR,QDD,QBB,QCC,HNS)
      DIMENSION AL(16),V(16),TT(16),A(5),B(5),C(5),D(5),E(5),XX(5,16),X(
     15)
      WRITE(3,100)
  100 FORMAT(1H1,4X,'TOWER PROFILE'/5X,'STAGE NO.      TEMPERATURE    LIQ
     1UID RATE      VAPOR RATE'/21X,'(DEG F)',6X,'(MOLES/HR)',6X,'(MOLES/
     2HR)')
  101 FORMAT(8X,I3,9X,F9.4,6X,F9.4,6X,F9.4)
  105 FORMAT(10X,'STAGE NO.      ',I3,/5X,'LIQUID MOLE FRAC.',2X,'VAPOR M
     1OLE FRAC.')
  106 FORMAT(8X,F10.8,6X,F10.8)
  107 FORMAT(4X,'DISTILLATE',10X,'FEED',/,4X,'MOLE FRAC.',10X,'MOLE FRAC
     1.')
  108 FORMAT(8X,F10.8,8X,F10.8)
      DO 1 I=1,NTT
    1 WRITE(3,101) I,TT(I),AL(I),V(I)
      Q=AL(NTT+1)+DDD
      R=Q-DDD
      WRITE(3,102) TT(NTT+1),Q,DDD,R
  102 FORMAT(5X,'CONDENSER       ',F9.4,6X,F9.4/21X,'DISTILLATE =   ',F9.
     14/21X,'REFLUX      =   ',F9.4/)
      WRITE(3,103) NF,TF
  103 FORMAT(2X,'STAGE 1 IS THE REBOILER',3X,'FEED STAGE IS',I3,/2X,'FEE
     1D TEMP. (DEGF) IS',F8.2,////)
      WRITE(3,104)
  104 FORMAT(4X,'MATERIAL BALANCE')
      DO 2 J=1,NTT
      WRITE(3,105) J
      DO 2 I=1,NC
      AK=A(I)+TT(J)*(B(I)+TT(J)*(C(I)+TT(J)*(D(I)+TT(J)*E(I))))
    5 Y=XX(I,J)*AK
      WRITE(3,106) XX(I,J),Y
    2 CONTINUE
      WRITE(3,107)
      DO 3 I=1,NC
    3 WRITE(3,108) XX(I,NTT+1),X(I)
      QIN=HNF+QR
      QOUT=QDD+QBB+QCC+HNS
      WRITE(3,109) HNF,QDD,QR,QBB,QCC,HNS,QIN,QOUT
  109 FORMAT(//,5X,'HEAT BALANCE'/21X,'(MM BTU/HR)',16X,'(MM BTU/HR)'/5X
     1,'FEED ENTHALPY =    ',F6.3,5X,'DISTILLATE =    ',F6.3/5X,
     2 'REBOILER      =    ',F6.3,5X,'BOTTOMS     =    ',F6.3/35X,'CONDE
     3NSER   =    ',F6.3/35X,'SIDE STEAM  =   ',F6.3
     4,/13X,'TOTAL =    ',F6.3,10X,'TOTAL =    ',F6.3//)
      RETURN
      END
```

Subroutine Calculate the Fractions for the Force-Fit Thiele-Geddes Method

```
      SUBROUTINE FIT(T1,T2,TF,TFP1,TSM1,TS,TN,R,DDD,F,S,NC,NS,NF,NTT,
     1FL10,WOD,ALD,VOB,     VV,AAL)
C  10/4/72
      DIMENSION WOD(5),ALD(5),VOB(5),         VV(16),AAL(16)
      COMMON A(5),B(5),C(5),D(5),E(5)
      VL=DDD+R*DDD
      WRITE(3,201)
      WRITE(3,1972)  TF,TS,TFP1,TSM1,AAL(NF+1),AAL(NS-1)
     1,VV(NS-1),VV(NF+1)
      TSM1=TS
      TFP1=TF
      WRITE(3,1972)  TF,TS,TFP1,TSM1,AAL(NF+1),AAL(NS-1)
     1,VV(NS-1),VV(NF+1)
  201 FORMAT(1H1,3X,'FORCE FIT FRACTIONS',///5X,'TOP SECTION OF THE COLU
     1MN')
      ALV1=R*DDD/VL
      NN=NTT-NS+1
      DO 1 I=1,NC
      AMA=                (A(I)+TN*(B(I)+TN*(C(I)+TN*(D(I)+TN*E(I)))))
      AMA=AAL(NTT)/(VV(NTT)*AMA)
      AMI=     (A(I)+TS*(B(I)+TS*(C(I)+TS*(D(I)+TS*E(I)))))
      AMI=(AAL(NS)   )/(VV(NS)*AMI)
      WRITE(3,103) AMA,AMI
  103 FORMAT(6X, 'MAX. ABSORPTION FACTOR=',E15.8,/6X,'MIN. ABSORPTION FA
     1CTOR=',E15.8)
      AM1=AMA*ALV1*VV(NTT)/AAL(NTT)
      AM2=AMI*ALV1*VV(NS)/(AAL(NS)   )
      WRITE(3,104) AM1,AM2
  104 FORMAT (3X,'ABSORPTION FACTORS BASED ON CONSTANT MOLAL OVERFLOW',
     1/6X,'MAX.=',E15.8,/6X,'MIN=',E15.8)
   10 AA=(AMA+AMI)*.5
      A1=AA
      AA=(AA**(NN+1)-AA)/(AA-1.)+R*AA**NN
      AA=AA*S/(R*DDD)
      WRITE(3,101) AA,WOD(I)
  101 FORMAT(2(6X,E15.8))
      IF(ABS(AA-WOD(I))/AA-.00001  ) 2,2,3
    3 IF(AA-WOD(I)) 4,4,5
    4 AMI=A1
      GO TO 10
    5 AMA=A1
      GO TO 10
    2 FRAC=(A1-AM2)/(AM1-AM2)
      WRITE(3,102) I,  FRAC,A1
  102 FORMAT(//6X,'COMP. NO.=',I5,                   /10X,'FRAC=',E15.8
     1,/10X,'AVE. ABSORPTION FACTOR=',E15.8)
    1 CONTINUE
```

```
      WRITE(3,1972)  TF,TS,TFP1,TSM1,AAL(NF+1),AAL(NS-1)
     1,VV(NS-1),VV(NF+1)
C   SECOND TOWER SECTION
      ALV1=(R*DDD-S)/VL
      NN=NS-NF
      DO 21 I=1,NC
      AMI= AAL(NF+1)/(VV(NF+1)*
     1(A(I)+TFP1*(B(I)+TFP1*(C(I)+TFP1*(D(I)+TFP1*E(I))))))
      AMA=AAL(NS-1)/(VV(NS-1)*
     1(A(I)+TSM1*(B(I)+TSM1*(C(I)+TSM1*(D(I)+TSM1*E(I))))))
      WRITE(3,1972)  TF,TS,TFP1,TSM1,AAL(NF+1),AAL(NS-1)
     1,VV(NS-1),VV(NF+1)
 1972 FORMAT(6X,E15.8)
      WRITE(3,103) AMA,AMI
      AM2=AMI*ALV1*VV(NF+1)/AAL(NF+1)
      AM1=AMA*ALV1*VV(NS-1)/AAL(NS-1)
      WRITE(3,104) AM1,AM2
   30 AA=(AMA+AMI)*.5
      A1=AA
      AA=AA**(NN-1)*(WOD(I)*R*DDD/S-WOD(I))
     1                                   +(1.+WOD(I))*((AA**NN-AA)/(AA-1.))
      WRITE(3,101) AA,ALD(I)
      IF(ABS(AA-ALD(I))/AA-.00001   ) 22,22,23
   23 IF(AA-ALD(I)) 24,24,25
   24 AMI=A1
      GO TO 30
   25 AMA=A1
      GO TO 30
   22 FRAC=(A1-AM2)/(AM1-AM2)
      WRITE(3,102) I,  FRAC,A1
   21 CONTINUE
      WRITE(3,200)
  200 FORMAT(1H1,6X,'BOTTOM SECTION OF COLUMN')
      VL=VL-F*(1.-FLIQ)
      ALV1=VL/(R*DDD+F*FLIQ-S)
      DO 41 I=1,NC
      AMA=(A(I)+T2*(B(I)+T2*(C(I)+T2*(D(I)+T2*E(I)))))
     1*VV(2)/AAL(2)
      AMI=(A(I)+TF*(B(I)+TF*(C(I)+TF*(D(I)+TF*E(I)))))
     1*VV(NF)/AAL(NF)
      WRITE(3,105) AMA,AMI
  105 FORMAT(6X,'MAX. STRIPPING FACTOR=',E15.8,/6X,'MIN. STRIPPING FACTO
     1R=',E15.8)
      AM1=AMA*AAL(2)*ALV1/VV(2)
      AM2=AMI*AAL(NF)*ALV1/VV(NF)
      WRITE(3,106) AM1,AM2
  106 FORMAT(3X,'STRIPPING FACTORS BASED ON CONSTANT MOLAL OVERFLOW',
     1/6X,'MAX.=',E15.8,/6X,'MIN.=',E15.8)
   50 AA=(AMA+AMI)*.5
      A1=AA
      AA=(AA**NF-AA)/(AA-1.)+AA**(NF-1)*(A(I)+T1*(B(I)+T1*(C(I)+T1*(D(I)
     1+T1*E(I)))))*VL/(F-DDD-S)
      WRITE(3,101) AA,VOB(I)
      IF(ABS(AA-VOB(I))/AA-.00001)42,42,43
   43 IF(AA-VOB(I)) 44,44,45
   45 AMA=A1
      GO TO 50
   44 AMI=A1
      GO TO 50
   42 FRAC=(A1-AM2)/(AM1-AM2)
      WRITE(3,102) I,  FRAC,A1
   41 CONTINUE
      RETURN
      END
```

Subroutine Calculates Either Dew or Bubble Points using the Newton Method

```
      SUBROUTINE BUBBA (A,B,C,D,E,X,T,N,J)
      DIMENSION A(5),B(5),C(5),D(5),E(5),X(5)
    9 SUM=0.
      SUM1=0.
      DO 6 I=1,N
      AKC=A(I)+B(I)*T+C(I)*T*T+D(I)*T*T*T+E(I)*T*T*T*T
      AKPC=B(I)+2.*C(I)*T+3.*D(I)*T*T+4.*E(I)*T*T*T
      IF(J) 1,2,1
    2 SUM=   X(I)*AKC      +SUM
      SUM1=   X(I)*AKPC      +SUM1
      GO TO 3
    1 SUM=SUM+X(I)/AKC
      SUM1=SUM1-X(I)*AKPC/AKC**2
    3 CONTINUE
    6 CONTINUE
      IF(ABS(SUM-1.)-.000001) 8,7,7
    7 T =T -(SUM-1.)/SUM1
      IF(T-101.)  21,21,9
   21 T=101.
      GO TO 9
    8 CONTINUE
      RETURN
      END
```

Program for Both the Stand-Alone Simplified Thiele-Geddes Method and the Force-Fit Thiele-Geddes Method

```
C    SIMPLIFIED THIELE GEDDES PROCEDURE
      DIMENSION A(5),B(5),C(5),D(5),E(5),X(5),XL(5),XV(5),DS(5),BS(5),
     1WS(5),ALD( 5) ,VOB( 5),WOD( 5),       FRAC1(5),FRAC2(5),FRAC3(5)
      AK (AA,BB,CC,DD,EE,TT)    =AA+TT*(BB+TT *(CC+TT*(DD+TT*EE)))
   76 READ(2,100)  NC,NTT,NS,NF,IFF
      READ(2,101) (A(I),I=1,NC)
      READ(2,101) (B(I),I=1,NC)
      READ(2,101) (C(I),I=1,NC)
      READ(2,101) (D(I),I=1,NC)
      READ(2,101) (E(I),I=1,NC)
      READ(2,102) (X(I)                  , I=1,NC)
      READ(2,102) F,DDD,R,S,FLIQ,TN,TS,T1,TF,T2
      WRITE(3,205)
      WRITE(3,300)  NC,NTT,NS,NF
      ATF=0.
      VL=DDD+R*DDD
      ALV1=R*DDD/VL
      ALV2=(R*DDD-S)/VL
      VL=VL-F*(1.-FLIQ)
      AVL3=VL/(R*DDD+F*FLIQ-S)
   69 ANN= NS-NF
      ANN=(TF-TS)/ANN
      TFP1=TF-ANN
      TSM1=TS+ANN
C   CALCULATE (L/D) NS
      NN=NTT-NS
      ANN=NN
      WRITE(3,700) T1,T2,TF,TFP1,TSM1,TS,TN
      IF(S)12,13,12
   13 TS=TF
      NS=NF+1
   12 IF(IFF) 31,39,30
   30 READ(2,103) (FRAC1(I),FRAC2(I),FRAC3(I),I=1,NC)
      WRITE(3,206) (FRAC1(I),FRAC2(I),FRAC3(I),I=1,NC)
      IFF=-1
      GO TO 31
   39 DO 1 I=1,NC
      AK1=AK(A(I),B(I),C(I),D(I),E(I), TN)
      AK2=AK(A(I),B(I),C(I),D(I),E(I), TS)
      PROD=ALV1/AK2
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      WOD(I)=PROD
      AIN=ALV1/ANN*(1./AK1-1./AK2)
      AK2=ALV1/AK2
      DO 2 J=1,NN
      AN=J
      PROD=PROD*(AK2+AIN*AN)
    2 WOD(I)=WOD(I)+PROD
    1 WOD(I)=WOD(I)+PROD*R
C   CALCULATE (L/D) F+1
      IF(S) 15,16,15
   16 DO 14 I=1,NC
      ALD(I)=WOD(I)
   14 WOD(I)=0.
      GO TO 17
   15 NN=NS-NF-2
      ANN=NN
      DO 3 I=1,NC
      AK1=AK(A(I),B(I),C(I),D(I),E(I),TSM1)
      AK2=AK(A(I),B(I),C(I),D(I),E(I),TFP1)
      PROD=ALV2/AK2
      ALD(I)=PROD
      AIN=ALV2/ANN*(1./AK1-1./AK2)
      AK2=ALV2/AK2
      DO 4 J=1, NN
      AN=J
      PROD=PROD*(AK2+AIN*AN)
    4 ALD(I)=ALD(I)+PROD
      AIN=WOD(I)*S/(R*DDD)
      WOD(I)=WOD(I) -AIN
      ALD(I)=PROD*(WOD(I)-AIN)+(1.+AIN)*ALD(I)
    3 WOD(I)=AIN
C   CALCULATE (V/B)F
   17 NN=NF-2
      ANN=NN
      DO 5 I=1,NC
      AK1=AK( A(I),B(I),C(I),D(I),E(I),TF)
      AK2=AK( A(I),B(I),C(I),D(I),E(I),T2)
      PROD=AVL3*AK1
      VOB(I)=PROD
      AIN=AVL3*(AK2-AK1)/ANN
      AK1=AVL3*AK1
      DO 6 J=1,NN
      AN=J
      PROD=PROD*(AK1+AN*AIN)
    6 VOB(I)=VOB(I)+PROD
      AK1=AK(A(I),B(I),C(I),D(I),E(I),T1)
    5 VOB(I)=VOB(I)+PROD *AK1*VL/(F-DDD-S)
      GO TO 38
C   FORCE FIT
   31 NN=NLT-NS+1
      DO 33 I=1,NC
      AK1=AK(A(I),B(I),C(I),D(I),E(I),TN)
      AK2=AK(A(I),B(I),C(I),D(I),E(I),TS)
      AK1=ALV1/AK2+FRAC1(I)*ALV1*(1./AK1-1./AK2)
      WOD(I)=(AK1**(NN+1)-AK1)/(AK1-1.)+R*AK1**NN
   33 WOD(I)=WOD(I)*S/(R*DDD)
      DO 34 I=1,NC
      AK1=AK(A(I),B(I),C(I),D(I),E(I),TS)
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      AK2=AK(A(I),B(I),C(I),D(I),E(I),TF)
      AK1=ALV2/AK2+FRAC2(I)*ALV2*(1./AK1-1./AK2)
   34 ALD(I)=AK1**(NS-NF-1) *(WOD(I)*R*DDD/S-WOD(I))
     1                          *(1.+WOD(I))*((AK1**(NS-NF)-AK1)/(AK1-1.))
      NN=NF-1
      DO 35 I=1,NC
      AK1=AK(A(I),B(I),C(I),D(I),E(I),T1)
      AK1=AK1*VL/(F-DDD-S)
      AK2=AK(A(I),B(I),C(I),D(I),E(I),T2)
      AK3=AK(A(I),B(I),C(I),D(I),E(I),TF)
      AK2=AK3*AVL3+AVL3*FRAC3(I)*(AK2-AK3)
   35 VOB(I)=(AK2**NF-AK2)/(AK2-1.)+AK1*AK2**NN
C FORCE FRACTION END
   36 IJK=0
      THETW=1.
   49 DCAL=0.
      WCAL=0.
      BCAL=0.
      DO 7 I=1,NC
      BOD=(ALD(I)+XL(I)/(F*X(I)))*(1.+WOD(I)))
     1                                          /(VOB(I)+XV(I)/(F*X(I)))
      DS(I)=F*X(I)/(1.+BOD+WOD(I))
      WS(I)=WOD(I)*DS(I) *THETW
      BS(I)=F*X(I)-DS(I)-WS(I)
      DCAL=DS(I)+DCAL
      BCAL=BS(I)+BCAL
    7 WCAL=WS(I)+WCAL
      IF(IJK) 41,42,41
   42 IF(S) 43,41,43
   43 THETW=S/WCAL
      IJK=1
      GO TO 49
   41 DO 8 I=1,NC
      WS(I)=WS(I)/WCAL
      BS(I)=BS(I)/BCAL
    8 DS(I)=DS(I)/DCAL
      J=1
      WRITE(3,203) DCAL,BCAL,WCAL
      TNA=TN
      T1A=T1
      TSA=TS
      T2A=T2
      TXT=TN
      CALL BUBBA(A,B,C,D,E,DS,TN  ,NC,J)
      J=0
      TXB=T1
      CALL BUBBA(A,B,C,D,E,BS,T1,NC,J)
C  CALCULATE TS,T2,TN
      IF(S) 18,19,18
   18 CALL BUBBA (A,B,C,D,E,WS,TS,NC,J)
C  GET L2 AND CALCULATE T2
   19 AL22=BCAL+VL
      DO 10 I=1,NC
      AK1=AK(A(I),B(I),C(I),D(I),E(I),T1)
   10 WOD(I)=(AK1*BS(I)*VL-BCAL*BS(I))/AL22
      CALL BUBBA (A,B,C,D,E,WOD,T2,NC,J)
      IF(ABS(TNA-TN)/TN-.0005 ) 71,71,69
   71 IF(ABS(T1A-T1)/T1-.0005 ) 72,72,69
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   72 IF(ABS(TSA-TS)/TS-.0005 ) 73,73,69
   73 IF(ABS(T2A-T2)/T2-.0005 )74,74,69
   74 IF(ABS(DDD-DCAL)/DCAL-    .0005) 68,68,22
   68 WRITE(3,204)
      WRITE(3,669)    THETW
      WRITE(3,201)
      DO 9 I=1,NC
    9 WRITE(3,202) I,BS(I),DS(I),WS(I)
      GO TO 76
   22 IF(ATF) 26,25,26
   25 IF(DDD-DCAL) 81,82,82
   82 ATF=TF
      ADD=DCAL
      TF=TF-2.
      GO TO 69
   81 ATF=TF
      ADD=DCAL
      TF=TF+2.
      GO TO 69
   26 ANN=TF
      TF=(ATF-TF)/(ADD-DCAL)*(DDD-DCAL)+TF
      ATF=ANN
      ADD=DCAL
      GO TO 69
  100 FORMAT(4I5)
  101 FORMAT(5E15.9)
  102 FORMAT(8F10.0)
  103 FORMAT(3F10.0)
  201 FORMAT(3X,'BOTTOMS COMPOSITION',6X'DISTILLATE COMPOSITION', 6X,'SI
     1DE STREAM COMPOSITION')
  203 FORMAT(/6X,'DISTILLATE=',F10.4,/6X,'BOTTOMS=',F10.4,
     1/6X,'SIDE STREAM=',F10.4)
  202 FORMAT(20X,I3,E14.7,1X,E14.7,1X,E14.7)
  204 FORMAT(/'****FINISHED****')
  205 FORMAT(1H1,6X,'***MODIFIED THIELE GEDDED PROGRAM***',///)
  206 FORMAT (              6X,'***FRACTION INPUT METHOD BEING USED***',
     1    ///,8X,'FOLLOWING FRACTIONS HAVE BEEN INPUTED',/2X,3(6X,E15.8))
  300 FORMAT(     12X,'INPUT SPECIFICATIONS',/3X,'***NOTE TRAY 1 IS THE R
     1EBOILER***',/6X,'NUMBER OF COMPONENTS=',  10X,I3,/6X,'NUMBER OF TR
     2AYS (INCLUDING THE REBOILER)=',2X,I3,/6X,'SIDE STREAM PLATE NUMBER
     3=',8X   ,I3,/6X,'FEED TRAY NUMBER=',8X,I3)
  700 FORMAT(6X,'T1=',E15.8,/6X,'T2=',E15.8,/6X,'TF=',E15.8,/6X,
     1'TFP1=',E15.8,/6X,'TSM1=',E15.8,/6X,'TS=',E15.8,/6X,'TN=',E15.8)
  669 FORMAT(6X,'THETW=',E15.8)
      END
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APPENDIX B

Input for the Base Case (Case 1) using the Rigorous Thiele-Geddes Program

Equilibrium and enthalpy data are fitted to a polynomial of the following form:

$$K_{t,i} = A_i + B_i t + C_i t^2 + D_i t^3 + E_i t^4$$

$$H_{t,i} = A_i + B_i t + C_i t^2 + D_i t^3 + E_i t^4$$

$$h_{t,i} = A_i + B_i t + C_i t^2 + D_i t^3 + E_i t^4$$

where: A, B, C, D, E, are inputed coefficients for component i and t is the temperature in degrees fahrenheit

$H_{t,i}$ = vapor enthalpy at temperature t for component i

$h_{t,i}$ = liquid enthalpy at temperature t for component i

$K_{t,i}$ = equilibrium constant at temperature t for component i

Card #1

Columns		Inserted Value
1 - 5	Number of Components	5
6 - 10	Total Number of stages including the reboiler	10
11 - 15	*Number of Sidestream draw-off stage	8
16 - 20	*Number of feed stage	5

*Stage 1 is the reboiler

Card #2 Coefficient equilibrium constant for component number one

Columns	Inserted Value
1 - 15	0.28531998E 00
16 - 30	0.82878992E-02
31 - 45	0.37041988E-04
46 - 60	-0.63860000E-04
61 - 75	0.71090994E-10

Card #3

Columns	Inserted Value
1 - 15	0.27804995E 00
16 - 30	-0.11902999E-02
31 - 45	0.62290987E-04
46 - 60	-0.12023997E-06
61 - 75	0.10241999E-09

Card #4

Columns	Inserted Value
1 - 15	0.22200996E 00
16 - 30	-0.18502998E-02
31 - 45	0.54022996E-04
46 - 60	-0.81239989E-07
61 - 75	0.53332991E-10

Card #5

Columns	Inserted Value
1 - 15	0.15309995E 00
16 - 30	-0.22649998E-02

Columns	Inserted Value
31 - 45	0.21813989E-04
46 - 60	-0.20709997E-07
61 - 75	-0.40599999E-12

Card #6

Columns	Inserted Value
1 - 15	0.16042995E 00
16 - 30	-0.26387000E-02
31 - 45	0.28703987E-04
46 - 60	-0.88699998E-08
61 - 75	-0.14969997E-10

There would be additional cards for additional components.

Card #7

Columns		Inserted Value
1 - 10	Mole fraction of component 1 in the feed	.05
11 - 20	Mole fraction of component 2 in the feed	.15
21 - 30	Mole fraction of component 3 in the feed	.25
31 - 40	Mole fraction of component 4 in the feed	.20
41 - 50	Mole fraction of component 5 in the feed	.35

There would be additional numbers for more components.

Card #8

Columns		Inserted Value
1 - 10	Initial assumed temperatures for stage 1	220.
11 - 20	Initial assumed temperatures for stage 2	210.

Columns		Inserted Value
21 - 30	Initial assumed temperatures for stage 3	200.
31 - 40	Initial assumed temperatures for stage 4	190.
41 - 50	Initial assumed temperatures for stage 5	180.
51 - 60	Initial assumed temperatures for stage 6	170.
61 - 70	Initial assumed temperatures for stage 7	160.
71 - 80	Initial assumed temperatures for stage 8	150.

Card #9

Columns		Inserted Value
1 - 10	Initial assumed temperatures for stage 9	145.
11 - 20	Initial assumed temperatures for stage 10	140.

There would be additional numbers for more stages.

Card #10 Coefficient for liquid enthalpy for component number one

Columns	Inserted Value
1 - 15	0.44835997E 01
16 - 30	0.2688299E-01
31 - 45	0.64745000E-05
46 - 60	0.32505998E-07
61 - 76	-0.52879992E-10

Card #11 Coefficient for liquid enthalpy for component number two

Columns	Inserted Value
1 - 15	0.52091999E 01
16 - 30	0.40495998E-01

Columns	Inserted Value
31 - 45	-0.57048988E-04
46 - 60	0.25799994E-06
61 - 75	-0.32644998E-09

Card #12 Coefficient for liquid enthalpy for component number three

Columns	Inserted Value
1 - 15	0.64442997E 01
16 - 30	0.14100999E-01
31 - 45	0.16052999E-03
46 - 60	-0.49556996E-06
61 - 75	0.61558980E-09

Card #13 Coefficient for liquid enthalpy for component number four

Columns	Inserted Value
1 - 15	0.67343998E 01
16 - 30	0.43812998E-01
31 - 45	-0.22595996E-04
46 - 60	0.13574999E-06
61 - 75	-0.16938999E-09

Card #14 Coefficient for liquid enthalpy for component number five

Columns	Inserted Value
1 - 15	0.83587999E 01
16 - 30	0.80696978E-02
31 - 45	0.26773987E-03

Columns	Inserted Value
46 - 60	-0.86588000E-06
61 - 75	0.10789998E-08

There would be additional cards for additional components.

Card #15 Coefficients for vapor enthalpy for component number one

Columns	Inserted Value
1 - 15	0.13575000E 02
15 - 30	-0.27656998E-01
31 - 45	0.37013995E-03
46 - 60	-0.12388991E-05
61 - 75	0.15431998E-08

Card #16 Coefficients for vapor enthalpy for component number two

Columns	Inserted Value
1 - 15	0.15278999E 02
16 - 30	-0.60739964E-02
31 - 45	0.23645999E-03
46 - 60	-0.75789995E-06
61 - 75	0.94283981E-09

Card #17 Coefficients for vapor enthalpy for component number three

Columns	Inserted Value
1 - 15	0.13910999E 02
16 - 30	0.46811998E-01
31 - 45	-0.19588000E-03
46 - 60	0.74338999E-06
61 - 75	-0.92781982E-09

Card #18 Coefficients for vapor enthalpy for component number four

Columns	Inserted Value
1 - 15	0.19401998E 02
16 - 30	-0.93661994E-02
31 - 45	0.30484982E-03
46 - 60	-0.97820975E-06
61 - 75	0.12168999E-08

Card #19 Coefficients for vapor enthalpy for component number five

Columns	Inserted Value
1 - 15	0.21092987E 02
16 - 30	-0.35334997E-01
31 - 45	0.52449-92E-03
46 - 60	-0.17495995E-05
61 - 75	0.21789999E-08

There would be additional cards for additional components.

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3. Tomme, W. J., "A Convergence Method for Distillation Systems," Ph. D. dissertation, A. and M. College of Texas, College Station, Texas, 1963.