MINIMUM REFLUX IN FRACTIONATING COLUMNS

A NEW AND IMPROVED SHORT-CUT METHOD

BY

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ABSTRACT

A short-cut method is presented for calculating the minimum reflux rate for multicomponent systems. This new method is best suited for use on the computer and gives a very accurate estimate of this important factor in the design of fractionating columns. It does so without going to the tedious and time-consuming calculations of the rigorous methods.

The calculation approach is based on a simplification of the Thiele and Geddes method for fractionating columns under minimum reflux conditions.

The program is written in Fortran IV language and was used on an IBM 370 computer. Input specifications include the split of the light and heavy key components and feed conditions and composition. The liquid rate at the rectifying pinch zone, which represents the constant internal minimum reflux, is then calculated.

This method is an iterative procedure and the program assumes constant molal overflow between the rectifying and stripping pinch zones. The overall material balance for every trial is based on temperatures calculated from the composition of the previous trial. However, the liquid rate at the rectifying pinch zone temporarily remains constant until convergence is obtained on the distillate composition and pinch zone temperatures. The liquid rate is then changed in the direction of convergence on the key component specifications and the calculations are repeated until converged.

The true minimum reflux was calculated on a rigorous plate-to-plate program by a parameter study of the actual required reflux for a series of column designs with increasing stages and with each design making the same separation for the key components. These values were asymtotically extrapolated to the case for infinite stages, and the minimum reflux value obtained was compared with the results given by the new procedure. The results demonstrated the reliability and usefulness of this new short-cut method.

APPROVAL OF THESIS

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NOMENCLATURE

A	Component absorption factor for the specific stage or section of the column. A_{R*} = component absorption factor at the rectifying pinch.
A_A	Average component absorption factor in the specific section.
b	Component molar flow rate in the bottoms.
B	Bottom molar flow rate.
C	Total number of components; the least volatile component.
d	Component molar flow rate in the distillate.
D	Distillate molar flow rate.
f	Feed stage.
f_F	Total component molar flow rate in the feed.
F	Total molar flow rate of feed.
h	Enthalpy of one mole of the liquid leaving the specific stage or section of the column.
H	Enthalpy of one mole of the vapor leaving the specific stage or section of the column.
HK	Heavy key component.
IHS	First component separated from the distillate.
ILS	First component separated from the bottoms.
K	Component vapor-liquid equilibrium constant ($y = Kx$), in the specific stage or section of the column.
ℓ	Component liquid molar flow rate leaving the specific stage.
ℓ_{f+1}	Component liquid molar flow rate onto stage f.
ℓ_F	Component molar flow rate in liquid feed.
L	Total liquid molar flow rate in the specific section.
L_F	Total liquid molar flow rate of feed.
L_R	External reflux.

L_{Rm}	External minimum reflux.
L_{R*}	Internal minimum reflux; liquid rate at the rectifying pinch.
LK	Light key component.
M	Number of stages between the stripping pinch and stage f.
N	Number of stages between the rectifying pinch and stage f+1.
N_m	Minimum number of stages of a column.
Q_C	Condenser duty.
Q_R	Reboiler duty.
R*	Rectifying pinch.
S	Component stripping factor for the specific stage or section of the column. $S_{\underline{S}*}$ = component stripping factor at the stripping pinch.
S_A	Average component stripping factor in the specific section.
$\underline{S}*$	Stripping pinch.
T	Temperature in °F.
v	Component vapor molar flow rate leaving the specific stage.
$\bar{v}_f$	Component vapor molar flow rate as it enters stage f+1.
v_F	Component molar flow rate in vapor feed.
V	Total vapor molar flow rate in the specific section.
V_1	Total molar flow rate of the vapor from the top stage of the column.
V_F	Total vapor molar flow rate of feed.
x	Component mole fraction in the liquid phase.
y	Component mole fraction in the vapor phase.
α	Relative volatility.
θ	Multiplier used to correct the (b/d) ratios.

Subscripts

A	Average value.
c	Total number of components.
F	Feed.
$f+1$	Stage above the feed stage.
f	Feed stage.
HK	Heavy key.
i	Component number. Components are numbered in the order of decreasing volatility.
L	Liquid part of a stream.
LK	Light key.
$R*$	Rectifying pinch.
$\underline{S}*$	Stripping pinch.
V	Vapor part of a stream.

CHAPTER I

INTRODUCTION

The minimum reflux ratio is the lowest reflux which can give a specified separation for two key components from a fixed feed to a fractionating column. To obtain that separation, an infinite number of equilibrium stages is required in both the rectifying section and the stripping section of the column.

This imaginary operation, that cannot be duplicated in practice, is of interest as a limiting case since it provides an effective variable for the selection of an economic operating reflux in the real design of the fractionating column.

A small increase in the value of the reflux ratio at values near the minimum gives a marked reduction in the number of stages, but as the value of this reflux ratio increases further, the effect on the number of stages becomes much less.

A large reflux ratio increases the operating costs, since large quantities of liquid are recirculated to the column resulting in higher cooling and heating duties. A low reflux ratio requires a greater number of stages and the investment cost increases. The most economic reflux ratio usually lies between 1.2 and 1.5 times the minimum reflux ratio.

Many methods have been presented for calculating the minimum reflux value for multicomponent distillation separations.

The purpose of this work was to develop a method for calculating the minimum reflux ratio for multicomponent fractionating columns, which will give a more accurate estimate of the minimum reflux without going to the tedious and time-consuming rigorous methods. This new method consists of a simplification of the Thiele and Geddes (30) plate-to-plate procedure applied to the calculation for infinite stages and, therefore, minimum reflux.

To obtain the rigorous solution of the minimum reflux a parameter study was made by calculating the reflux required for a series of column designs with increasing stages and with each design making the same separation for the key components. These values were asymptotically extrapolated to the case for infinite stages and, then, the true minimum reflux value obtained was compared with the results given by the new simplified procedure and with the traditional Underwood method.

The programs used have been written in Fortran IV language and are listed in the Appendix B. The calculations were carried out on an IBM 370 computer.

CHAPTER II

A FRACTIONATING COLUMN

The purpose of a fractionating column is the separation of two or more components which are present in a feed stream to give an overhead product (D) and a bottom product (B) meeting certain specifications. Figure 2-1 illustrates a fractionating column having one feed.

The components upon which the specifications are made are commonly referred to as the light and the heavy keys.

The split, light and heavy key components will appear in both, the distillate and the bottoms products and therefore, these are, by definition, distributed components. Components lighter than the light key which appear in the distillate and heavier than heavy key which appear in the bottoms are also, distributed components. Components which appear only in one product are called separated components.

The conventional procedure for the design of a fractionating column frequently involves the calculation of two limits. One is the minimum number of stages required for the separation if practically no product is withdrawn from the column. This condition is called total reflux. The other is the requirement of an infinite height column and this leads to the calculation of the minimum reflux. Therefore, a practical operation lies in between these two conditions.

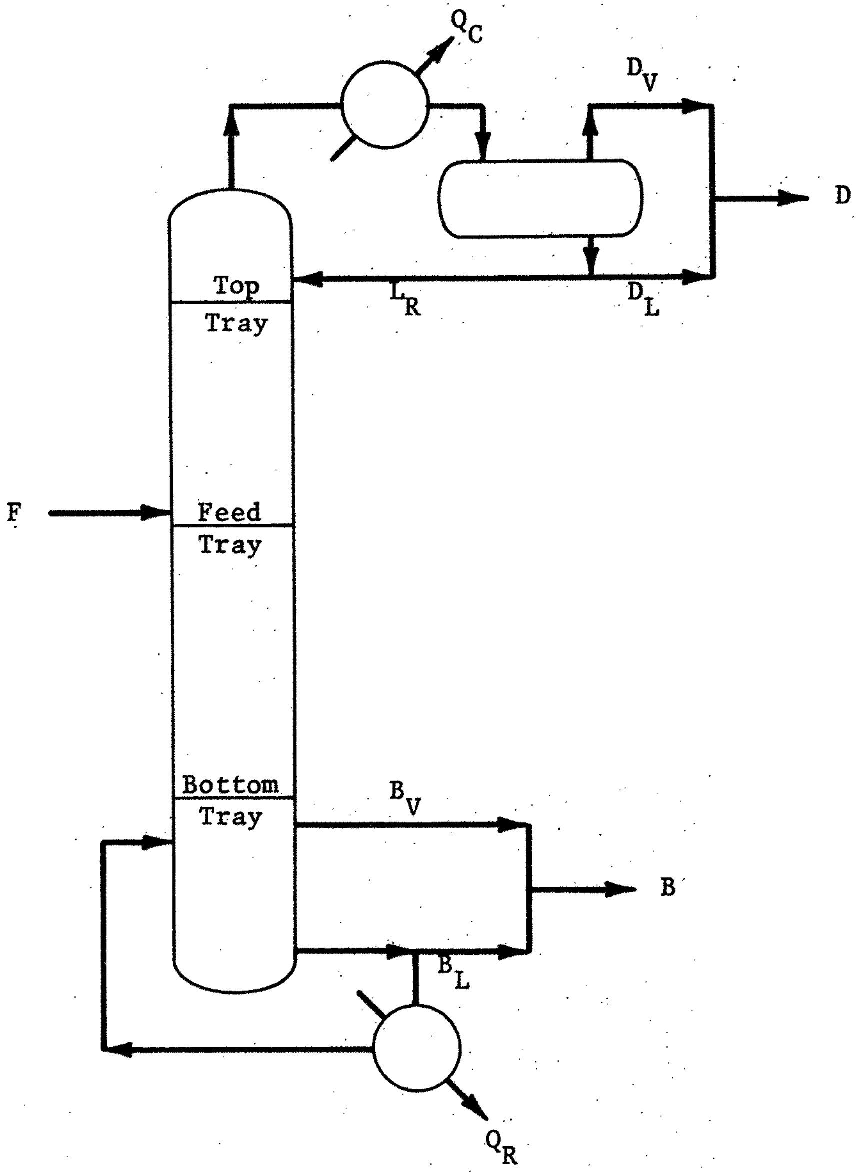


FIGURE 2-1. A fractionating column having one feed.

CHAPTER III

BEHAVIOR OF A COLUMN AT MINIMUM REFLUX

A fractionating column in the state of minimum reflux presents a maximum of six distinct column sections. This type of infinite column is represented in Figure 3-1 and corresponds to separations where some of the components of the feed are completely separated from the top product and some others are completely separated from the bottom product.

At minimum reflux no separation occurs at some point in the column. This point will originate what is called a "pinch" zone.

Sections II and V, where the "pinch" zones occur, are the uniform sections. The temperatures, stream compositions and molal overflow remain constant throughout these sections.

The points of infinitude or pinches of the type of column shown in Figure 3-1 occur away from the feed stage. Hence, two other sections are to be distinguished between the pinch zones in the rectifying and stripping sections and the feed stage: Section III, which is an intermediate section between the feed and the stripping pinch, and Section IV, which is an intermediate section between the feed and the rectifying pinch. Stream compositions, as well as temperatures and molal overflow may change considerably over the intermediate trays between the feed and the constant composition zones. The compositions of the liquid and vapor phases of the feed differ from the liquid and vapor stream compositions in the pinch zones for all feed conditions.

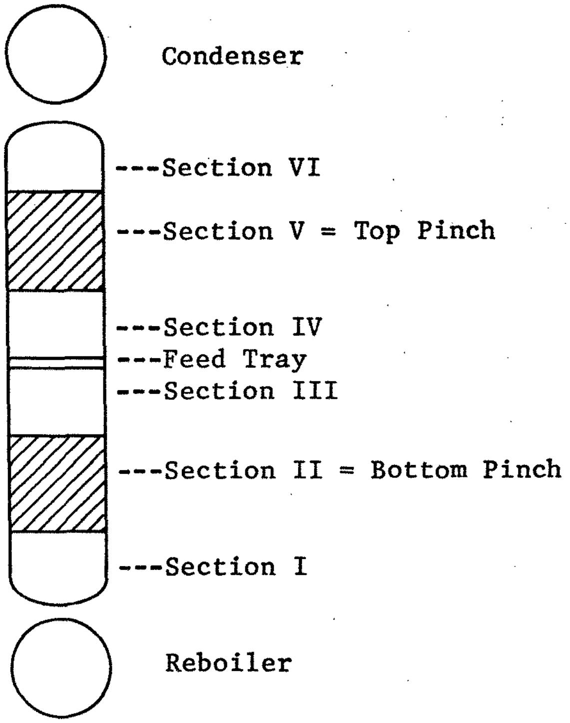


FIGURE 3-1. The six typical sections of an infinite column. Both pinch zones occur away from the feed tray.

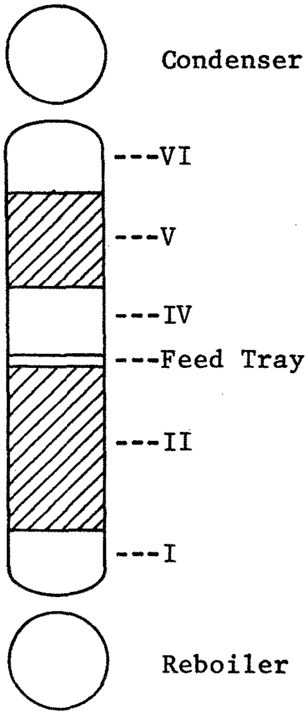


FIGURE 3-2. An infinite column with five distinct sections. The rectifying pinch occurs away from the feed tray.

Stripping and absorption occur again near the reboiler (Section I) and near the condenser (Section VI) respectively.

If the bottom product contains all the light components of the feed but some of the heavy components are separated from the top product, the pinch zone in the rectifying section will still be at an intermediate point away from the feed stage, similar to that section of the column in Figure 3-1. However, the pinch zone in the stripping section terminates in the feed stage. This type of column is schematically represented in Figure 3-2.

A similar statement can be applied to the case where all the heavy components of the feed are present in the distillate but some of the light components are separated from the bottoms product. In this case, the pinch zone occurs away from the feed plate in the stripping section, while the rectifying section pinch zone terminates at the feed stage. This type of column is schematically represented in Figure 3-3.

The paragraphs above describe three different types of fractionating columns at minimum reflux in which at least one of the pinch zones occurs away from the feed stage. Separations of these types fall under the Class II category such that, with infinite stages, some of the components are separated completely from the top product, or completely from the bottom product, or from both products.

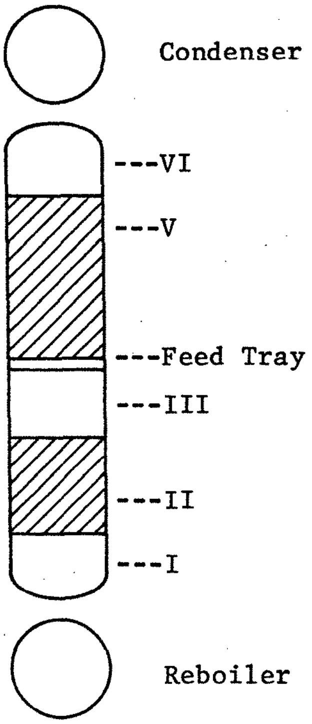


FIGURE 3-3. An infinite column with five distinct sections. The stripping pinch occurs away from the feed tray.

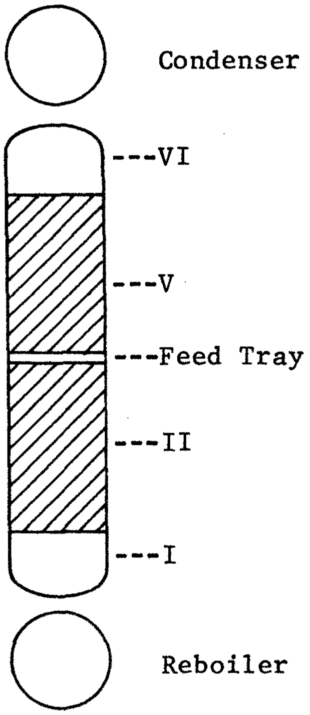


FIGURE 3-4. An infinite column with four distinct sections. Typical case of a bynary mixture.

If all the components in the feed are distributed to both the top and bottom products, both pinch zones terminate in the feed stage and only four sections are present in this column (Figure 3-4). This system is analogous to that of a bynary mixture and is classified under the Class I separations. The composition of the liquid and vapor phases of the feed are respectively identical with the liquid and vapor compositions in the constant composition zones except for superheated-vapor and subcooled-liquid feeds.

Since three different types of fractionating columns at minimum reflux are classified under Class II separations, it is possible to subclassify them according to the pinch zone occurrence at the rectifying and stripping sections of the column, as shown in Table 1.

TABLE 1. TYPES OF COLUMN SECTIONS AT MINIMUM REFLUX

CLASS OF SEPARATION	COMPONENT DISTRIBUTION	TYPE OF COLUMN SECTION
I	All Distributed	Rectifying-Type I Stripping-Type I
II-A	Lightest Separated Others Distributed	Rectifying-Type I Stripping-Type II
II-B	Heaviest Separated Others Distributed	Rectifying-Type II Stripping-Type I
II-C	Lightest Separated Heaviest Separated Others Distributed	Rectifying-Type II Stripping-Type II

The compositions of the pinch zones at the rectifying section and the stripping section are given by the familiar relationships (5):

$$\left(\frac{\ell}{d}\right)_{R*} = \frac{\left(\frac{L}{VK}\right)_{R*}}{1 - \left(\frac{L}{VK}\right)_{R*}} = \frac{A_{R*}}{1 - A_{R*}} \tag{3-1}$$

$$\left(\frac{v}{b}\right)_{\underline{S}*} = \frac{\left(\frac{VK}{L}\right)_{\underline{S}*}}{1 - \left(\frac{VK}{L}\right)_{\underline{S}*}} = \frac{S_{\underline{S}*}}{1 - S_{\underline{S}*}} \tag{3-2}$$

where ℓ = component liquid molar rate;

v = component vapor molar rate;

d = component molar rate in the distillate;

b = component molar rate in the bottoms;

L = liquid molar rate in the specific section;

V = vapor molar rate in the specific section;

K = component equilibrium constant in the specific section;

$R*$ = bottom stage of the rectifying pinch zone;

$\underline{S}*$ = top stage of the stripping pinch zone;

A_{R*} = component absorption factor for the rectifying pinch zone;

$S_{\underline{S}*}$ = component stripping factor for the stripping pinch zone.

In these equations and the following ones, the subscript "i" is understood for all terms.

These equations easily explain the existence of four types of fractionating columns when minimum reflux ($N = \infty$) is approached: A component present in the feed stream is distributed to both the top and bottom products (or constant composition zones), only if the factors A_{R*} and $S_{\underline{S}*}$ are both less than unity. A separated heavy component ($d_i = 0$) is one for which $A_{R*} \geq 1.0$. Similarly for a separated light component ($b_i = 0$), the factor $S_{\underline{S}*} \geq 1.0$. It is obvious that A_{R*} for the heavy key and $S_{\underline{S}*}$ for the light key must be less than 1.0 in order to meet the required specifications for these two components.

In binaries or narrow cut multicomponent systems, where all components are distributed, the absorption factor at the rectifying pinch, A_{R*}, and the stripping factor at the stripping pinch, $S_{\underline{S}*}$, of the column for all components are less than unity. However, this is not true for wide boiling feeds and Class II minimum reflux situations result for such systems.

For rigorous calculations, the minimum reflux can be approximated as an asymptote of the stages-reflux curve which results of a parameter study of the actual reflux required for a series of column designs with increasing stages for the same given separation of the key components. Such a curve is shown in Figure 3-5.

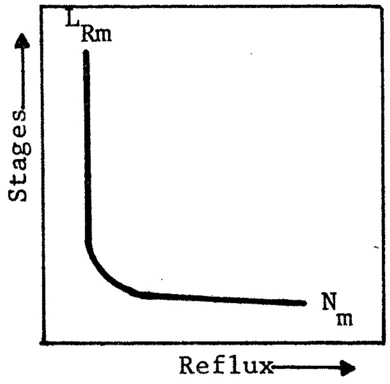


FIGURE 3-5. Typical Stages-Reflux curve.

If a parameter study is made and the column design case which represents the minimum reflux is chosen, a plot of temperature vs stage number will explain the behavior of the four different types of fractionating columns discussed above. These temperature plots are shown in Figure 3-6 through Figure 3-9. Similar curves can be obtained from plots of stream compositions or total molal overflow vs stage number.

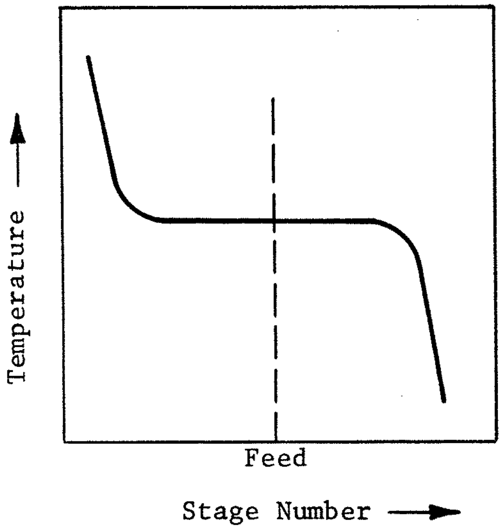


FIGURE 3-6. Class I

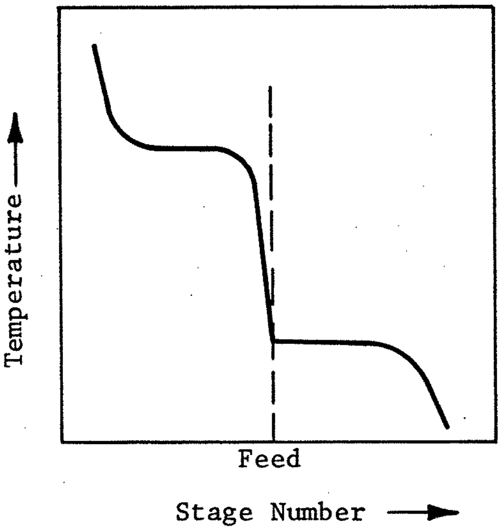


FIGURE 3-7. Class II-A

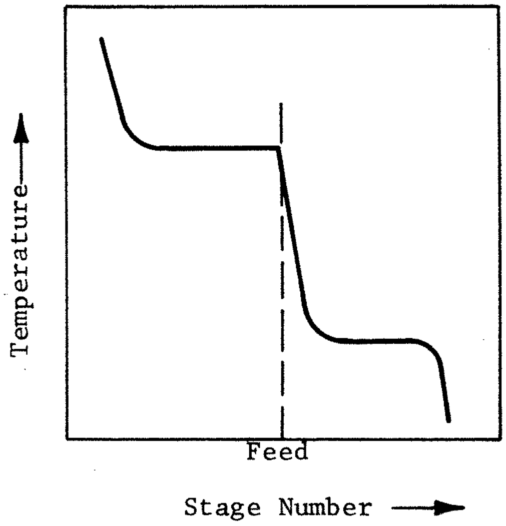


FIGURE 3-8. Class II-B

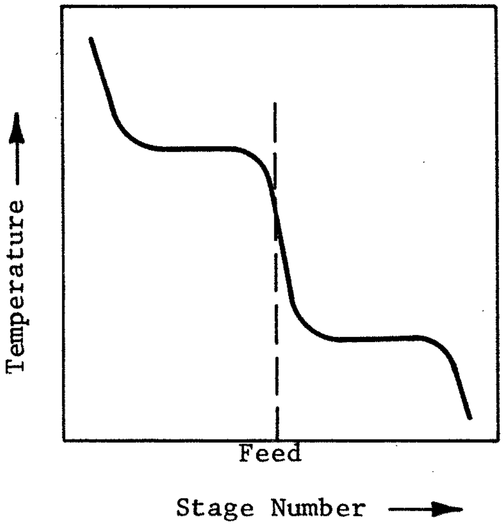


FIGURE 3-9. Class II-C

CHAPTER IV

LITERATURE SURVEY

There exist in the literature several methods for determining the minimum reflux ratio for a multicomponent system. Many of these methods are very complex. The estimation of the feed plate composition is essential in order to compute the minimum reflux required for the separation between distillate and feed plate, and between feed plate and bottoms.

Underwood (31) and Fenske (13) independently developed an equation for the minimum reflux required to attain a certain composition of the key components in the rectifying section. This equation is not accurate unless the compositions of the key components are known on the plate where the equation is applied. Underwood's equation (31) is applicable to binary mixtures or to completely distributed systems only, since it assumes that the composition on the stages immediately above and below the feed stage are approximately equal. This is true only if the liquid feed composition is the same as the liquid on the feed stage.

A false assumption that the ratio of the fractions of the key components in the liquid on the feed plate is the same as that of the same components in the liquid feed at minimum reflux has been presented in other methods (5,12,15).

Many of the methods developed (1,6,9,14,17,19) involve tedious trial and error.

Later, Underwood (32) developed equations for the determination of the minimum reflux for a multicomponent system based on constant volatility and constant molal overflow. These assumptions used by some investigators (14,22,32) are some of the most common ones made for short-cut techniques. These short-cut methods involve some loss of accuracy, but are used widely in preliminary design calculations.

Scheibel and Montross (27) have presented an empirical equation which eliminates the trial and error procedures. The procedure was modified by Bailey and Coates (3) to be applied to systems with varying volatility, but tedious trial and error is used.

Empirical correlations of the minimum and operating reflux ratios and equilibrium stages have been proposed as a short-cut design procedure by Brown and Martin (5), Gilliland (14), Erbar and Maddox (12), Maxwell (21), Colburn (6), and Gray (16).

Mayfield and May (23) assume a complete separation and no components lighter than the light key or heavier than the heavy key are present.

Many articles (10,11,12,26,28,29) have dealt with minor modifications or rearrangements of a second Underwood's minimum reflux method (33). Much of the work is of little consequence in advancing the techniques used to find minimum reflux.

An exact calculation of the minimum reflux for the Class II separations for which the simplifying assumptions of constant volatility and constant molal overflow are not valid has been carried out by Brown and Holcomb (4). Their method is an adaptation to minimum reflux of the Lewis and Matheson (20) plate-to-plate procedure for calculation of finite plates and reflux. The method assumes distribution of the key components only. If several components other than the key components are distributing, the operations are time consuming.

Shiras, Hanson and Gibson (28) presented methods which distinguish between systems with all components of the feed being distributed (Class I Separations) and systems on which some components have been separated (Class II Separations). This latter method is a rigorous plate-to-plate calculation.

Another plate-to-plate procedure which does not require pre-estimation of component distribution, but still is too time-consuming, is the method of Thiele and Geddes (30), adapted to the calculation of minimum reflux. Some authors (1,2,28) have suggested the use of this method which is outlined by Holland (18) including convergence methods proposed by McDonough (24) and McDonough and Holland (25).

Edmister (7,8) calculated the fractionation in each section of the column by short-cut equations based on a simplification of the rigorous Thiele and Geddes series solutions.

CHAPTER V

THEORY AND DEVELOPMENT OF EQUATIONS

The proposed method presented in this paper was guided by Dr. Ralph Cecchetti. In this work, his development of the simplified Thiele and Geddes procedure for the design of fractionating columns has been extended to the calculation of minimum reflux conditions. Some of the equations of the proposed new method have been presented by Edmister (7,8) for the calculation of theoretical stages and component distribution for multi-component fractionation. Holland (18) uses the general plate-to-plate calculational procedure of Thiele and Geddes for the calculation of minimum reflux and applies the Θ Method of Convergence (24,25) to the specified working conditions of the column.

The following sections contain the derivation of the short-cut equations that relate the component rates at the pinches and the component rates at the feed stage with the distillate composition and the number of stages between these sections of the column. The procedure employed in this new method will also calculate the number of stages between the pinches for each section, i.e., rectifying and stripping, and the feed stage.

Material Balances for the Rectifying Section

Distributed and light separated components. As discussed in Chapter III, the Equation (3-1) relating the rectifying pinch zone composition for distributed and light separated components is given by:

$$\left(\frac{\ell}{d}\right)_{R*} = \frac{A_{R*}}{1-A_{R*}}$$

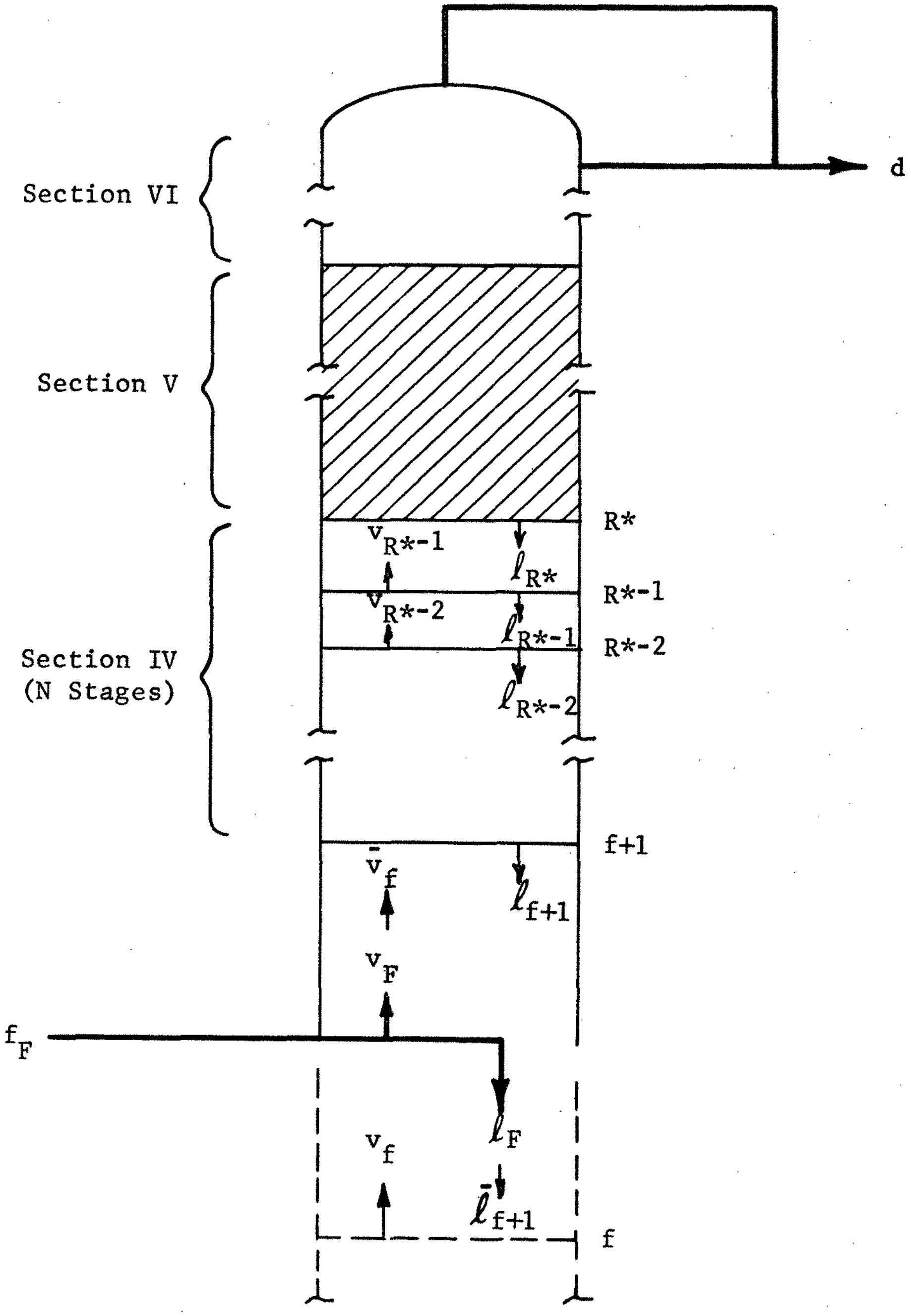


FIGURE 5-1. Component rates in the rectifying section of a fractionating column at minimum reflux conditions.

For the stages, N, between the feed and the rectifying pinch zones, an equation can be developed for the composition on the bottom stage of the rectifying section, f+1, by material balances enclosing the top of the column, the bottom stage of the rectifying pinch, R*, through to the bottom stage of the rectifying section.

By an inspection of Figure 5-1, the component liquid rate leaving stage R* of the top infinite section of the column is given by:

$$\ell_{R*} = v_{R*-1} - d \tag{5-1}$$

Since $v_{R*-1} = \dfrac{\ell_{R*-1}}{A_{R*-1}}$, Equation (5-1) may be expressed as follows:

$$\left(\frac{\ell}{d}\right)_{R*-1} = A_{R*-1}\left[\left(\frac{\ell}{d}\right)_{R*} + 1\right] \tag{5-2}$$

or

$$\left(\frac{\ell}{d}\right)_{R*-1} = A_{R*-1}\left(\frac{\ell}{d}\right)_{R*} + A_{R*-1} \tag{5-3}$$

Similarly, for the R^{*-2} stage:

$$\left(\frac{\ell}{d}\right)_{R*-2} = A_{R*-2}\left[\left(\frac{\ell}{d}\right)_{R*-1} + 1\right]$$

Substituting for $(\ell/d)_{R*-1}$ with Equation (5-2) gives:

$$\left(\frac{\ell}{d}\right)_{R*-2} = A_{R*-2}\left\{A_{R*-1}\left[\left(\frac{\ell}{d}\right)_{R*} + 1\right] + 1\right\} \tag{5-4}$$

or

$$\left(\frac{\ell}{d}\right)_{R*-2} = A_{R*-2}\,A_{R*-1}\left(\frac{\ell}{d}\right)_{R*} + A_{R*-2}\,A_{R*-1} + A_{R*-2} \tag{5-5}$$

This procedure can continue until stage f+1 is reached, which gives the general expression:

$$\left(\frac{\ell}{d}\right)_{f+1} = A_{f+1}\cdots A_{R*-1}\left(\frac{\ell}{d}\right)_{R*} + A_{f+1}\cdots A_{R*-1} + A_{f+1}\cdots A_{R*-2} + \ldots + A_{f+1} \tag{5-6}$$

where A = absorption factors subscripted for each stage.

This equation is completely rigorous and requires the component absorption factor, A, on each stage of that section of the column for its solution.

If an average component absorption factor can be determined, such that it gives the identical solution as the rigorous equation, Equation (5-6) simplifies as follows:

$$\left(\frac{\ell}{d}\right)_{f+1} = A_A^N\left(\frac{\ell}{d}\right)_{R*} + A_A^N + A_A^{N-1} + \ldots + A_A \tag{5-7}$$

where N = number of stages between stage R* of the top infinite section and stage f+1;

A_A = average absorption factor for the component in the N-stage section.

Simplifying further,

$$\left(\frac{\ell}{d}\right)_{f+1} = A_A^N\left(\frac{\ell}{d}\right)_{R*} + \frac{A_A^{N+1} - A_A}{A_A - 1} \tag{5-8}$$

By utilizing Equation (3-1), $(\ell/d)_{R*}$ is substituted in Equations (5-6), (5-7) or (5-8), and the value of $(\ell/d)_{f+1}$ can be found. The use of Equation (3-1) requires that the absorption factor at the rectifying pinch, A_{R*}, be less than 1, which is true only for distributed components and light separated components. The liquid rates, ℓ_{R*}, of the heavy separated components at the rectifying pinch can be determined by Equations (5-14) or (5-15). The derivation of these equations follows.

Heavy separated components. A material balance enclosing the bottom of the column and the feed stage, f, (Figure 5-2) gives:

$$v_f + b = \bar{\ell}_{f+1} = \ell_{f+1} + \ell_F \tag{5-9}$$

since

$$f_F = \ell_F + v_F \tag{5-10}$$

Therefore,

$$v_f + b + v_F = \ell_{f+1} + f_F \tag{5-11}$$

where f_F = total component molar rate in feed;

ℓ_F = component molar rate in liquid feed;

v_F = component molar rate in vapor feed;

Since $b=f_F$ for a heavy separated component, Equation (5-11) becomes:

$$\ell_{f+1} = v_f + v_F \tag{5-12}$$

Equation (5-6) can be modified to give:

$$\ell_{f+1} = A_{f+1}\cdots A_{R*-1}\left(\ell_{R*}\right) + A_{f+1}\cdots A_{R*-1}(d) + A_{f+1}\cdots A_{R*-2}(d) +\ldots+ A_{f+1}(d)$$

Since d=o, the above expression becomes:

$$\ell_{f+1} = A_{f+1}\cdots A_{R*-1}\left(\ell_{R*}\right) \tag{5-13}$$

Substitution of Equation (5-13) into Equation (5-12), gives:

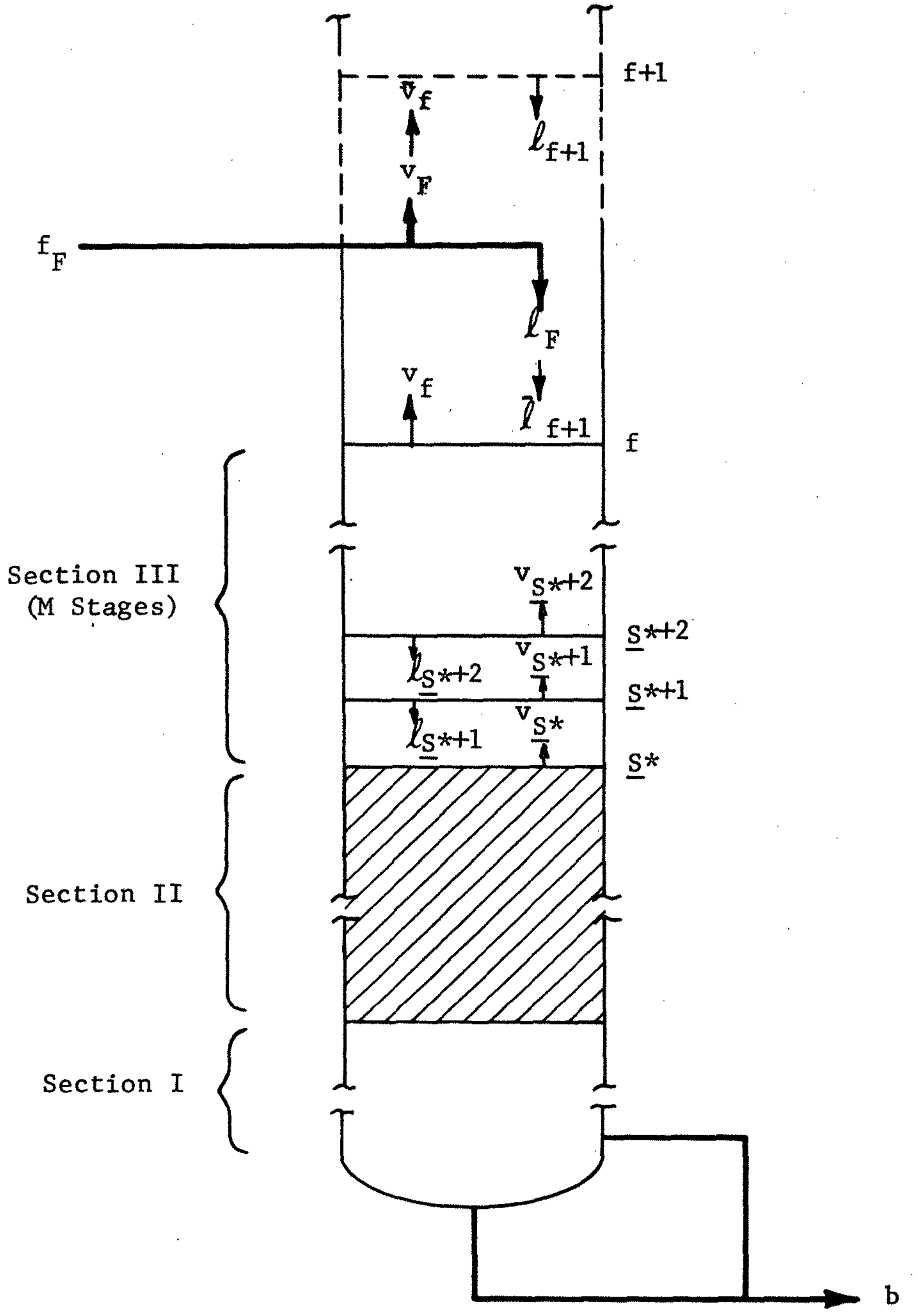


FIGURE 5-2. Component rates in the stripping section of a fractionating column at minimum reflux conditions.

$$\ell_{R*} = \frac{1}{A_{f+1}} \cdots \frac{1}{A_{R*-1}} (v_f + v_F)$$

or

$$\ell_{R*} = S_{f+1} \cdots S_{R*-1} (v_f + v_F) \qquad (5\text{-}14)$$

If an average stripping (or absorption) factor is used, Equation (5-14) may be written as:

$$\ell_{R*} = S_A^N (v_f + v_F) \qquad (5\text{-}15)$$

These equations are applicable to a heavy separated component to give the liquid rate from the bottom stage of the rectifying section, ℓ_{f+1}, and the liquid rate from the pinch of that section, ℓ_{R*}, provided the vapor rate of that component from the feed stage, v_f, is known.

The development of Equations (5-19), (5-20) and (5-21) to determine v_f, or $(v/b)_f$, similar to equations (5-6), (5-7) and (5-8) respectively, for distributed and heavy separated components will be given on the following section.

<u>Material Balances for the Stripping Section</u>

<u>Distributed and heavy separated components</u>. As discussed in Chapter III, the Equation (3-2) relating the stripping pinch zone composition for distributed and heavy separated components is given by:

$$\left(\frac{v}{b}\right)_{\underline{S}*} = \frac{S_{\underline{S}*}}{1-S_{\underline{S}*}}$$

In the event that M stages exist between the feed and the stripping pinch zones, an equation similar to Equation (5-6), relating the component vapor rates in these two sections of the column, is necessary.

By a material balance around the bottom of the column and the top stage of the stripping pinch, $\underline{S}*$, through the feed stage, f, the component vapor rate leaving stage $\underline{S}*$ of the bottom infinite section of the column (Figure 5-2) is:

$$v_{\underline{S}*} = \ell_{\underline{S}*+1} - b \tag{5-16}$$

Since $\ell_{\underline{S}*+1} = \dfrac{v_{\underline{S}*+1}}{S_{\underline{S}*+1}}$, Equation (5-16) becomes:

$$\left(\frac{v}{b}\right)_{\underline{S}*+1} = S_{\underline{S}*+1}\left[\left(\frac{v}{b}\right)_{\underline{S}*} + 1\right]$$

or

$$\left(\frac{v}{b}\right)_{\underline{S}*+1} = S_{\underline{S}*+1}\left(\frac{v}{b}\right)_{\underline{S}*} + S_{\underline{S}*+1} \tag{5-17}$$

For the $\underline{S}*+2$ stage:

$$\left(\frac{v}{b}\right)_{\underline{S}*+2} = S_{\underline{S}*+2}\left\{S_{\underline{S}*+1}\left[\left(\frac{v}{b}\right)_{\underline{S}*} + 1\right] + 1\right\}$$

or

$$\left(\frac{v}{b}\right)_{\underline{S}*+2} = S_{\underline{S}*+2}\,S_{\underline{S}*+1}\left(\frac{v}{b}\right)_{\underline{S}*} + S_{\underline{S}*+2}\,S_{\underline{S}*+1} + S_{\underline{S}*+2} \tag{5-18}$$

Similarly, for the successive stages up to stage f, the general expression is obtained:

$$\left(\frac{v}{b}\right)_{f} = S_{f}\ldots S_{\underline{S}*+1}\left(\frac{v}{b}\right)_{\underline{S}*} + S_{f}\ldots S_{\underline{S}*+1} + S_{f}\ldots S_{\underline{S}*+2} + \ldots + S_{f} \tag{5-19}$$

where S = stripping factors subscripted for each stage.

Component stripping factors, S, are required on each stage of that section of the column to solve the above rigorous equation. The following equation results when an average component stripping factor is used:

$$\left(\frac{v}{b}\right)_f = S_A^M \left(\frac{v}{b}\right)_{\underline{S}*} + S_A^M + S_A^{M-1} + \ldots + S_A \qquad (5\text{-}20)$$

where M = number of stages between $\underline{S}$* of the bottom infinite section and stage f;

S_A = average stripping factor for the component in the M-stage section.

Simplifying further,

$$\left(\frac{v}{b}\right)_f = S_A^M \left(\frac{v}{b}\right)_{\underline{S}*} + \frac{S_A^{M+1} - S_A}{S_A - 1} \qquad (5\text{-}21)$$

To solve these equations, $(v/b)_{\underline{S}*}$ must be determined by Equation (3-2), which applies for distributed components and heavy separated components. The derivation of the equations for the determination of $v_{\underline{S}*}$ for the light separated components follows.

<u>Light separated components</u>. Since b = o, Equation (5-9) gives:

$$v_f = \ell_{f+1} + \ell_F \qquad (5\text{-}22)$$

Equation (5-19 can be modified to give:

$$v_f = S_f \ldots S_{\underline{S}*+1} \left(v_{\underline{S}*}\right) + S_f \ldots S_{\underline{S}*+1} (b) + S_f \ldots S_{\underline{S}*+2} (b) + \ldots + S_f (b)$$

Since b = o, the above expression becomes:

$$v_f = S_f \ldots S_{\underline{S}*+1} \left(v_{\underline{S}*}\right) \qquad (5\text{-}23)$$

If Equation (5-23) is substituted into Equation (5-22), it yields:

$$v_{\underline{S}*} = \frac{1}{S_f} \cdots \frac{1}{S_{f+1}} \left(\ell_{f+1} + \ell_F \right)$$

or

$$v_{\underline{S}*} = A_f \cdots A_{f+1} \left(\ell_{f+1} + \ell_F \right) \qquad (5\text{-}24)$$

If an average absorption (or stripping) factor is used, Equation (5-24) becomes:

$$v_{\underline{S}*} = A_A^M \left(\ell_{f+1} + \ell_F \right) \qquad (5\text{-}25)$$

The liquid rate from the bottom stage of the rectifying section, ℓ_{f+1}, is determined by Equations (5-6), (5-7) or (5-8) for the light separated components.

Feed Plate Match

The feed plate match equation for the short-cut procedure is identical to that used in the rigorous Thiele and Geddes method.

This equation is obtained from Equation (5-9) which can be expressed as follows:

$$v_f + b = \ell_{f+1} + \ell_F \left(\frac{b + d}{f_F} \right)$$

and

$$v_f + b - \frac{\ell_F \, b}{f_F} = \ell_{f+1} + \frac{\ell_F \, d}{f_F}$$

$$b \left[\frac{v_f}{b} + 1 - \frac{\ell_F}{f_F} \right] = d \left[\frac{\ell_{f+1}}{d} + \frac{\ell_F}{f_F} \right]$$

which can be solved for (b/d) to give:

$$\frac{b}{d} = \frac{\left(\frac{\ell}{d}\right)_{f+1} + \frac{\ell_F}{f_F}}{\left(\frac{v}{b}\right)_f + \frac{v_F}{f_F}} \tag{5-26}$$

For all liquid feed $(\ell_F/f_F) = 1$ and $(v_F/f_F) = 0$, and Equation (5-26) becomes:

$$\frac{b}{d} = \frac{\left(\frac{\ell}{d}\right)_{f+1} + 1}{\left(\frac{v}{b}\right)_f} \tag{5-27}$$

For all vapor feed, $(v_F/f_F) = 1$ and $(\ell_F/f_F) = 0$, and Equation (5-26) gives:

$$\frac{b}{d} = \frac{\left(\frac{\ell}{d}\right)_f}{\left(\frac{v}{b}\right)_f + 1} \tag{5-28}$$

CHAPTER VI

METHOD OF CALCULATION

This chapter describes the calculational procedure used to calculate the minimum reflux for the four different types of column that can occur as a result of component distributions.

The primary interest of this work is the determination of the liquid rate at the rectifying pinch zone, L_{R*}, which represents the constant internal minimum reflux of the column.

The external reflux, L_R, can then be obtained by overall heat balance calculations as will be seen later on this chapter.

The proposed method uses the rectifying pinch and the stripping pinch sections of the column to obtain the material balance which will give the component distribution.

This method is a trial and error procedure, and in order to initiate the calculations, values for the liquid rate at the rectifying pinch, L_{R*}, and the total distillate rate, D, are assumed. The other internal loadings in the column are then determined by overall material balance and the assumption of constant molal overflow between the rectifying and stripping pinch stages:

$$V_{R*} = L_{R*} + D \qquad (6\text{-}1)$$

$$L_{\underline{S}*} = L_{R*} + L_F \qquad (6\text{-}2)$$

$$V_{\underline{S}*} = V_{R*} - V_F \qquad (6\text{-}3)$$

and the bottom rate is:

$$B = F - D \qquad (6\text{-}4)$$

where L_{R*} = liquid molar rate at the rectifying pinch;

V_{R*} = vapor molar rate at the rectifying pinch;

$L_{\underline{S}*}$ = liquid molar rate at the stripping pinch;

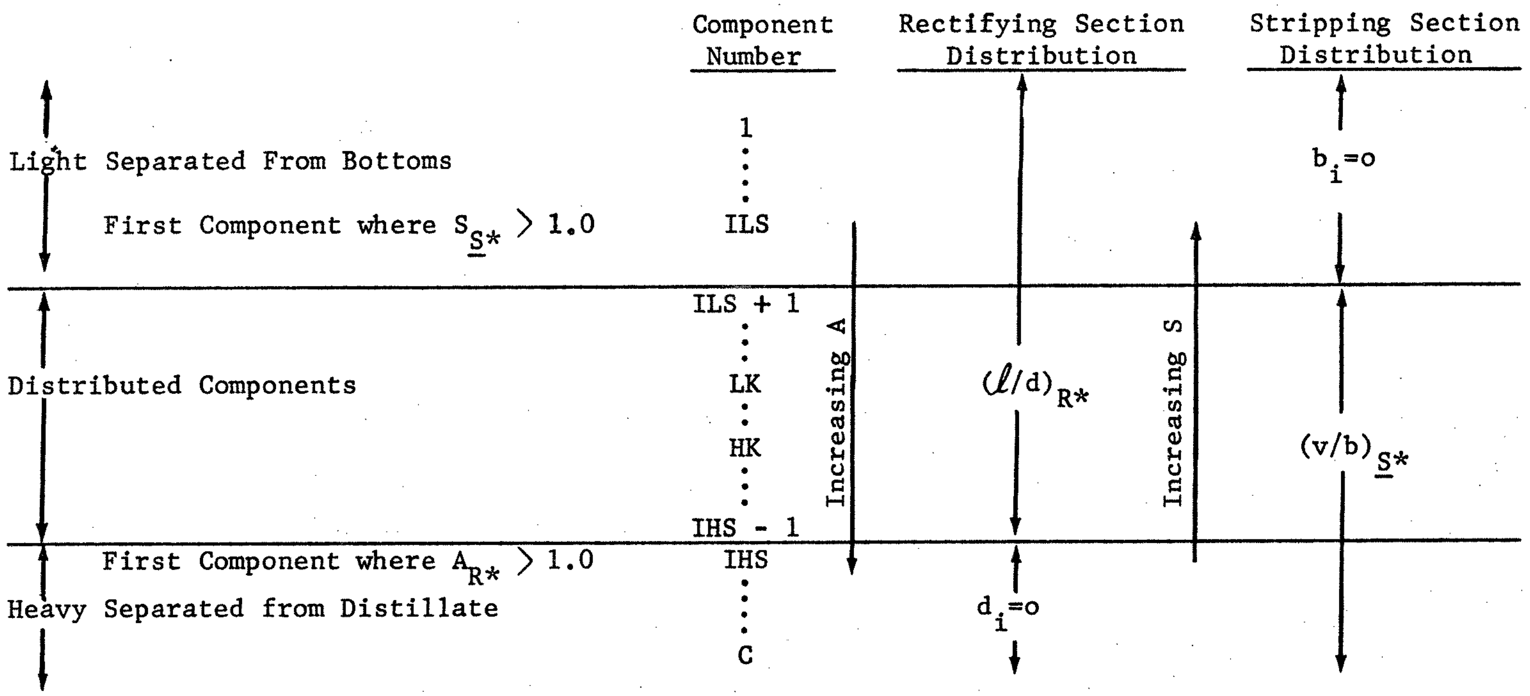
$V_{\underline{S}*}$ = vapor molar rate at the stripping pinch;

L_F = liquid molar flow rate of feed;

V_F = vapor molar flow rate of feed.

In the next step, values are assumed for temperatures at the feed locations, T_f and T_{f+1}, and at the pinch locations, T_{R*} and $T_{\underline{S}*}$. The K values at these temperatures combined with the respective L/V's give the component absorption factors or stripping factors at these points of the column.

The component distribution and the type of column section is then determined by inspection of the absorption factors at the rectifying pinch, A_{R*}, and the stripping factors at the stripping pinch, $S_{\underline{S}*}$: light separated components are those with values of $S_{\underline{S}*}$ greater than 1.0, while heavy separated components are those with values of A_{R*} greater than 1.0. This is shown on the following diagram:


Component Number
Rectifying Section Distribution
Stripping Section Distribution
Light Separated From Bottoms
First Component where $S_{\underline{S}*} > 1.0$
1
ILS
b_i=o
ILS + 1
Distributed Components
LK
HK
IHS - 1
Increasing A
$(\ell/d)_{R*}$
Increasing S
$(v/b)_{\underline{S}*}$
First Component where $A_{R*} > 1.0$
IHS
Heavy Separated from Distillate
d_i=o
C

Therefore, the four different types of column occur under the following circumstances:

- If ILS = 0 and IHS = C + 1
    - All components are distributed
    - Rectifying and Stripping sections are Type I
- If ILS = 0 and IHS $<$ C + 1
    - All light components are distributed
    - Some heavy components are separated from the distillate
    - Rectifying section is Type II and Stripping section is Type I
- If ILS $>$ 0 and IHS = C + 1
    - Some light components are separated from the bottoms.
    - All heavy components are distributed
    - Rectifying section is Type I and Stripping section is Type II
- If ILS $>$ 0 and IHS $<$ C + 1
    - Some light components are separated from bottoms
    - Some heavy components are separated from distillate
    - Rectifying and Stripping sections are Type II

Type I in Both Column Sections

In systems with type I in both sections, the minimum reflux can be calculated directly by Underwood's Equations (31). If these equations are applied to the two key components whose specified distributions (b/d), define the separation, they give an exact solution for the minimum reflux for Class I separations.

These equations are presented here for convenient reference.

For a partially vaporized feed:

$$L_{R*} = \frac{L_F\left[\left(\frac{d}{\ell_F}\right)_A - \left(\frac{d}{\ell_F}\right)_B \alpha_{AB}\right]}{\alpha_{AB} - 1} \qquad (6\text{-}5)$$

where A,B = specific components

α_{AB} = relative volatility for the key components at the feed stage conditions.

For all liquid feed:

$$L_{R*} = \frac{F\left[\left(\frac{d}{f_F}\right)_A - \left(\frac{d}{f_F}\right)_B \alpha_{AB}\right]}{\alpha_{AB} - 1} \qquad (6\text{-}6)$$

since $L_F = F$ and $\ell_F = f_F$.

For all vapor feed:

$$L_{R*} = \frac{F\left[\alpha_{AB}\left(\frac{d}{f_F}\right)_A - \left(\frac{d}{f_F}\right)_B\right]}{\alpha_{AB}} - 1 \qquad (6\text{-}7)$$

The traditional approach has been to use the feed temperature for the values of K_f or α_{AB}. However, the preferred solution is to calculate the component distributions (b/d), with the assumed temperatures at the feed location ($T_f = T_{f+1}$) to give K values and solve by the following:

$$\frac{b}{d} = \frac{L_{R*}\ (1-K_f) + F - DK_f}{L_{R*}\ (K_f-1) + DK_f} \qquad (6\text{-}8)$$

for a liquid feed.

And for a vapor feed:

$$\frac{b}{d} = \frac{L_{R*}\ (1-K_f) + FK_f - DK_f}{L_{R*}\ (K_f-1) + DK_f} \qquad (6\text{-}9)$$

The values of (b/d) can then be used to determine the individual component distillate rate, d, by:

$$d = \frac{f_F}{1 + \left(\frac{b}{d}\right)} \tag{6-10}$$

Since the rectifying pinch occurs at the feed stage, $T_{f+1} = T_{R*}$, and the liquid rate at the stage above the feed stage, f+1, can be calculated by Equation (3-1) which becomes:

$$\left(\frac{\ell}{d}\right)_{f+1} = \frac{A_{f+1}}{1 - A_{f+1}} \tag{6-11}$$

The values of ℓ_{f+1} are determined and normalized to give reflux compositions at the feed stage. The bubble point is calculated and the resulting K values or α values used for the next trial to determine L_{R*}. Convergence results when T_{R*} reaches a constant value.

Type II in Rectifying Section, Type I in Stripping Section

The objective for this type of system is to calculate the number of stages N, between the rectifying pinch, R*, and the stage above the feed stage, f+1. This is done by applying Equation (5-6) or Equation (5-8) to the heavy key component.

If the calculations are done by hand, a good approximation results by using Equation (5-8). If a computer program is used, as the one presented in this paper, Equation (5-6) can be used for better results, assuming a linear profile of the absorption factors between the calculated values at the f+1 and R* locations.

The ratios $(\ell/d)_{R^*,HK}$, and $(v/b)_{\underline{S}^*,HK}$ are calculated by Equation (3-1) and Equation (3-2) respectively as discussed in Chapter V. Note that $(v/b)_f = (v/b)_{\underline{S}^*}$ in this case.

The Feed Plate Match Equation (5-26) is then used to determine $(b/d)_{HK}$ for the heavy key component.

Starting with N = 0, the value of N is varied until the specified $(b/d)_{HK}$ is calculated. Interpolation can be used between trials to find N.

Type I in Rectifying Section, Type II in Stripping Section

The objective in this case is to calculate the number of stages M, between the stripping pinch, $\underline{S}^*$, and the feed stage, f.

Equations (5-19) or (5-21) are applied to the light key component. Again, Equation (5-19) can be used for better results with a linear profile between the calculated stripping factors at the $\underline{S}^*$ and f locations.

The ratios $(v/b)_{\underline{S}^*,LK}$, and $(\ell/d)_{R^*,LK}$ are calculated by Equation (3-2) and Equation (3-1) respectively as discussed in Chapter V. Note that $(\ell/d)_{f+1} = (\ell/d)_{R^*}$.

The Feed Plate Match Equation (5-26) is again used here, to determine $(b/d)_{LK}$ for the light key component.

Starting with M = 0, the value of M is varied until the specified $(b/d)_{LK}$ is calculated. Interpolation can be used between trials to find M.

Type II in Both Sections

This case is actually the general one. The discussed previous cases are special situations where N, M or both were zero.

The objective is to calculate N and M. The calculation of $(\ell/d)_{R*}$ and $(v/b)_{\underline{S}*}$ is the same as discussed in the previous sections except that these values are determined for both the key components. The solution of N and M is the simultaneous solution of Equation (5-6) and Equation (5-19) for both key components.

This in effect, gives two (b/d) equations, one for the light key and one for the heavy key in the two unknowns N and M.

Material Balances Calculation Procedure

The following stepwise procedure is self-explanatory:

1. Evaluate Equation (3-1) to obtain $(\ell/d)_{R*}$ for the distributed and light separated components.
2. Calculate $(\ell/d)_{f+1}$:
   a. If $N = 0$, the rectifying section is Type I and $IHS = C+1$ (see diagram on page 30). It results in this case that $(\ell/d)_{f+1} = (\ell/d)_{R*}$.
   b. If $N > 0$, $IHS < C+1$ and the rectifying section is Type II. In this case, $(\ell/d)_{f+1}$ is calculated by Equation (5-6).
3. Determine $(v/b)_{\underline{S}*}$ for the distributed and heavy separated components by Equation (3-2).

4. Calculate $(v/b)_f$:

   a. If M = 0, the stripping section is Type I and ILS = 0 (see diagram on page 30). Therefore, $(v/b)_{\underline{S}*} = (v/b)_f$.

   b. If M > 0, ILS > 0 and the stripping section is Type II. Here, $(v/b)_f$ is calculated by Equation (5-19).

5. Calculate (b/d) for the distributed components by Equation (5-26). Correct $(b/d)_{LK}$ and $(b/d)_{HK}$ to be consistent with the specifications. This is done by using the multiplier θ, such that,

$$(b/d)_{LK,\ spec.} = \theta_{LK}\ (b/d)_{LK,\ calc.}$$

and

$$(b/d)_{HK,\ spec.} = \theta_{HK}\ (b/d)_{HK,\ calc.}$$

6. Determine the distillate rate $D_{calc.} = \sum_c d$. For the light separated components, $d = f_F$. For the separated heavies, d = o. The flow rates for all distributed components are evaluated by an overall material balance which yields,

$$d = \frac{f_F}{1 + \left(\frac{b}{d}\right)}$$

The specified values of (b/d) are used for the light and heavy key components.

7. Calculate the liquid rate at the rectifying pinch zone, $L_{R*,\ calc.}$. This is done as follows:

   a. For the distributed and light separated components, determine ℓ_{R*} by,

$$\ell_{R*} = \left(\frac{\ell}{d}\right)_{R*} d$$

b. For the heavy separated components, ℓ_{R*} is determined by Equation (5-14).

c. Determine $L_{R*,\ calc.} = \sum_c \ell_{R*}$.

At this point, check for convergence on the specified value of L_{R*}:

- If $L_{R*,\ calc.} = L_{R*,\ spec.}$, "converge" = 1
- If $L_{R*,\ calc.} \neq L_{R*,\ spec.}$, "converge" = 0

8. Calculate liquid rates on f+1, and vapor rates on S_f and $\underline{S}*$ by the following procedure:

a. For the distributed and light separated components,

$$\ell_{f+1} = \left(\frac{\ell}{d}\right)_{f+1} d$$

v_f is determined by Equation (5-22) and $v_{\underline{S}*}$ by Equation (5-24).

b. For the separated heavies, ℓ_{f+1} is determined by Equation (5-12). Here also,

$$v_f = \left(\frac{v}{b}\right)_f b$$

and

$$v_{\underline{S}*} = \left(\frac{v}{b}\right)_{\underline{S}*} b$$

c. Then, the sum of the calculated component flow rates gives

$$L_{f+1} = \sum_c \ell_{f+1}$$

$$V_f = \sum_c v_f$$

$$V_{\underline{S}*} = \sum_c v_{\underline{S}*}$$

9. Mole fraction compositions on stages R*, f+1, f and $\underline{S}$* are calculated by normalizing the component molar rates with the total molar rates calculated in step 8-c.

10. T_{f+1} and T_{R*} are determined by bubble point calculations. T_f and $T_{\underline{S}*}$ are found by dew point calculations.

11. Check convergence.

    - If the calculated temperatures are different from the values used in the trial, the new values are used to calculate absorption and stripping factors, determine the type of column sections and then repeat the stepwise procedure just outlined. The value of $D_{calc.}$ from this trial is used for the next trial, but L_{R*} must not be changed. New values of V_{R*}, $L_{\underline{S}*}$ and B are also determined.
    - If the calculated temperatures are the same as the values used in the trial, check "converge" (see step 7). The trial should be repeated if "converge" = 0.
    - If the calculated temperatures are the same and "converge" = 1, this is a converged case for the specified value of L_{R*}.

12. When the calculations are converged for the value of L_{R*}, the value of θ_{LK} and θ_{HK} are a measure of the deviation from convergence to the specified (b/d) for the key components. For the second iteration on L_{R*} an arbitrary change is made in the direction of convergence, i.e., bringing the θ values to 1.0. After the second iteration, interpolation on $\Delta\theta$ and ΔL_{R*} can be used to estimate the next iteration on L_{R*}. This procedure converges all systems with Type I in either or both sections of the column.

For Type II systems in both sections, the Θ values become equal to 1.0 when the value of L_{R*} is in the vicinity of the true minimum reflux. However, this is not necessarily the final answer. The number of stages N and M can adjust the key component compositions, so that the specified separation is made at a reflux higher than the minimum. Successively, lower values of L_{R*} are then assumed and this results in lower values of N and M. The total calculation is converged when the values of N and M reach a minimum, i.e., lower values of L_{R*} give non-convergence on the specified key components split.

Enthalpy Balance

The external minimum reflux was calculated by use of the following enthalpy balance. Enclosing the rectifying pinch and the top plate of the column, it gives:

$$V_{R*}H_{R*} + L_{Rm}h_{Rm} = V_1H_1 + L_{R*}h_{R*} \qquad (6\text{-}12)$$

where V_1 = molar flow rate of the vapor from the top stage of the column;

H = enthalpy of one mole of the vapor leaving the specific stage or section of the column;

h = enthalpy of one mole of the liquid leaving the specific stage or section of the column.

Since:

$$V_1 = L_{Rm} + D$$

and

$$V_{R*} = L_{R*} + D$$

Equation (6-12) reduces to:

$$L_{Rm} = \frac{L_{R*} \ (H_{R*} - h_{R*}) \ + \ D \ (H_{R*} - H_1)}{(H_1 - h_{Rm})} \tag{6-13}$$

CHAPTER VII

DISCUSSION OF ILLUSTRATIVE EXAMPLES

The minimum reflux was calculated for four hydrocarbons mixtures which at minimum reflux conditions fall into each possible combination of Class I or Class II separations.

The true minimum reflux was determined by a plot of the actual reflux required to make the specified separation of the key components vs the number of stages specified. Such a plot approaches the minimum reflux at a value of stages that is 10-20 times the minimum number of stages required for the specified separation. An example of such a plot is shown in Figure A-1.

The actual reflux required to make the separation for various stages from 8 to 100 was determined by a plate-to-plate procedure available to the author through Esso Research and Engineering Company. This program uses a Newton-Raphson algorithim. One option in the program allows the user to specify stages and key component split and the program then calculate the required reflux.

The internal minimum reflux was then calculated by the short-cut method outlined in this work, through a computer program as listed in Appendix B. The values obtained by this method were then compared with the rigorous plate-to-plate minimum reflux at the constant composition zone. These results are shown in Table A-10. The results obtained by the short-cut method are in agreement with those obtained by the plate-to-plate procedure. Only in the case for a Type II situation in both sections of the column, the values are off by 7.6% as compared with the plate-to-plate values.

The external minimum reflux calculated by an enthalpy balance was also in agreement with the one obtained by the plate-to-plate procedure (see Table A-10). Enthalpies were calculated using a composition independent procedure available to the author through Esso Research and Engineering Company. This procedure is the same one used by the plate-to-plate program.

The short-cut method for minimum reflux that is most commonly used is the method of Underwood. This procedure gives the value of the reflux at the stage above the feed. However, the Underwood value is frequently taken as the external minimum reflux. This can lead to a significant error when the actual external reflux is specified as a ratio to the Underwood minimum reflux for the design of a fractionating column. Underwood's values for the four examples are also given in Table A-10.

Specifications for Examples 1, 2, 3, and 4 are presented in Table A-1. The key components split is the same for all four examples.

Example 1 is a typical case of Class II separations which presents a Type I rectifying section and a Type II stripping section. In this example, light components are separated in the distillate while the keys and heavier are distributed to both products. This is shown in Table A-2. Temperature profiles from the various plate-to-plate cases are plotted in Figure A-2. These temperature profiles illustrate the typical behavior of this type of column as minimum reflux conditions are approached.

Example 2 and 3 are also Class II separations, and although the rectifying section is Type II for both cases, the stripping section is Type I for Example 2 and Type II for Example 3. Tables A-4 and A-6 respectively, show the distribution of the components for these two cases. Example 2 is similar to Example 1 except that in this case, a heavy component is separated in the bottoms. In Example 3, only the key components are distributed.

Example 4 is the typical case of Class I separations, and therefore, both sections of the column are Type I. Table A-8 shows all components distributed in both products.

Temperature profiles for Examples 2, 3, and 4 are shown in Figures A-3, A-4, and A-5. These plots were obtained from plate-to-plate cases with 100 stages each, since this number of stages was high enough to develop the plateaus and approximate the rigorous value of the minimum reflux. Cases with 200 stages were obtained and no change in the minimum reflux value was observed.

Tables A-3, A-5, A-7, and A-9 tabulate the flow rates and temperatures at the key locations of the column as they were obtained by the short-cut procedure and by the plate-to-plate program. By an inspection of these Tables, the values of the internal flow rate, obtained for Examples 1, 2, and 4 are in agreement with the values obtained by the plate-to-plate procedure. Small differences are due to the pinches for the intermediate trials. The internal flow rates calculated for Type II systems in both column sections show some disagreement with the values obtained by the plate-to-plate procedure. (See Table A-7). Enthalpy balances to establish L_{f+1} and $L_{\underline{S}*}$ rather than using constant molal overflow would probably eliminate most if not all of this error. This case, with only two distributed components was the most difficult to converge.

The same vapor-liquid equilibrium ratio (K) values were used for the rigorous plate-to-plate solution as for the short-cut procedures. Five values for each component at five different temperatures and the column pressure were taken from the plate-to-plate results and read in the input cards to the computer program used. A polynomial curve-fit was used to obtain K values at other temperatures. This is done by a sub-routine program listed in Appendix B.

Other sub-routine programs were written for the calculation of bubble point, dew point and to solve the linear series Equations (5-6), (5-14), (5-19), and (5-24). All these programs are listed in Appendix B.

CHAPTER VIII

CONCLUSIONS

The new minimum reflux method presented in this paper is very accurate for computing the minimum reflux when the split of two components is specified. In the examples presented here these two components, the light key and the heavy key, are adjacent, but the method is not limited to this case.

The values from the plate-to-plate procedure were chosen as the correct minimum reflux because they are based on a rigorous solution of a column with a large number of stages. The Underwood minimum reflux is probably the most widely used method today. It is also presented here for the sake of comparison and the minimum reflux values are not as accurate as the proposed procedure.

The assumption made by some authors that all components lighter than the light key and heavier than the heavy key are separated from the products at minimum reflux conditions is not valid as it can be seen in Examples 1, 2, and 4. In these cases some lighter and heavier components are distributed along with the keys. Example 3, with only the two keys distributed was found to be the most difficult to converge. Class I separations are the easiest to converge with very good results as illustrated by Example 4, Tables A-8 and A-9. In this case the Underwood method is also very reliable.

The minor discrepancies found in some of the results are mainly due to the assumption of constant molal overflow between the pinch zones. The method does calculate the liquid rate from the stage above the feed, and the vapor from the feed stage, as well as the liquid and vapor in the pinches by material balance. However, these values were not used in successive iterations since they were not restricted by enthalpy balance considerations. The material balances were only used to obtain normalized compositions and these were then used for temperature determination.

CHAPTER IX

RECOMMENDATIONS

The primary contribution of this work is the short-cut calculation of the minimum reflux for systems under the Class II separations category. Underwood's method gives good results for the Class I separations systems.

Improvements in the accuracy of the program would result from the addition of enthalpy balances to calculate the internal loadings in the column for the successive trials. It was expected that the calculation procedure would become very sensitive and the rate of convergence decrease if the internal loadings calculated by material balance in one trail were used in the next one.

More work should be done to demonstrate the accuracy of the method with feeds of more than five components, with totally and partially vaporized feeds and with non-ideal systems.

APPENDIX A

TABLE A-1. SPECIFICATIONS FOR EXAMPLES 1, 2, 3, AND 4

Component	Example 1		Example 2		Example 3		Example 4	
	Comp. No.	Feed Rate	Comp. No.	Feed Rate	Comp. No.	Feed Rate	Comp. No.	Feed Rate
C_3H_8	1	5			1	5		
EX34 (*)			1	20			1	20
i-C_4H_{10}	2	15			2	15		
n-C_4H_{10} (LK)	3	25	2	25	3	25	2	25
i-C_5H_{12} (HK)	4	20	3	20	4	20	3	20
n-C_5H_{12}	5	35					4	35
EX23 (*)			4	35	5	35		
Temperature °F		181.73		204.46		191.25		193.27

Total Feed Rate = 100 Moles/Hr
Feed Condition = Boiling Point Liquid
Column Pressure = 120 Lb/Sq.In.Abs.
Distillate Condition = Boiling Point Liquid
LK Specification, (b/d) = 0.1933
HK Specification, (b/d) = 5.7340

(*) Hypothetical components with K values that give the desired type of separation.

TABLE A-2. MOLAR FLOW RATES AND CONDITIONS OF PRODUCTS FOR EXAMPLE 1

Component Number	Short-cut in This Work		Plate-to-Plate	
	Distillate	Bottoms	Distillate	Bottoms
1	5.00	-	5.00	-
2	15.00	-	15.00	-
3 - LK	20.95	4.05	20.95	4.05
4 - HK	2.97	17.03	2.97	17.03
5	0.98	34.02	0.97	34.03
Total	44.90	55.10	44.89	55.11
Temperature, °F	141.27	226.50	141.26	226.47

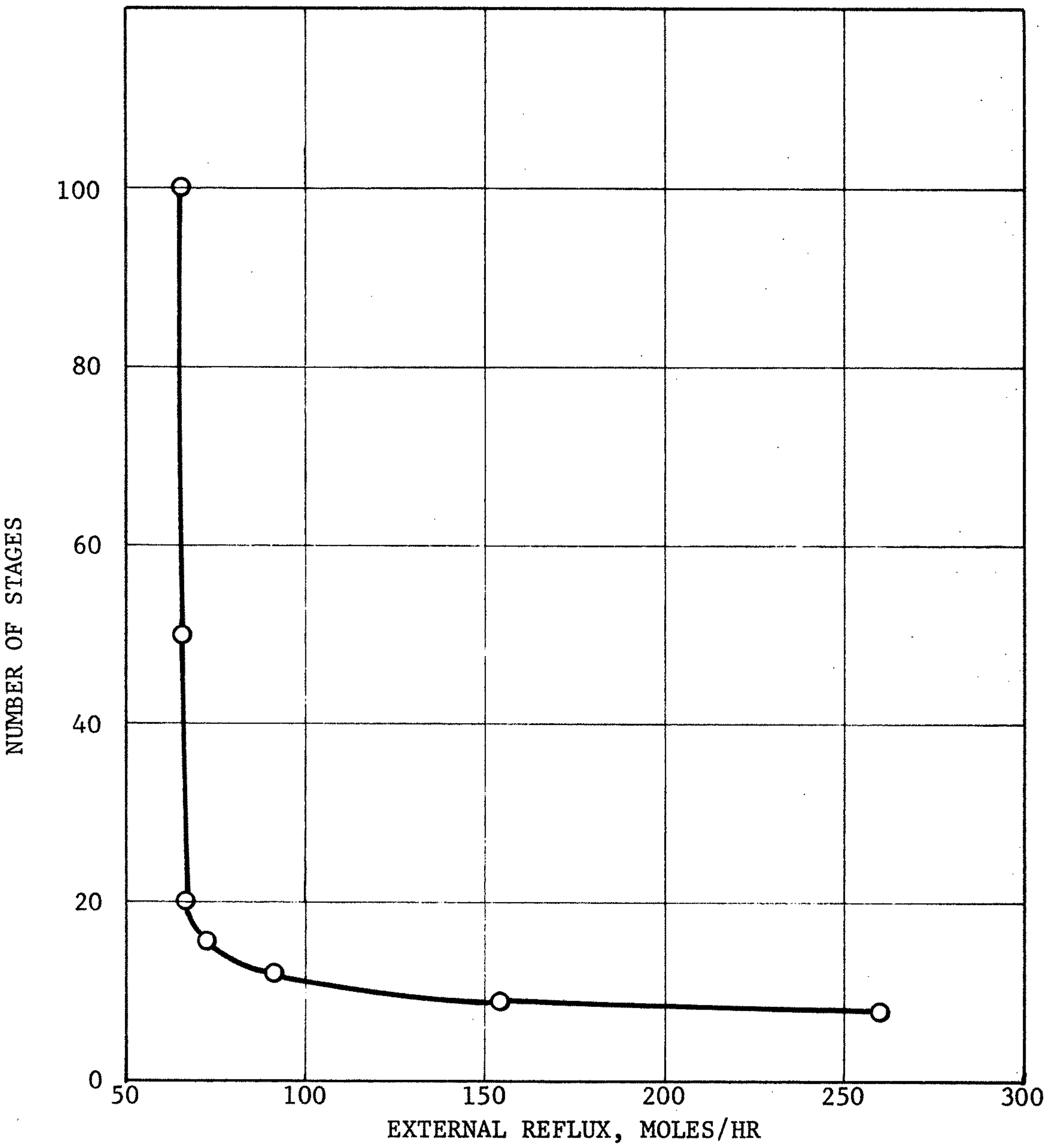


FIGURE A-1. Typical stages - reflux curve for Example 1

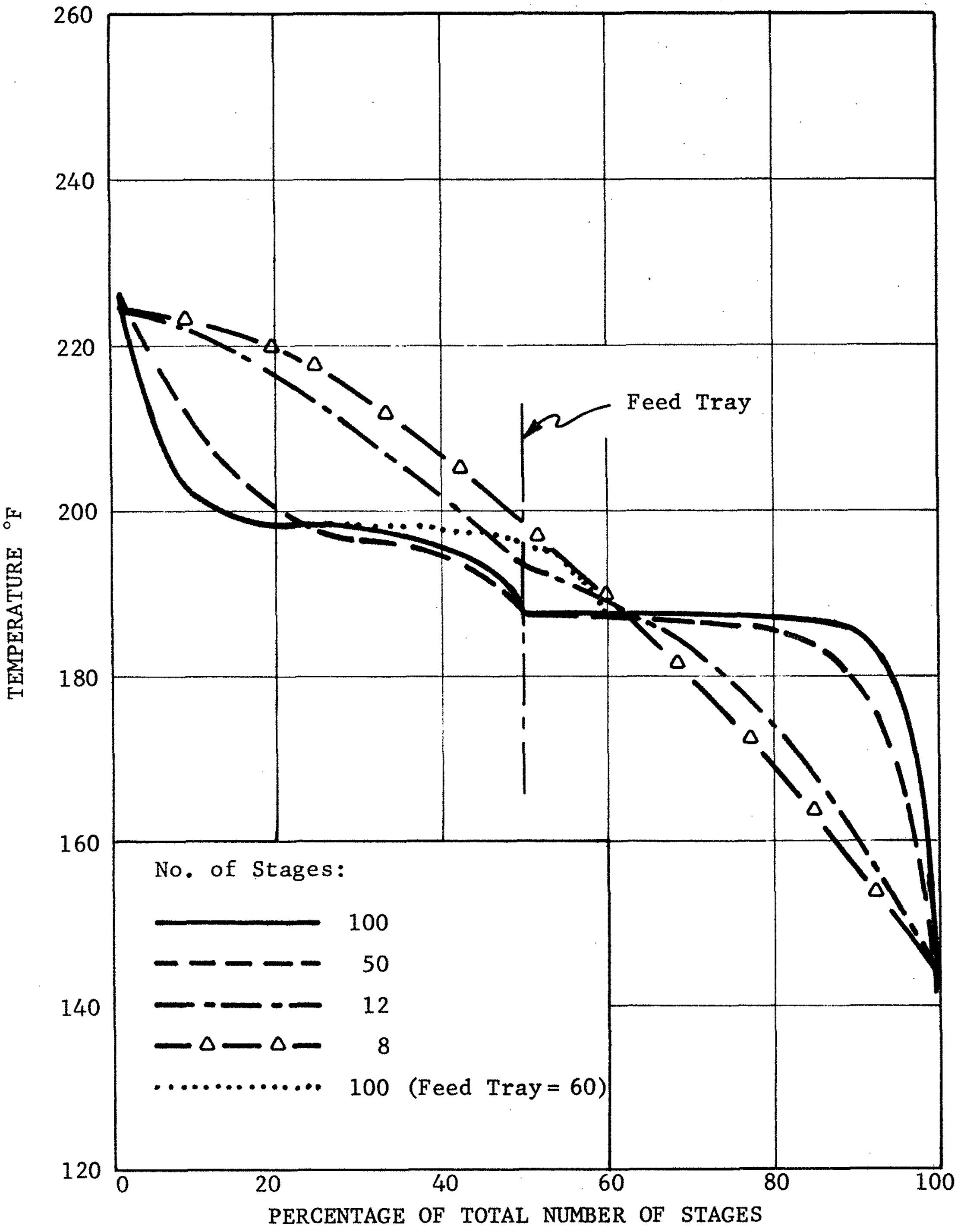


FIGURE A-2. Temperature profiles for Example 1.

TABLE A-3. MOLAR FLOW RATES AND CONDITIONS AT KEY COLUMN LOCATIONS FOR EXAMPLE 1

Component Number	Short-cut in This Work				Plate-to-Plate			
	L_{R*}	L_{f+1}	V_f	$V_{\underline{S}*}$	L_{R*}	L_{f+1}	V_f	$V_{\underline{S}*}$
1	1.25	1.25	6.25	0.03	1.25	1.25	6.25	0.00
2	8.45	8.45	23.45	12.78	8.46	8.46	23.45	4.06
3 - LK	16.40	16.40	37.35	51.18	16.43	16.42	37.37	58.00
4 - HK	12.12	12.12	15.09	18.19	12.18	12.16	15.12	18.32
5	21.12	21.12	22.10	26.48	21.11	21.14	22.11	26.60
Total	59.34	59.34	104.24	108.66	59.43	59.43	104.30	106.98
Temperature °F	187.53	187.53	187.53	195.63	187.54	187.55	187.55	197.28

TABLE A-4. MOLAR FLOW RATES AND CONDITIONS OF PRODUCTS FOR EXAMPLE 2

Component Number	Short-cut in This Work		Plate-to-Plate	
	Distillate	Bottoms	Distillate	Bottoms
1	17.88	2.12	17.61	2.39
2	20.95	4.05	20.95	4.05
3	2.97	17.03	2.97	17.03
4	-	35.00	-	35.00
Total	41.80	58.20	41.53	58.47
Temperature °F	161.79	248.81	161.82	248.23

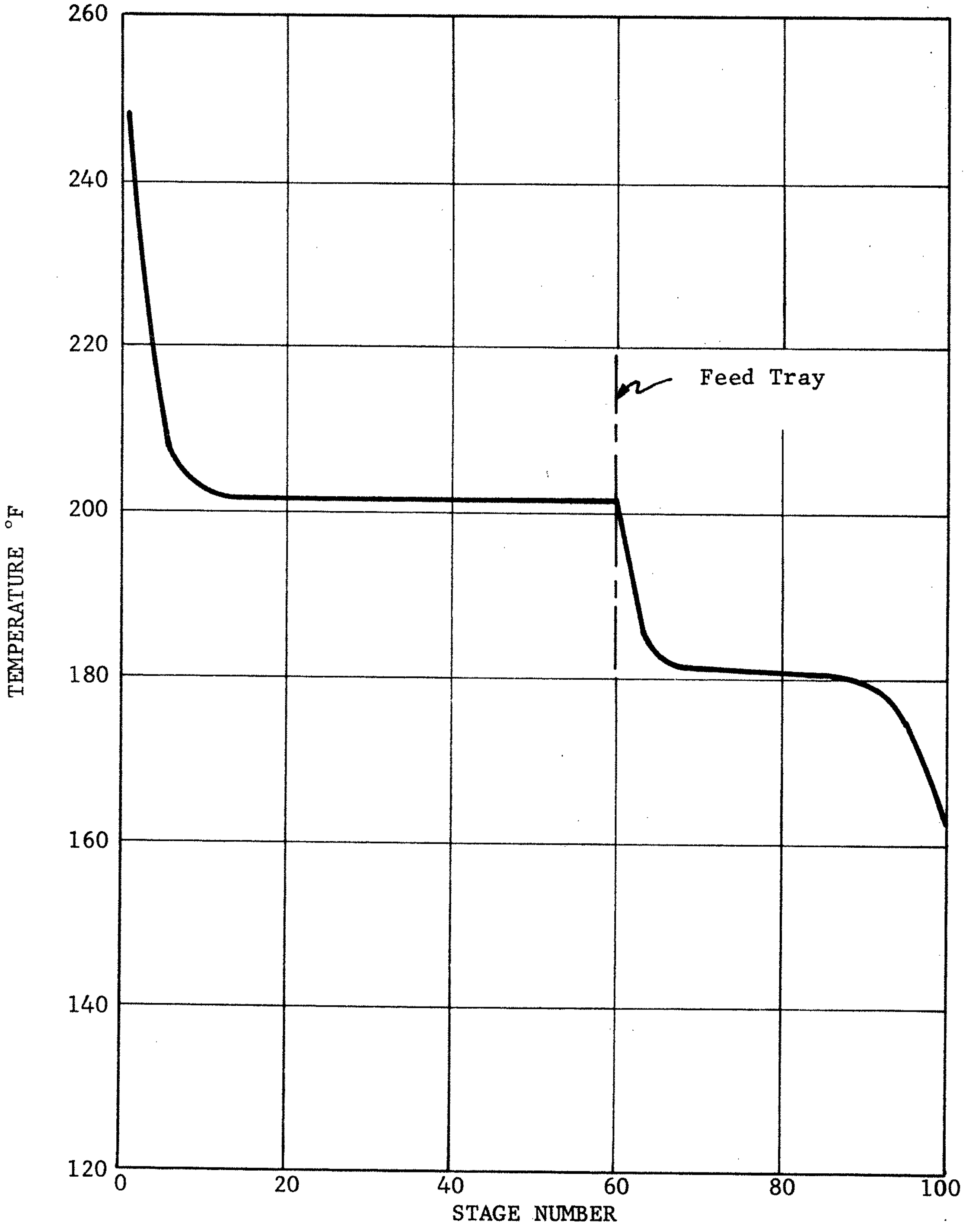


FIGURE A-3. Temperature profile for Example 2.

TABLE A-5. MOLAR FLOW RATES AND CONDITIONS AT KEY COLUMN LOCATIONS FOR EXAMPLE 2

Component Number	Short-cut in This Work				Plate-to-Plate			
	L_{R*}	L_{f+1}	V_f	$V_{\underline{S}*}$	L_{R*}	L_{f+1}	V_f	$V_{\underline{S}*}$
1	15.61	12.95	30.83	30.83	15.41	11.63	29.24	29.21
2	19.34	15.99	40.10	40.10	19.39	14.57	35.52	35.50
3	23.96	14.57	17.54	17.54	24.13	14.29	17.26	17.24
4	0.06	12.07	12.07	12.07	0.01	12.01	12.01	12.00
Total	58.97	55.57	100.54	100.54	58.94	52.50	94.03	93.95
Temperature °F	180.58	193.58	199.51	199.51	180.68	195.59	201.37	201.38

TABLE A-6. MOLAR FLOW RATES AND CONDITIONS OF PRODUCTS FOR EXAMPLE 3

Component Number	Short-cut in This Work		Plate-to-Plate	
	Distillate	Bottoms	Distillate	Bottoms
1	5.00	-	5.00	-
2	15.00	-	15.00	-
3	20.95	4.05	20.95	4.05
4	2.97	7.03	2.97	17.03
5	-	5.00	-	35.00
Total	43.92	56.08	43.92	56.08
Temperature °F	139.73	253.95	139.73	253.97

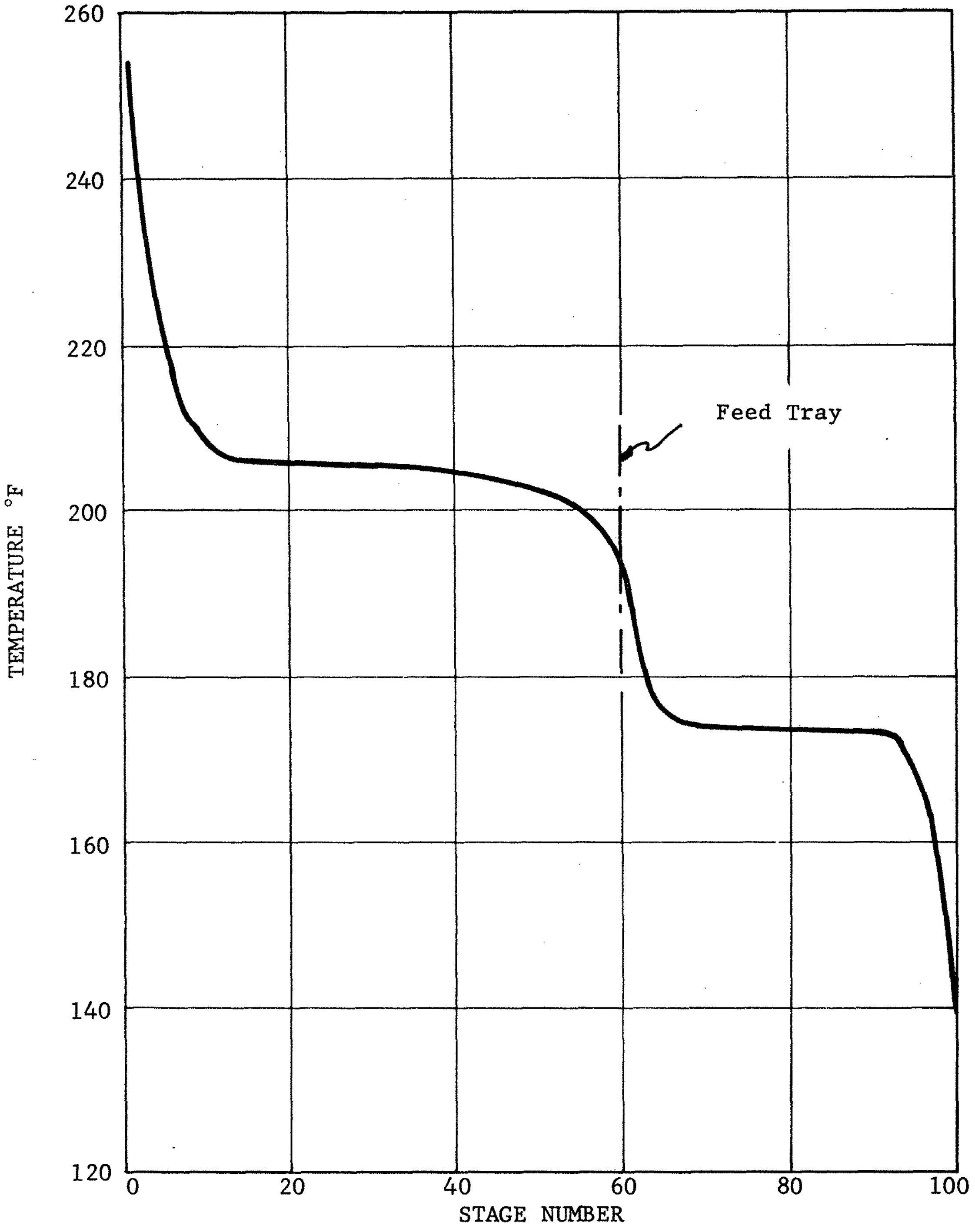


FIGURE A-4. Temperature profile for Example 3.

TABLE A-7. MOLAR FLOW RATES AND CONDITIONS AT KEY COLUMN LOCATIONS FOR EXAMPLE 3

Component Number	Short-cut in This Work				Plate-to-Plate			
	L_{R*}	L_{f+1}	V_f	$V_{\underline{S}*}$	L_{R*}	L_{f+1}	V_f	$V_{\underline{S}*}$
1	1.25	1.12	6.11	0.35	1.30	1.06	6.06	0.00
2	8.74	7.44	22.45	17.03	9.12	6.98	21.98	0.43
3	17.52	14.44	35.39	40.80	18.38	13.49	34.44	59.24
4	17.85	12.75	15.72	17.77	21.46	12.16	15.13	19.08
5	1.06	10.90	10.90	12.30	0.00	10.60	10.60	13.00
Total	46.42	46.65	90.57	88.25	50.26	44.29	88.21	91.75
Temperature °F	172.80	187.97	194.47	202.65	173.51	188.78	194.30	205.80

TABLE A-8. MOLAR FLOW RATES AND CONDITIONS OF PRODUCTS FOR EXAMPLE 4

Component Number	Short-cut in This Work		Plate-to-Plate	
	Distillate	Bottoms	Distillate	Bottoms
1	18.24	1.76	18.23	1.77
2	20.95	4.05	20.95	4.05
3	2.97	17.03	2.97	17.03
4	0.60	34.40	0.64	34.36
Total	42.76	57.24	42.79	57.21
Temperature °F	161.39	223.75	161.45	223.73

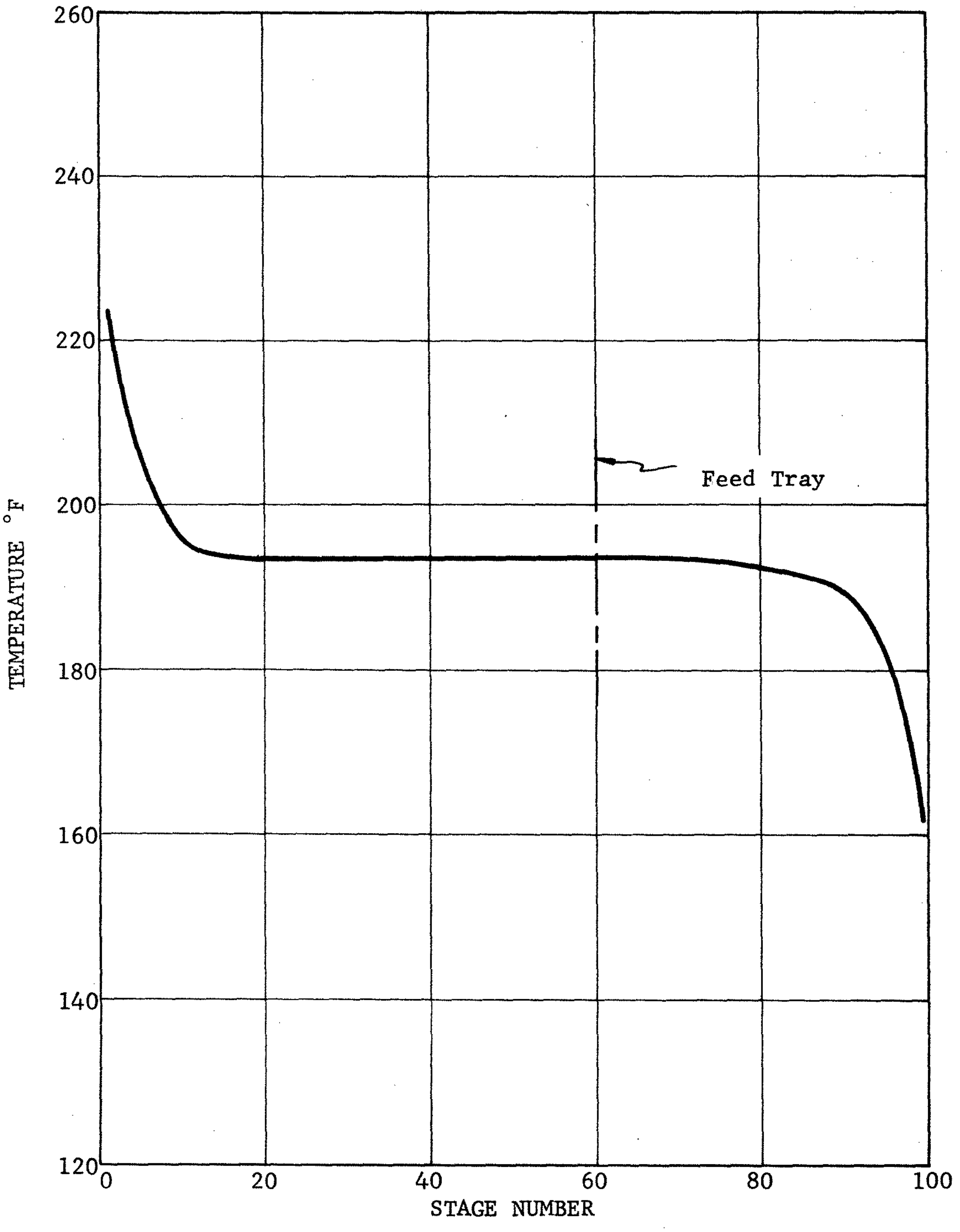


FIGURE A-5. Temperature profile for Example 4.

TABLE A-9. MOLAR FLOW RATES AND CONDITIONS AT KEY COLUMN LOCATIONS FOR EXAMPLE 4

Component Number	Short-cut in This Work				Plate-to-Plate			
	L_{R*}	L_{f+1}	V_f	$V_{\underline{S}*}$	L_{R*}	L_{f+1}	V_f	$V_{\underline{S}*}$
1	14.02	14.02	32.25	32.25	14.01	14.01	32.24	32.24
2	17.53	17.53	38.33	38.33	17.53	17.53	38.48	38.50
3	13.93	13.93	17.03	17.03	14.09	14.06	17.03	17.04
4	24.54	24.54	25.13	25.13	24.41	24.45	25.10	25.10
Total	70.02	70.02	112.74	112.74	70.04	70.05	112.85	112.88
Temperature °F	193.31	193.31	193.39	193.39	193.31	193.32	193.34	193.34

TABLE A-10. MINIMUM REFLUX RESULTS FOR EXAMPLES 1, 2, 3, AND 4

Case	Short-cut in This Work		Plate-to-Plate		Underwood
	L_{R*}	L_{Rm}	L_{R*}	L_{Rm}	L_{R*}
Example 1	59.34	66.12	59.43	66.09	55.80
Example 2	58.97	63.50	58.94	63.32	55.30
Example 3	46.42	50.45	50.26	54.05	46.90
Example 4	70.02	79.35	70.04	79.28	70.00

APPENDIX B

PROGRAM 1. MAIN EXECUTOR

```
      COMMON    / SHRTCT /                                              MNR00100
     A   AA(100),        AB(100),        AC(100),        AD(100),       MNR00120
     B  B(50),         BDI(50),        BFLOW,          BN(50),          MNR00140
     C  D(50),         DCALC,          DCON,           DELBAR(100),     MNR00160
     D   DELF(100),      DL,             DLS(50),        DLST,          MNR00180
     E   DN(50),         DSPEC,          DV,             DVS,           MNR00200
     F   DVX(50),        DVXT,           FNTH,           ER,            MNR00220
     G   FACT(100),      FEND(50,6),     FFLOW,          FL(50),        MNR00240
     H  FLTOT,         FMAXA,          FMAXS,          FMINA,           MNR00260
     I  FMINS,         FP,             FRVAP,          FT,              MNR00280
     J  FTOT(50),      FV(50),         FVTOT,          ICON,            MNR00300
     K  ID,            IP,             ISEC,           MTRY,            MNR00320
     L  ISTAGE,        KODE(10),       KSEC,           LFD(50),         MNR00340
     M   LFFX(50),       LV(6),          NABSR,          NCOMP,         MNR00360
     N   NFSTG,          NITER,          NS(5),          NSTRP,         MNR00380
     O   P(6),           R,              S2(50),         S3(50),        MNR00400
     P   S4(50),         S5(50),         T(6),           THETA,         MNR00420
     Q  VFB(50),       VFFX(50),    NTRY,    IHK,    ILK                MNR00440
      INTEGER ER                                                        MNR00460
      CALL WIPE ( AA(1), ILK )                                          MNR00480
C                                                                       MNR00500
      CALL RELOC                                                        MNR00520
      CALL INPUT                                                        MNR00540
C                                                                       MNR00560
      END                                                               MNR00580
```

```
                              MAIN

*OPTIONS IN EFFECT*  ID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP
*OPTIONS IN EFFECT*  NAME = MAIN    , LINECNT =       55
*STATISTICS*    SOURCE STATEMENTS =        6,PROGRAM SIZE =      332
*STATISTICS*  NO DIAGNOSTICS GENERATED
```

PROGRAM 2. BUBBLE POINT CALCULATIONS

```
      SUBROUTINE BUB(PBP,TBP,L)
C
C     SUBROUTINE TO PERFORM BUBBLE POINT CALCULATIONS
C     L         LIQUID COMPONENT RATES
C     RATE      TOTAL LIQUID RATE
C
      COMMON /KVALUE/ AK(50),          DK(50),          DDK(50)
      COMMON   / SHRTCT /
     A    AA(100),        AB(100),        AC(100),        AD(100),
     B   B(50),          BDI(50),        BFLOW,          BN(50),
     C   D(50),          DCALC,          DCON,           DELBAR(100),
     D    DELF(100),      DL,             DLS(50),        DLST,
     E    DN(50),         DSPEC,          DV,             DVS,
     F    DVX(50),        DVXT,           ENTH,           ER,
     G    FACT(100),      FEND(50,6),     FFLOW,          FL(50),
     H   FLTOT,          FMAXA,          FMAXS,          FMINA,
     I   FMINS,          FP,             FRVAP,          FT,
     J   FTOT(50),       FV(50),         FVTOT,          ICON,
     K   ID,             IP,             ISEC,           MTRY,
     L   ISTAGE,         KODE(10),       KSEC,           LFD(50),
     M    LFFX(50),       LV(6),          NABSR,          NCOMP,
     N    NFSTG,          NITER,          NS(5),          NSTRP,
     O    P(6),           R,              S2(50),         S3(50),
     P     S4(50),         S5(50),         T(6),           THETA,
     Q   VFB(50),        VFFX(50),   NTRY,   IHK,    ILK
      REAL L(50)
      INTEGER ER
C
C     SUM LIQUID COMPONENT RATES
      RATE = 0.0
      DO 100 I=1,NCOMP
      RATE = RATE + L(I)
  100 CONTINUE
C
C     START BUBBLE POINT CALCULATIONS
C
      DO 500 ITER=1,50
C
C     CALCULATE THE SUMS OF  LK, LDK, AND LDDK
C
      SKL  = 0.0
      DF   =  0.0
      DDF  =  0.0
      CALL KVAL(PBP,TBP,IER)
      DO 200 I=1,NCOMP
      SKL = SKL + L(I) * AK(I)
      DF   = DF    + L(I) * DK(I)
      DDF  = DDF   + L(I) * DDK(I)
  200 CONTINUE
      F = -1.0 + SKL / RATE
      IF ( ABS(F) .LT.0.00001) GO TO 600
C
C     CALCULATE CORRECTED TEMPERATURE  USING RICHMOND METHOD
```

BUB

```
C                                                                               MNR01660
      TBP = TBP - 1.0 / (( DF/(F * RATE))- ( 0.5 * DDF / DF ))                  MNR01680
  500 CONTINUE                                                                  MNR01700
C      SOLUTION NOT CONVERGING                                                  MNR01720
      ER    = 1                                                                 MNR01740
      CALL ERROR                                                                MNR01760
C                                                                               MNR01780
  600 RETURN                                                                    MNR01800
C                                                                               MNR01820
      END                                                                       MNR01840
```

```
FORTRAN IV G LEVEL  21                    BUB

  *OPTIONS IN EFFECT*  ID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP
  *OPTIONS IN EFFECT*  NAME = BUB      , LINECNT =       55
  *STATISTICS*    SOURCE STATEMENTS =        27,PROGRAM SIZE =       756
  *STATISTICS*  NO DIAGNOSTICS GENERATED
```

PROGRAM 3. DEW POINT CALCULATIONS

```
      SUBROUTINE DEW(PDW,TDW,V)                                         MNR01860
C                                                                       MNR01880
C     SUBROUTINE TO PERFORM DEW POINT CALCULATIONS                      MNR01900
C     V         VAPOR COMPONENT RATES                                   MNR01920
C                                                                       MNR01940
      COMMON /KVALUE/ AK(50),            DK(50),          DDK(50)       MNR01960
      COMMON    / SHRTCT /                                              MNR01980
     A    AA(100),        AB(100),        AC(100),        AD(100),      MNR02000
     B   B(50),          BDI(50),        BFLOW,          BN(50),        MNR02020
     C   D(50),          DCALC,          DCON,           DELBAR(100),   MNR02040
     D    DFLF(100),      DL,             DLS(50),        DLST,         MNR02060
     E    DN(50),         DSPEC,          DV,             DVS,          MNR02080
     F    DVX(50),        DVXT,           ENTH,           ER,           MNR02100
     G    FACT(100),      FEND(50,6),     FFLOW,          FL(50),       MNR02120
     H   FLTOT,          FMAXA,          FMAXS,          FMINA,         MNR02140
     I   FMINS,          FP,             FRVAP,          FT,            MNR02160
     J   FTOT(50),       FV(50),         FVTOT,          ICON,          MNR02180
     K   ID,             IP,             ISEC,           MTRY,          MNR02200
     L   ISTAGE,         KODE(10),       KSEC,           LFD(50),       MNR02220
     M    LFFX(50),       LV(6),          NABSR,          NCOMP,        MNR02240
     N    NFSTG,          NITER,          NS(5),          NSTRP,        MNR02260
     O    P(6),           R,              S2(50),         S3(50),       MNR02280
     P    S4(50),         S5(50),         T(6),           THETA,        MNR02300
     Q   VFB(50),        VFFX(50),   NTRY,    IHK,    ILK               MNR02320
C                                                                       MNR02340
      DIMENSION V(50)                                                   MNR02360
      INTEGER ER                                                        MNR02380
C                                                                       MNR02400
C                                                                       MNR02420
C     SUM VAPOR COMPONENT RATES                                         MNR02440
      RATE = 0.0                                                        MNR02460
      DO 100 I=1,NCOMP                                                  MNR02480
      RATE = RATE + V(I)                                                MNR02500
  100 CONTINUE                                                          MNR02520
C                                                                       MNR02540
C                                                                       MNR02560
      DO 500 ITER=1,50                                                  MNR02580
C                                                                       MNR02600
C     CALCULATE THE SUMS OF  F,DFYDT,D2F/DT2                            MNR02620
C                                                                       MNR02640
      SKV  = 0.0                                                        MNR02660
      DF   =  0.0                                                       MNR02680
      DDF  =  0.0                                                       MNR02700
      CALL KVAL(PDW,TDW,IER)                                            MNR02720
      DO 200 I=1,NCOMP                                                  MNR02740
      AK2  =  AK(I)**2                                                  MNR02760
      SKV  = SKV + V(I) / AK(I)                                         MNR02780
      DF   =  DF  - V(I)*DK(I)/AK2                                      MNR02800
      DDF  =  DDF - V(I)*(DDK(I)/AK2 - 2.*DK(I)**2/AK2*AK(I))           MNR02820
  200 CONTINUE                                                          MNR02840
      F = -1.0 + SKV / RATE                                             MNR02860
      IF ( ABS(F) .LT.0.00001) GO TO 600                                MNR02880
C                                                                       MNR02900
```

```
C     CALCULATE CORRECTED TEMPERATURE  USING RICHMOND METHOD             MNR02920
C                                                                        MNR02940
      TDW = TDW - 1.0 / (( DF / ( F * RATE )) - ( 0.5 * DDF / DF ))      MNR02960
  500 CONTINUE                                                           MNR02980
C     SOLUTION NOT CONVERGING                                            MNR03000
      ER    = 2                                                          MNR03020
      CALL ERROR                                                         MNR03040
C                                                                        MNR03060
  600 RETURN                                                             MNR03080
C                                                                        MNR03100
      END                                                                MNR03120
```

```
FORTRAN IV G LEVEL  21                    DEW

  *OPTIONS IN EFFECT*  ID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP
  *OPTIONS IN EFFECT*  NAME = DEW     , LINECNT =       55
  *STATISTICS*    SOURCE STATEMENTS =       28,PROGRAM SIZE =      812
  *STATISTICS*  NO DIAGNOSTICS GENERATED
```

PROGRAM 4. ROUTINE TO READ ALL INPUT

```
      SUBROUTINE INPUT                                                  MNR03140
C                                                                       MNR03160
C     INPUT ROUTINE - READ, STORE, & PRINT INPUT DATA                   MNR03180
C                                                                       MNR03200
      COMMON /COMPNM/ CMPNAM(3,50)                                      MNR03220
C                                                                       MNR03240
      COMMON / FNSKOP /  IREF,          REFRCL,         FNM,            MNR03260
     1    REFRCH,        DEST,                                          MNR03280
     2    LRSTAR,        FNAME(3),      DUMDUM(100)                     MNR03300
C                                                                       MNR03320
      COMMON    / SHRTCT /                                              MNR03340
     A    AA(100),       AB(100),       AC(100),        AD(100),        MNR03360
     B   B(50),         BDI(50),       BFLOW,          BN(50),          MNR03380
     C   D(50),         DCALC,         DCON,           DELBAR(100),     MNR03400
     D    DELF(100),     DL,            DLS(50),        DLST,           MNR03420
     E    DN(50),        DSPEC,         DV,             DVS,            MNR03440
     F    DVX(50),       DVXT,          ENTH,           ER,             MNR03460
     G    FACT(100),     FEND(50,6),    FFLOW,          FL(50),         MNR03480
     H   FLTOT,         FMAXA,         FMAXS,          FMINA,           MNR03500
     I   FMINS,         FP,            FRVAP,          FT,              MNR03520
     J   FTOT(50),      FV(50),        FVTOT,          ICON,            MNR03540
     K   ID,            IP,            ISEC,           MTRY,            MNR03560
     L   ISTAGE,        KODE(10),      KSEC,           LFD(50),         MNR03580
     M    LFFX(50),      LV(6),         NABSR,          NCOMP,          MNR03600
     N    NFSTG,         NITER,         NS(5),          NSTRP,          MNR03620
     O    P(6),          R,             S2(50),         S3(50),         MNR03640
     P    S4(50),        S5(50),        T(6),           THETA,          MNR03660
     Q   VFB(50),       VFFX(50),  NTRY,   IHK,   ILK                   MNR03680
C                                                                       MNR03700
      COMMON /SYSTEM/ IREAD, IWRITE                                     MNR03720
C                                                                       MNR03740
      COMMON /WHILE/ PERC,THTA1,THTA2,TT1,TT2, CLV(5),DELPC,DELP        MNR03760
C                                                                       MNR03780
      COMMON /ZALPHA/ KZ(160)                                           MNR03800
C                                                                       MNR03820
      DIMENSION NAME(3,8), DATA(10)                                     MNR03840
      DIMENSION             PNAME(2,50), RNAME(2,50)                    MNR03860
C                                                                       MNR03880
      DIMENSION  COEF(5), W(5), DUMY(5), XK(5)                          MNR03900
      DIMENSION   TCF(5),  PCF(5), CFKV(30,5)                           MNR03920
C                                                                       MNR03940
      DATA NAME / '*360', '1   ', '    ',                               MNR03960
     1            '*CMP', '    ', '    ',                               MNR03980
     2            '*KCO', 'EF  ', '    ',                               MNR04000
     3            '*KDA', 'TA  ', '    ',                               MNR04020
     4            '*FEE', 'D   ', '    ',                               MNR04040
     5            '*BAS', 'E CA', 'SE  ',                               MNR04060
     6            '*COM', 'PR  ', '    ',                               MNR04080
     7            '*DES', 'IGN ', '    ' /                              MNR04100
C                                                                       MNR04120
      DATA  W / 5*1. /                                                  MNR04140
C                                                                       MNR04160
      REAL LFD,LV,LFFX,LRSTAR                                           MNR04180
```

INPUT

```
C                                                                       MNR04200
C     INITIALIZE                                                        MNR04220
C                                                                       MNR04240
C     VARIABLES                                                         MNR04260
C                                                                       MNR04280
      ENTH = 0.                                                         MNR04300
      FFLOW = 0.                                                        MNR04320
      FLTOT = 0.                                                        MNR04340
      FVTOT = 0.                                                        MNR04360
      FTF = 0.0                                                         MNR04380
      ID = 0                                                            MNR04400
      IP = 0                                                            MNR04420
      IREAD = 5                                                         MNR04440
      IWRITE = 6                                                        MNR04460
      NCOMP = 0                                                         MNR04480
C                                                                       MNR04500
C     INPUT CARD CHECKING COUNTERS                                      MNR04520
C                                                                       MNR04540
      ICOEF = 0                                                         MNR04560
      IDATA = 0                                                         MNR04580
      IFD = 0                                                           MNR04600
      IK = 0                                                            MNR04620
      IR = 0                                                            MNR04640
      KERROR = 0                                                        MNR04660
      KVC = 0                                                           MNR04680
      TTC = 0.                                                          MNR04700
C                                                                       MNR04720
C                                                                       MNR04740
      DO 5 J=1,50                                                       MNR04760
      D(J) = 0.                                                         MNR04780
      DLS(J) = 0.                                                       MNR04800
      DVX(J) = 0.0                                                      MNR04820
    5 CONTINUE                                                          MNR04840
C                                                                       MNR04860
   10 CALL ZCARD ( Z, &50 )                                             MNR04880
C                                                                       MNR04900
C     ERROR MSG - * CARD SEQUENCE ERROR                                 MNR04920
C                                                                       MNR04940
      PRINT 20                                                          MNR04960
C                                                                       MNR04980
      KERROR = KERROR + 1                                               MNR05000
      STOP                                                              MNR05020
C                                                                       MNR05040
C     PACK FIRST 12 WORDS INTO 3                                        MNR05060
C                                                                       MNR05080
   50 DUMMY = ZPACK ( KZ(1), KZ(81), 12 )                               MNR05100
C                                                                       MNR05120
C     CHECK FOR TYPE OF CARD FOUND                                      MNR05140
C                                                                       MNR05160
      DO 100 I = 1,10                                                   MNR05180
      IT = I                                                            MNR05200
      IF ( KZ(81) - NAME(1,I))100, 150, 100                             MNR05220
  100 CONTINUE                                                          MNR05240
```

```
C                                                                       MNR05260
C     NO MATCH FOUND                                                    MNR05280
C                                                                       MNR05300
      WRITE (IWRITE,120) (KZ(I), I=1,80)                                MNR05320
C                                                                       MNR05340
      KERROR = KERROR + 1                                               MNR05360
      STOP                                                              MNR05380
C                                                                       MNR05400
C     MATCH FOUND - GO TO PROPER STATEMENT FOR PROCESSING               MNR05420
C                                                                       MNR05440
C             TITL CMP KCF KDA FD  BC  CPR DES                          MNR05460
  150 GO TO (200,250,300,350,400,450,500,550 ),IT                       MNR05480
C                                                                       MNR05500
C     *3601 TITLE CARD FOUND                                            MNR05520
C                                                                       MNR05540
  200 TTC = TTC + 1                                                     MNR05560
      IF ( TTC .EQ. 1 ) GO TO 210                                       MNR05580
C                                                                       MNR05600
      WRITE (IWRITE,2000)(KZ(I), I=1,80)                                MNR05620
C                                                                       MNR05640
      GO TO 220                                                         MNR05660
C                                                                       MNR05680
  210 WRITE (IWRITE,2010)(KZ(I), I=1,80)                                MNR05700
C                                                                       MNR05720
  220 CALL ZCARD ( Z, &50 )                                             MNR05740
C                                                                       MNR05760
C                                                                       MNR05780
      GO TO 220                                                         MNR05800
C                                                                       MNR05820
C     *CMP COMPONENT CARD FOUND                                         MNR05840
C                                                                       MNR05860
  250 PRINT 2020                                                        MNR05880
C                                                                       MNR05900
  260 CALL ZCARD ( Z, &270 )                                            MNR05920
C                                                                       MNR05940
      GO TO 280                                                         MNR05960
C                                                                       MNR05980
C     EITHER NO CD OR UNRECOGNIZABLE CD CARD FOUND - PRINT MESSAGE      MNR06000
C                                                                       MNR06020
  270 WRITE (IWRITE,2030)                                               MNR06040
C                                                                       MNR06060
      KERROR = KERROR + 1                                               MNR06080
C                                                                       MNR06100
      GO TO 50                                                          MNR06120
C                                                                       MNR06140
C     CHECK FOR CD CARDS                                                MNR06160
C                                                                       MNR06180
  280 IF( TEST( 2, KZ(81),1, 1, 'CD   ', 1, 1 ).EQ.0.0 ) GO TO 290      MNR06200
C                                                                       MNR06220
      GO TO 270                                                         MNR06240
C                                                                       MNR06260
  290 NCOMP = NCOMP + 1                                                 MNR06280
      DUMMY = ZPACK ( KZ(5), CMPNAM(1,NCOMP), 12 )                      MNR06300
```

```
C
      WRITE (IWRITE,2000)(KZ(I), I=1,80)
      CALL ZCARD ( Z, &50 )
      GO TO 280
C
C     *KCOEF CARD FOUND
C
C     GENERATE DATA TYPE IDENTIFIER, IK
C
  300 IK = 1
C
      X = ZINTGR ( KZ(13), KSEC, 12 )
C
C     DETERMINE WHICH SECTION BEING PROCESSED
C
      KVC = KVC + 1
      IF ( KSEC .EQ. 0 .AND. KVC .EQ. 1 ) KSEC = 1
      IF ( KSEC .EQ. 0 .AND. KVC .EQ. 2 ) KSEC = 2
C
C     CHECK FOR KV CARDS
C
  310 CALL ZCARD ( Z, &320)
C
      GO TO 330
C
C     EITHER NO KC OR UNRECOGNIZABLE KC CARD FOUND - PRINT MESSAGE
C
  320 WRITE (IWRITE,2040)
C
      KERROR = KERROR + 1
C
      GO TO 50
C
C     CHECK FOR KC CARDS
C
  330 IF( TEST( 2, KZ(81),1, 1, 'KC  ', 1, 1 ).EQ.0.0 ) GO TO 340
C
      GO TO 320
C
  340 ICOEF = ICOEF + 1
C
      DO 342 K = 1,4
      X = ALFA ( DATA(K), KZ(7+(K-1)*18), 18, 1, 8 )
  342 CONTINUE
C
      ISLOT = (KSEC-1)*50 + ICOEF
C
      AA(ISLOT) = DATA(1)
      AB(ISLOT) = DATA(2)
      AC(ISLOT) = DATA(3)
      AD(ISLOT) = DATA(4)
C
      CALL ZCARD ( Z, &50 )
```

```
C
      GO TO 330
C
C     *KDATA CARD FOUND
C
C     GENERATE DATA TYPE IDENTIFIER, IK
C
  350 IK = 2
C
C     CHECK FOR * CARD
      CALL ZCARD ( Z, &370 )
C
      GO TO 372
C
  370 WRITE (IWRITE,2055)
C
      KERROR = KERROR + 1
C
      GO TO 50
C
C     STORE TEMPERATURE DATA, TCF
C
  372 DO 374 K = 1,5
      X = ZREAL ( KZ(13+(K-1)*12), TCF(K), IU, 12 )
  374 CONTINUE
C
      CALL ZCARD ( Z, &370 )
C
C     STORE PRESSURE DATA, PCF
C
      DO 376 K = 1,5
      X = ZREAL ( KZ(13+(K-1)*12), PCF(K), UI, 12 )
  376 CONTINUE
C
      CALL ZCARD ( Z, &370 )
C
C     CHECK FOR KV CARDS
C
  380 IF( TEST( 2, KZ(81),1, 1, 'KV  ', 1, 1 ).EQ.0.0 ) GO TO 390
C
      GO TO 370
C
  390 IDATA = IDATA + 1
C
C     STORE COMPONENT-TRAY K-VALUES
C
      DO 392 K = 1,5
      X = ZREAL ( KZ(13+(K-1)*12),CFKV(IDATA,K),IU, 12 )
  392 CONTINUE
C
      CALL ZCARD ( Z, &50)
C
      GO TO 380
```

INPUT

```
C                                                                       MNR08440
C      *FEED CARD FOUND                                                 MNR08460
C                                                                       MNR08480
  400 DUMMY = ZPACK ( KZ(13), FNAME(1),12)                              MNR08500
C                                                                       MNR08520
      DO 402 K = 1,4                                                    MNR08540
      X = ZREAL ( KZ(25+(K-1)*12),DATA(K), IU, 12 )                     MNR08560
  402 CONTINUE                                                          MNR08580
C                                                                       MNR08600
      FFLOW = DATA(1)                                                   MNR08620
      NFSTG = DATA(2)                                                   MNR08640
      FT = DATA(3)                                                      MNR08660
      FRVAP = DATA(4)                                                   MNR08680
C                                                                       MNR08700
      CALL ZCARD (Z, &420 )                                             MNR08720
C                                                                       MNR08740
      GO TO 430                                                         MNR08760
C                                                                       MNR08780
  420 WRITE (IWRITE,2050)                                               MNR08800
C                                                                       MNR08820
      KERROR = KERROR + 1                                               MNR08840
C                                                                       MNR08860
      GO TO 50                                                          MNR08880
C                                                                       MNR08900
  430 IF( TEST( 2, KZ(81),1, 1, 'COMP', 1, 1 ).EQ.0.0 ) GO TO 440       MNR08920
C                                                                       MNR08940
      GO TO 420                                                         MNR08960
C                                                                       MNR08980
  440 IFD = IFD + 1                                                     MNR09000
C                                                                       MNR09020
      DO 442 K = 1,2                                                    MNR09040
      X = ZREAL ( KZ(13+(K-1)*12),DATA(K), IU, 12 )                     MNR09060
  442 CONTINUE                                                          MNR09080
C                                                                       MNR09100
      FTOT(IFD) = DATA(1)                                               MNR09120
      FV(IFD) = DATA(2)                                                 MNR09140
      FL(IFD) = FTOT(IFD) - FV(IFD)                                     MNR09160
      FVTOT = FVTOT + FV(IFD)                                           MNR09180
      FLTOT = FLTOT + FL(IFD)                                           MNR09200
      FTF = FTF + FTOT(IFD)                                             MNR09220
C                                                                       MNR09240
      CALL ZCARD ( Z, &50)                                              MNR09260
C                                                                       MNR09280
      GO TO 430                                                         MNR09300
C      *COMPR CARD FOUND                                                MNR09320
C                                                                       MNR09340
C      CHECK FOR * CARD                                                 MNR09360
  500 CALL ZCARD( Z, &520 )                                             MNR09380
C                                                                       MNR09400
      GO TO 530                                                         MNR09420
C                                                                       MNR09440
  520 WRITE ( IWRITE, 2070 )                                            MNR09460
C                                                                       MNR09480
```

```
      KERROR = KERROR + 1
      GO TO 50
C
  530 IF( TEST( 2, KZ(81),1, 1, 'RATI', 1, 1 ).EQ.0.0 ) GO TO 540
C
      GO TO 520
C
  540 IR = IR + 1
      DO 542 K = 1,2
      X = ZREAL ( KZ(13+(K-1)*12), DATA(K), IU, 12 )
  542 CONTINUE
C
C     TRANSFER L(F+1)/D AND V(F)/B COMPONENT RATIO INFORMATION
C
      LFD(IR) = DATA(1)
      VFB(IR) = DATA(2)
C
      CALL ZCARD ( Z, &50 )
C
      GO TO 530
C
C     *BASE CASE CARD FOUND
C
C     READ SPECIAL OPERATING CODES
C
  450 DO 452 K = 1,10
      X = ZINTGR  ( KZ(13+(K-1)*4), KODE(K), 4 )
  452 CONTINUE
C
C     CHECK FOR * CARD
C
      CALL ZCARD(Z, &470)
C
      GO TO 480
C
  470 WRITE ( IWRITE, 2060)
C
      KERROR = KERROR + 1
      GO TO 50
C
  480 IF( TEST( 2, KZ(81),1, 1, 'B1  ', 1, 1 ).EQ.0.0 ) GO TO 490
C
      GO TO 470
C
  490 DO 492 K = 1,5
      X = ZREAL ( KZ(9+(K-1)*12), DATA(K), IU, 12 )
  492 CONTINUE
C
C     TRANSFER GENERAL INFORMATION FROM B1 CARD
C
      ISTAGE = DATA(1)
      ISEC = DATA(2)
      R = DATA(3)
```

```
      P(5) = DATA(4)                                                    MNR10560
      DELP = DATA(5)                                                    MNR10580
C                                                                       MNR10600
C     CHECK FOR *CARD                                                   MNR10620
C                                                                       MNR10640
      CALL ZCARD( Z, &470)                                              MNR10660
C                                                                       MNR10680
      IF( TEST( 2, KZ(81),1, 1, 'B2  ', 1, 1 ).EQ.0.0 ) GO TO 493       MNR10700
C                                                                       MNR10720
      GO TO 470                                                         MNR10740
C                                                                       MNR10760
  493 DO 494 K = 1,5                                                    MNR10780
      X = ZREAL ( KZ(9+(K-1)*12), DATA(K), IU, 12 )                     MNR10800
  494 CONTINUE                                                          MNR10820
C                                                                       MNR10840
C     TRANSFER CONDENSER INFORMATION FROM B2 CARD                       MNR10860
      DSPEC = DATA(1)                                                   MNR10880
      DELPC = DATA(2)                                                   MNR10900
      ICON = DATA(3)                                                    MNR10920
      DL = DATA(4)                                                      MNR10940
      DV = DATA(5)                                                      MNR10960
C                                                                       MNR10980
C     CHECK FOR * CARD                                                  MNR11000
C                                                                       MNR11020
      CALL ZCARD ( Z, &470 )                                            MNR11040
C                                                                       MNR11060
      IF( TEST( 2, KZ(81),1, 1, 'B3  ', 1, 1 ).EQ.0.0 ) GO TO 495       MNR11080
C                                                                       MNR11100
      GO TO 470                                                         MNR11120
C                                                                       MNR11140
C     READ LIQUID/VAPOR MOLAR RATIOS FROM B3 CARD                       MNR11160
C                                                                       MNR11180
  495 DO 496 K = 1,5                                                    MNR11200
      X = ZREAL ( KZ(9+(K-1)*12), LV(K), IU, 12 )                       MNR11220
  496 CONTINUE                                                          MNR11240
C                                                                       MNR11260
C     CHECK FOR * CARD                                                  MNR11280
C                                                                       MNR11300
      CALL ZCARD ( Z, &470)                                             MNR11320
C                                                                       MNR11340
      IF( TEST( 2, KZ(81),1, 1, 'B4  ', 1, 1 ).EQ.0.0 ) GO TO 497       MNR11360
C                                                                       MNR11380
      GO TO 470                                                         MNR11400
C                                                                       MNR11420
C     READ STAGE TEMPERATURES FROM B4 CARD                              MNR11440
C                                                                       MNR11460
  497 DO 498 K = 1,6                                                    MNR11480
      X = ZREAL ( KZ(9+(K-1)*12), T(K), IU, 12 )                        MNR11500
  498 CONTINUE                                                          MNR11520
C                                                                       MNR11540
      GO TO 600                                                         MNR11560
C                                                                       MNR11580
C     *DESIGN CARD FOUND                                                MNR11600
```

```
C                                                                       MNR11620
  550 ID = 1                                                            MNR11640
C                                                                       MNR11660
      DO 552 K = 1,10                                                   MNR11680
      X = ZINTGR ( KZ(13+(K-1)*4), KODE(K), 4 )                         MNR11700
  552 CONTINUF                                                          MNR11720
C                                                                       MNR11740
C     CHECK FOR * CARD                                                  MNR11760
C                                                                       MNR11780
      CALL ZCARD ( Z, &570 )                                            MNR11800
C                                                                       MNR11820
      GO TO 580                                                         MNR11840
C                                                                       MNR11860
  570 WRITE ( IWRITE, 2080)                                             MNR11880
C                                                                       MNR11900
      KERROR = KERROR + 1                                               MNR11920
      GO TO 50                                                          MNR11940
C                                                                       MNR11960
  580 IF( TEST( 2, KZ(81),1, 1, 'D1   ', 1, 1 ).EQ.0.0 ) GO TO 590      MNR11980
C                                                                       MNR12000
      GO TO 570                                                         MNR12020
C                                                                       MNR12040
  590 DO 592 K = 1,6                                                    MNR12060
      X = ZREAL ( KZ(9+(K-1)*12), DATA(K), IU, 12 )                     MNR12080
  592 CONTINUE                                                          MNR12100
C                                                                       MNR12120
C     TRANSFER GENERAL INFORMATION FROM D1 CARD                         MNR12140
C                                                                       MNR12160
      ISTAGE = DATA(1)                                                  MNR12180
      ISEC = DATA(2)                                                    MNR12200
      R = DATA(3)                                                       MNR12220
      P(5) = DATA(4)                                                    MNR12240
      DELP = DATA(5)                                                    MNR12260
      NTRY = DATA(6)                                                    MNR12280
C     CHECK FOR *CARD                                                   MNR12300
C                                                                       MNR12320
      CALL ZCARD ( Z, &570)                                             MNR12340
C                                                                       MNR12360
      IF( TEST( 2, KZ(81),1, 1, 'D2   ', 1, 1 ).EQ.0.0 ) GO TO 593      MNR12380
C                                                                       MNR12400
      GO TO 570                                                         MNR12420
C                                                                       MNR12440
  593 DO 594 K = 1,6                                                    MNR12460
      X = ZREAL ( KZ(9+(K-1)*12), DATA(K), IU, 12 )                     MNR12480
  594 CONTINUF                                                          MNR12500
C                                                                       MNR12520
C     TRANSFER CONDENSER INFORMATION FROM D2 CARD                       MNR12540
C                                                                       MNR12560
      DSPEC = DATA(1)                                                   MNR12580
      DELPC = DATA(2)                                                   MNR12600
      ICON = DATA(3)                                                    MNR12620
      DL = DATA(4)                                                      MNR12640
      DV = DATA(5)                                                      MNR12660
```

```
      FACMAX = DATA(6)
C     CHECK FOR *CARD
C
      CALL ZCARD ( Z, &570)
C
      IF( TEST( 2, KZ(81),1, 1, 'D3   ', 1, 1 ).EQ.0.0 ) GO TO 595
C
      GO TO 570
C
C     READ LIQUID/VAPOR MOLAR RATIOS FROM D3 CARD
C
  595 DO 596 K = 1,5
      X = ZREAL ( KZ(9+(K-1)*12), LV(K), IU, 12 )
  596 CONTINUE
C
C     CHECK FOR *CARD
C
      CALL ZCARD ( Z, &570 )
C
      IF( TEST( 2, KZ(81),1, 1, 'D4   ', 1, 1 ).EQ.0.0 ) GO TO 597
C
      GO TO 570
C
C     READ STAGE TEMPERATURES FROM D4 CARD
C
  597 DO 598 K = 1,6
      X = ZREAL ( KZ(9+(K-1)*12), T(K), IU, 12 )
  598 CONTINUE
C
C     CHECK FOR *CARD
C
      CALL ZCARD ( Z, &570 )
C
      IF( TEST( 2, KZ(81),1, 1, 'D5   ', 1, 1 ).EQ.0.0 ) GO TO 587
C
      GO TO 570
C
C     READ OPTIONAL DESIGN INFORMATION
C
  587 DO 588 K = 1,9
      X = ZREAL ( KZ(9+(K-1)*8 ), DATA(K), IU, 8   )
  588 CONTINUE
C
      IREF = DATA(1)
      REFRCL= DATA(2)
      FNM = DATA(3)
      REFRCH = DATA(4)
      DEST = DATA(5)
      ILK     = DATA(6)
      IHK     = DATA(7)
      LRSTAR = DATA(8)
      MTRY = DATA(9)
C     INPUT INFORMATION FORMATS
```

```
C
   20 FORMAT ( /5X, '*** ERROR *** REQUIRED ''*'' CARD NOT FOUND - RUN T
     1ERMINATED - CHECK DATA.' )
  120 FORMAT ( /5X, '*** ERROR *** NO RECOGNIZABLE INPUT DATA FOUND. FIR
     1ST CARD ENCOUNTERED IS: ', /5X, 80A1, ' RUN TERMINATED.' )
 2000 FORMAT ( /25X, 80A1 )
 2010 FORMAT ( 1H1,//25X, 80A1 )
 2020 FORMAT ( 1H1, 60X, 'COMPONENTS', /61X, 10('-'), // )
 2030 FORMAT ( /5X, '*** ERROR MESSAGE *** EITHER NO CD OR UNRECOGNIZABL
     1E CD CARD FOUND,EXECUTION WILL TERMINATE AFTER INPUT PROCESSING.')
 2040 FORMAT ( /5X, '*** ERROR MESSAGE *** EITHER NO KC OR UNRECOGNIZABL
     1E KC CARD FOUND,EXECUTION WILL TERMINATE AFTER INPUT PROCESSING.')
 2050 FORMAT ( /5X, '*** ERROR *** NO FEED FLOW CARDS SUBMITTED -
     1EXECUTION WILL TERMINATE AFTER INPUT PROCESSING.' )
 2055 FORMAT ( /5X, '*** ERROR MESSAGE *** UNRECOGNIZABLE CARD FOUND UND
     1ER *KDATA,EXECUTION WILL TERMINATE AFTER INPUT PROCESSING.' )
 2060 FORMAT ( /5X, '*** ERROR MESSAGE *** INCORRECT NUMBER OF BASE CASE
     1 CARDS. EXECUTION WILL TERMINATE AFTER INPUT PROCESSING.' )
 2070 FORMAT ( /5X, '*** ERROR MESSAGE *** UNRECOGNIZABLE CARD FOUND UND
     1ER *COMPR. EXECUTION WILL TERMINATE AFTER INPUT PROCESSING.' )
 2080 FORMAT ( /5X, '*** ERROR MESSAGE *** INCORRECT NUMBER OF *DESIGN 1
     1 CARDS. EXECUTION WILL TERMINATE AFTER INPUT PROCESSING.' )
C
  600 CONTINUE
C
C     CHECK INPUT COUNTERS AND ERROR GENERATION
C
C     CHECK NUMBER OF EQUILIBRIUM COEFFICIENT CARDS
C
      IF ( IK.NE.1 ) GO TO 604
C
      IF ( NCOMP.EQ.ICOEF ) GO TO 604
      WRITE ( IWRITE, 2100 ) ICOEF, NCOMP
      KERROR = KERROR + 1
C
  604 IF ( IK.NE.2 ) GO TO 606
C
C     CHECK THE NUMBER OF EQUILIBRIUM K-VALUE CARDS
C
      IF ( NCOMP.EQ.IDATA ) GO TO 606
      WRITE ( IWRITE, 2110 ) IDATA, NCOMP
      KERROR = KERROR + 1
C
C     BE SURE THAT EQUILIBRIUM DATA IS AVAILABLE
C
  606 IF ( IK.GE.1.AND.IK.LE.3 ) GO TO 608
      WRITE ( IWRITE, 2120 )
      KERROR = KERROR + 1
C
C     CHECK THE NUMBER OF FEED CARDS
C
  608 IF ( NCOMP.EQ.IFD ) GO TO 610
      WRITE ( IWRITE, 2130 ) IFD, NCOMP
```

```
      KERROR = KERROR + 1
C
  610 IF ( ID.EQ.1 ) GO TO 612
C
      IF ( NCOMP.EQ.IR ) GO TO 612
      WRITE ( IWRITE, 2135 ) IR, NCOMP
  612 IF ( KERROR.EQ.0 ) GO TO 620
      PRINT 2140, KERROR
      STOP
C
C     FORMATS FOR ERRORS IN NO. OF INPUT CARDS
 2100 FORMAT ( ///5X, '*** ERROR MESSAGE *** PLEASE CHECK INPUT DECK. TH
     1E NUMBER OF KC EQUILIBRIUM COEFFICIENT CARDS,', I3, ', DOES NOT MA
     2TCH THE NUMBER OF COMPONENT CARDS,', I3, '.' )
 2110 FORMAT ( ///5X, '*** ERROR MESSAGE *** PLEASE CHECK INPUT DECK. TH
     1E NUMBER OF KV EQUILIBRIUM CONSTANT CARDS,', I3, ', DOES NOT MATCH
     2 THE NUMBER OF COMPONENT CARDS,', I3, '.' )
 2120 FORMAT ( ///5X, '*** ERROR MESSAGE *** PLEASE CHECK INPUT DECK. YO
     1U HAVE FAILED TO SUBMIT OR ACCESS VAPOR/LIQUID EQUILIBRIUM DATA.')
 2130 FORMAT ( ///5X, '*** ERROR MESSAGE *** PLEASE CHECK INPUT DECK. TH
     1E NUMBER OF COMP FEED CARDS,', I3, ', DOES NOT MATCH THE NUMBER OF
     2 COMPONENT CARDS,', I3, '.' )
 2135 FORMAT ( ///5X, '*** ERROR MESSAGE *** PLEASE CHECK INPUT DECK. TH
     1E NUMBER OF COMPONENT RATIO CARDS,', I3, ', DOES NOT MATCH THE NUM
     2BER OF COMPONENT CARDS,', I3, '.' )
 2140 FORMAT ( //5X, 'INPUT PROCESSING COMPLETED - EXECUTION TERMINATED
     1DUE TO, ', I4, ', INPUT ERROR(S).' )
 2150 FORMAT ( ///5X, '*** ERROR MESSAGE *** THE DISTILLATE LIQUID AND/O
     1R THE DISTILLATE VAPOR RATES WERE NOT SPECIFIED FOR A PARTIAL COND
     2ENSER.' /27X, 'PLEASE CORRECT INPUT CARDS AND RESUBMIT.' )
 2160 FORMAT ( ///5X, '*** ERROR MESSAGE *** BOTH FEED TEMPERATURE ',
     1      F7.2, ' AND FRACTION VAPORIZED ', F7.4, ' WERE GIVEN.'
     2     /27X, 'RESUBMIT CASE WITH ONLY ONE GIVEN ON THE *FEED CARD.' )
C
  620 CONTINUE
C
      ISEC = 2
C
      IF ( IK.NE.1 ) GO TO 634
C
      PRINT 910
C
C
C     CHECK IF KVAL SECTION 2 FILLED IN
C
      IF ( KVC .EQ. 2 ) GO TO 633
C
      DO 632 J=1,NCOMP
C
      AA(J+50) = AA(J)
      AB(J+50) = AB(J)
      AC(J+50) = AC(J)
      AD(J+50) = AD(J)
```

```
C                                                                       MNR15860
  632 CONTINUE                                                          MNR15880
C                                                                       MNR15900
  633 CONTINUE                                                          MNR15920
C                                                                       MNR15940
C     PHYSICAL PROPERTIES                                               MNR15960
C     PRINT SECTION HEADING                                             MNR15980
C                                                                       MNR16000
      DO 950 I= 1,ISEC                                                  MNR16020
      PRINT 920, I                                                      MNR16040
C                                                                       MNR16060
C     PRINT K-VALUE COEFFICIENTS PER SECTION                            MNR16080
C                                                                       MNR16100
      DO 940 J=1,NCOMP                                                  MNR16120
      ISLOT = (I-1)*50+J                                                MNR16140
C                                                                       MNR16160
      PRINT 930, J, AA(ISLOT), AB(ISLOT), AC(ISLOT), AD(ISLOT)          MNR16180
  940 CONTINUE                                                          MNR16200
C                                                                       MNR16220
C                                                                       MNR16240
  950 CONTINUE                                                          MNR16260
C                                                                       MNR16280
  634 IF ( IK.NE.2 ) GO TO 846                                          MNR16300
C                                                                       MNR16320
C     CURVE-FIT K-DATA                                                  MNR16340
C                                                                       MNR16360
C     INITIALIZE                                                        MNR16380
C                                                                       MNR16400
      TLOW =  TCF(1) - ( TCF(1) * .1 )                                  MNR16420
      THIGH = TCF(5) + ( TCF(5) * .1 )                                  MNR16440
C                                                                       MNR16460
C     PRINT HEADING                                                     MNR16480
C                                                                       MNR16500
  830 PRINT  831                                                        MNR16520
C                                                                       MNR16540
      PRINT  832,  P(5)                                                 MNR16560
C                                                                       MNR16580
      DO  845   I = 1,NCOMP                                             MNR16600
      DO  840   J = 1,5                                                 MNR16620
      DUMY(J) = (( CFKV(I,J) * PCF(J) ) / (( TCF(J)+460. ) * P(5) ) )  MNR16640
     1          ** ( 1./3. )                                            MNR16660
  840 CONTINUE                                                          MNR16680
C                                                                       MNR16700
      SE  =  FITIT( TCF, DUMY, 5, 3, COEF, 1, 1, W )                    MNR16720
C                                                                       MNR16740
      AA(I) = COEF(2)                                                   MNR16760
      AB(I) = COEF(3)                                                   MNR16780
      AC(I) = COEF(4)                                                   MNR16800
      AD(I) = COEF(5)                                                   MNR16820
      AA(I+50) = AA(I)                                                  MNR16840
      AB(I+50) = AB(I)                                                  MNR16860
      AC(I+50) = AC(I)                                                  MNR16880
      AD(I+50) = AD(I)                                                  MNR16900
```

```
      XKLOW = ( TLOW + 460. ) * ( AA(I) + TLOW * ( AB(I) + TLOW * (     MNR16920
     1        AC(I) + TLOW * AD(I) ))) ** 3                             MNR16940
      XKHIGH = ( THIGH + 460. ) * ( AA(I) + THIGH * ( AB(I) + THIGH     MNR16960
     1         * ( AC(I) + THIGH * AD(I) )))  ** 3                      MNR16980
      DO  843 LL = 1,5                                                  MNR17000
      XK(LL) = ( TCF(LL) + 460. ) * ( AA(I) + TCF(LL) * ( AB(I) +       MNR17020
     1        TCF(LL) * ( AC(I) + TCF(LL) * AD(I) ))) ** 3              MNR17040
  843 CONTINUE                                                          MNR17060
C                                                                       MNR17080
      PRINT  842,    I, AA(I), AB(I), AC(I), AD(I), SE, TLOW, XKLOW,    MNR17100
     1   ( TCF(KK), XK(KK),  KK = 1,5 ), THIGH, XKHIGH                  MNR17120
C                                                                       MNR17140
  845 CONTINUE                                                          MNR17160
      KSEC = 1                                                          MNR17180
  846 CONTINUE                                                          MNR17200
C                                                                       MNR17220
  640 CONTINUE                                                          MNR17240
C                                                                       MNR17260
C     CALCULATE STAGE PRESSURES                                         MNR17280
C                                                                       MNR17300
      P(1) = P(5) + (ISTAGE-1     ) * DELP                              MNR17320
      P(2) = P(5) + (ISTAGE-2     ) * DELP                              MNR17340
      P(3) = P(5) + (ISTAGE-NFSTG) * DELP                               MNR17360
      P(4) = P(5) + (ISTAGE- (NFSTG+1)) * DELP                          MNR17380
      P(6) = P(5) - DELPC                                               MNR17400
      FP = P(3)                                                         MNR17420
C                                                                       MNR17440
C     DEFAULTS                                                          MNR17460
C                                                                       MNR17480
      NITER = KODE(1)                                                   MNR17500
      IF ( NITER.EQ.0 ) NITER = 10                                      MNR17520
      IF ( KODE(3).EQ.0 ) KODE(3) = 20                                  MNR17540
C                                                                       MNR17560
C     CONDENSER FLOWS AND DSPEC                                         MNR17580
C                                                                       MNR17600
      IF ( ICON.EQ.0 ) ICON = 1                                         MNR17620
C                                                                       MNR17640
      GO TO (650,670,660), ICON                                         MNR17660
C                                                                       MNR17680
C     LIQUID DISTILLATE                                                 MNR17700
C                                                                       MNR17720
  650 DL = DSPEC                                                        MNR17740
      DV = 0.0                                                          MNR17760
      GO TO 680                                                         MNR17780
C                                                                       MNR17800
C     VAPOR DISTILLATE                                                  MNR17820
C                                                                       MNR17840
  660 DL = 0.0                                                          MNR17860
      DV = DSPEC                                                        MNR17880
      GO TO 680                                                         MNR17900
C                                                                       MNR17920
C     PARTIAL CONDENSER                                                 MNR17940
C                                                                       MNR17960
```

```
  670 IF ( DL.NE.0.0.AND.DV.NE.0.0 ) GO TO 675
C
C     INPUT ERROR
C
      PRINT 2150
      KERROR = KERROR + 1
      GO TO 612
C
  675 DVD = DL + DV
      DL = DL * DSPEC / DVD
      DV = DV * DSPEC / DVD
C
  680 CONTINUE
      BFLOW = FFLOW - DSPEC
      DO 681 I = 1,NCOMP
      FTOT(I) = (FTOT(I)/FTF)*FFLOW
  681 CONTINUE
  686 FRVAP = FVTOT / ( FVTOT + FLTOT )
C
C
      DO 687  I=1,NCOMP
C
      IF ( FVTOT .EQ. 0.0 ) GO TO 1380
      FV(I) = (FV(I)/FTF)*FFLOW
 1380 IF ( FLTOT .EQ. 0.0 ) GO TO 687
      FL(I) = (FL(I)/FTF)*FFLOW
      LFFX(I) = FL(I)/FTOT(I)
      VFFX(I) = FV(I)/FTOT(I)
C
C
C
  687 CONTINUE
C
      GO TO 689
C     CALL TO FFLASH REPLACED BY A CONTINUE. USE LATER IF NEEDED.
  688 CONTINUE
C
C
  689 IF ( ID.EQ.1 ) GO TO 690
C
C     PRINT SUMMARY OF INPUT
C
      PRINT 1000
C
      PRINT 1010, ISTAGE, ISEC, R
C
      PRINT 1020, (FNAME(I), I=1,3), NFSTG
C
      PRINT 1030
C
      IS = 1
      PRINT 1040, DSPEC,IS,BFLOW
C
```

```
      PRINT 1050, P(5), DELPC, DELP, DELP                                MNR19040
C                                                                        MNR19060
C                                                                        MNR19080
      PRINT 1070                                                         MNR19100
C                                                                        MNR19120
      NS(1) = 1                                                          MNR19140
      NS(2) = 2                                                          MNR19160
      NS(3) = NFSTG                                                      MNR19180
      NS(4) = NFSTG + 1                                                  MNR19200
      NS(5) = ISTAGE                                                     MNR19220
C                                                                        MNR19240
      DO 1100 I=1,5                                                      MNR19260
      PRINT 1080,  NS(I), T(I), P(I), LV(I)                              MNR19280
 1100 CONTINUE                                                           MNR19300
      PRINT 1105, T(6), P(6)                                             MNR19320
      PRINT 1120, ( K, VFB(K), LFD(K), K = 1,NCOMP )                     MNR19340
 1120 FORMAT ( //5X, 'COMPOSITION RATIOS -', //10X,'COMPONENT NO.    SECMNR19360
     1TION NO.1     SECTION NO.2', 50(/12X, I4, 7X, 2(2X, E15.8)))       MNR19380
C                                                                        MNR19400
C                                                                        MNR19420
C     PRINT SUMMARY OF FEED STREAMS                                      MNR19440
C                                                                        MNR19460
  690 PRINT 1240                                                         MNR19480
C                                                                        MNR19500
C     PRINT STREAM DATA                                                  MNR19520
C                                                                        MNR19540
      PRINT 1270, (FNAME(I), I=1,3), FFLOW, FP                           MNR19560
C                                                                        MNR19580
      PRINT 1280, FT, ENTH, FRVAP                                        MNR19600
C                                                                        MNR19620
C                                                                        MNR19640
      PRINT 1370                                                         MNR19660
      PRINT 1310                                                         MNR19680
      DO 1400 I=1,NCOMP                                                  MNR19700
C                                                                        MNR19720
      PRINT 1330, I, (CMPNAM(J,I), J=1,3), FTOT(I), FV(I), FL(I)         MNR19740
C                                                                        MNR19760
 1400 CONTINUE                                                           MNR19780
      CALL MINR                                                          MNR19800
      STOP                                                               MNR19820
C                                                                        MNR19840
 1500 RETURN                                                             MNR19860
C                                                                        MNR19880
C     BASE CASE INPUT FORMATS                                            MNR19900
C                                                                        MNR19920
  831 FORMAT ( 1H1, 4X, 'PHYSICAL PROPERTIES', /, 5X, 19('-'),           MNR19940
     1     /,/, 5X, 'K-VALUE COEFFICIENTS  (K/T)**1/3',' = A + BT + ',   MNR19960
     2     'CT**2 + DT**3', / )                                          MNR19980
  832 FORMAT ( 5X, 'CURVE-FIT K-DATA FOR BOTH SECTIONS AT TOP STAGE REFEMNR20000
     1RENCE PRESSURE OF ', F6.1, ' PSIA', /,                             MNR20020
     2          10X, 'ASSUME P*K = CONSTANT', //,                        MNR20040
     3          10X, 'K-VALUES ARE TABULATED AT REFERENCE PRESSURE',/////)MNR20060
  842 FORMAT ( ////10X, 'COMPONENT NO.', I3, //,                         MNR20080
```

```
   1         15X, 'CURVE-FIT COEFFICIENTS', /, 20X, 'A = ', E15.8, /,  MNR20100
   2         20X, 'B = ', E15.8, /,20X, 'C = ', E15.8, /,20X, 'D = ',  MNR20120
   3         E15.8, /,20X, 'STANDARD ERROR OF THE COEFFICIENTS = ',    MNR20140
   4         E10.4, //,15X, 'TEMP (DEG.F)      K (CALC)', //, 30(17X,  MNR20160
   5         F7.2, 9X, F9.4, /) , ///// )                              MNR20180
 910 FORMAT ( 1H1,  4X, 'PHYSICAL PROPERTIES', /5X,  19('-'),//5X,     MNR20200
   1  'K-VALUE COEFFICIENTS  (K/T)**1/3 = A + BT + CT**2 + DT**3', / )MNR20220
 920 FORMAT ( /10X, 'SECTION = ', I4, //15X, 'COMPONENT NO.',10X,'A ', MNR20240
   1          18X, 'B ', 18X, 'C ', 18X, 'D ', / )                     MNR20260
 930 FORMAT ( 17X, I4, 2X, 4(2X,E18.8) )                               MNR20280
1000 FORMAT ( 1H1, 4X, 'SUMMARY OF BASE CASE INPUT', /5X, 26('-') )    MNR20300
1010 FORMAT ( //5X, 'GENERAL -', //10X, 'NUMBER OF STAGES      = ', I5,MNR20320
   1         /10X, 'NUMBER OF SECTIONS    = ', I5, /10X,               MNR20340
   2         'REFLUX RATIO            =  ', F10.5 )                    MNR20360
1020 FORMAT ( //5X, 'FEEDS -', //13X, 'NAME', 9X, 'STAGE NUMBER',      MNR20380
   1         /13X, 4('-'), 9X, 12('-'), //10X, 3A4, 6X, I5 )           MNR20400
1030 FORMAT ( //5X, 'PRODUCTS -', //13X, 'NAME', 9X, 'STAGE NUMBER',   MNR20420
   1         9X, 'RATE (MPH)', /13X, 4('-'), 9X, 12('-'), 9X, 10('-'))MNR20440
1040 FORMAT( /29X,'COND',13X,F10.5,/,29X,I4,13X,F10.5)                 MNR20460
1050 FORMAT ( //5X, 'PRESSURE DROPS -', //10X,                         MNR20480
   1         'PRESSURE OF THE TOP STAGE       = ', F12.5, ' PSIA',/10X,MNR20500
   2         'PRESSURE DROP ACROSS CONDENSER = ', F12.5, ' PSI', /10X,MNR20520
   3         'PRESSURE DROP ACROSS EACH TRAY = ', F12.5, ' PSI', /10X,MNR20540
   4         'PRESSURE DROP ACROSS REBOILER  = ', F12.5, ' PSI' )     MNR20560
1070 FORMAT (                                          ///5X,          MNR20580
   1        'PROFILES -', //10X, 'STAGE NUMBER    TEMPERATURE', 7X,   MNR20600
   2        'PRESSURE            L/V', / )                             MNR20620
1080 FORMAT ( /12X, I4, 4X, 3(4X,F12.5) )                              MNR20640
1105 FORMAT ( /12X, 'COND', 4X, 2(4X,F12.5) )                          MNR20660
1240 FORMAT ( 1H1, 4X, 'SUMMARY OF FEED STREAMS',           /5X, 23('-'MNR20680
   1     ), / )                                                        MNR20700
1270 FORMAT ( 10X, 'STREAM NAME', 20X, 3A4, //10X, 'FLOW RATE', 20X,   MNR20720
   1         F12.4, //10X, 'PRESSURE (PSIA)', 14X, F12.4 )             MNR20740
1280 FORMAT (/10X, 'TEMPERATURE (DEG.F)', 10X, F12.4, //10X,           MNR20760
   1         'ENTHALPY (MBTU/MOL)', 10X, F12.4, //10X,                 MNR20780
   2         'FRACTION VAPORIZED', 11X, F12.4 )                        MNR20800
1300 FORMAT( //10X, 'UNNORMALIZED COMPOSITIONS :' )                    MNR20820
1310 FORMAT (/10X, 'NO.     NAME', 22X, 'TOTAL', 17X, 'VAPOR', 17X,    MNR20840
   1         'LIQUID', / )                                             MNR20860
1330 FORMAT ( 8X, I4, 4X, 3A4, 3X, 3(2X,F20.4) )                       MNR20880
1370 FORMAT ( //10X, 'NORMALIZED COMPOSITIONS :', / )                  MNR20900
C                                                                      MNR20920
      END                                                              MNR20940
```

INPUT

```
*OPTIONS IN EFFECT*  ID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP
*OPTIONS IN EFFECT*  NAME = INPUT    , LINECNT =       55
*STATISTICS*    SOURCE STATEMENTS =       440,PROGRAM SIZE =    17468
*STATISTICS*  NO DIAGNOSTICS GENERATED
```

PROGRAM 5. EVALUATION OF THE POLYNOMIAL TO CALCULATE K VALUES

```
      SUBROUTINE KVAL(PK,TK,IER)                                        MNR20960
C                                                                       MNR20980
      COMMON /KVALUE/ AK(50),          DK(50),         DDK(50)          MNR21000
C                                                                       MNR21020
      COMMON   / SHRTCT /                                               MNR21040
     A   AA(100),        AB(100),        AC(100),        AD(100),       MNR21060
     B  B(50),          BDI(50),        BFLOW,          BN(50),         MNR21080
     C  D(50),          DCALC,          DCON,           DELBAR(100),    MNR21100
     D   DELF(100),      DL,             DLS(50),        DLST,          MNR21120
     E   DN(50),         DSPEC,          DV,             DVS,           MNR21140
     F   DVX(50),        DVXT,           ENTH,           ER,            MNR21160
     G   FACT(100),      FEND(50,6),     FFLOW,          FL(50),        MNR21180
     H  FLTOT,          FMAXA,          FMAXS,          FMINA,          MNR21200
     I  FMINS,          FP,             FRVAP,          FT,             MNR21220
     J  FTOT(50),       FV(50),         FVTOT,          ICON,           MNR21240
     K  ID,             IP,             ISEC,           MTRY,           MNR21260
     L  ISTAGE,         KODE(10),       KSEC,           LFD(50),        MNR21280
     M   LFFX(50),       LV(6),          NABSR,          NCOMP,         MNR21300
     N   NFSTG,          NITER,          NS(5),          NSTRP,         MNR21320
     O   P(6),          R,              S2(50),         S3(50),         MNR21340
     P   S4(50),        S5(50),          T(6),           THETA,         MNR21360
     Q  VFB(50),        VFFX(50),    NTRY,    IHK,    ILK               MNR21380
      PC   = P(5) / PK                                                  MNR21400
C                                                                       MNR21420
      JJ   = (KSEC - 1) * 50                                            MNR21440
C                                                                       MNR21460
      TA   = TK + 460.0                                                 MNR21480
C                                                                       MNR21500
      DO  500   I = 1,NCOMP                                             MNR21520
      KK   = JJ + I                                                     MNR21540
C                                                                       MNR21560
C     EVALUATE POLYNOMIAL AND DERIVATIVES                               MNR21580
C                                                                       MNR21600
      FCN = AA(KK) + TK*(AB(KK) + TK*(AC(KK) + AD(KK)*TK))              MNR21620
      DFN = AB(KK) + TK*(2.*AC(KK)+ TK*3.*AD(KK))                       MNR21640
      DDF = 2.*AC(KK)+ 6.0*AD(KK)*TK                                    MNR21660
C                                                                       MNR21680
C     EVALUATE K (AT CORRECT PRESSURE) AND DERIVATIVES                  MNR21700
C                                                                       MNR21720
      AK(I) =  TA * FCN**3 * PC                                         MNR21740
      DK(I) = (FCN**2)*(FCN + 3.0*TA*DFN) * PC                          MNR21760
      DDK(I)= 3.0*FCN*(FCN*(DFN + TA*DDF) + 2.0*TA*(DFN**2)) * PC       MNR21780
C                                                                       MNR21800
  500 CONTINUE                                                          MNR21820
C                                                                       MNR21840
      RETURN                                                            MNR21860
C                                                                       MNR21880
      END                                                               MNR21900
```

KVAL

```
*OPTIONS IN EFFECT*  ID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP
*OPTIONS IN EFFECT*  NAME = KVAL    , LINECNT =         55
*STATISTICS*    SOURCE STATEMENTS =        17,PROGRAM SIZE =       720
*STATISTICS*  NO DIAGNOSTICS GENERATED
```

PROGRAM 6. EVALUATION OF THE LINEAR SERIES EQUATIONS (5-6), (5-14), (5-19) AND (5-24)

```
      SUBROUTINE LINEAR ( XNM,LOCA, ICOMP )                             MNR21920
C                                                                       MNR21940
C     ADAPTED FROM DELFC AND FORCFT                                     MNR21960
C     KSEC = 1, STRIPPING SECTION S(AVG), XNM = STGM OR PSUEDO-STAGES   MNR21980
C     KSEC= 2, RECTIFYING SECTION A(AVG), XNM = STGN OR PSUEDO-STAGES   MNR22000
C                                                                       MNR22020
C                                                                       MNR22040
      COMMON / LINMIN /   SLFD, SVFB                                    MNR22060
C                                                                       MNR22080
      DIMENSION  SLFD(50),  SVFB(50)                                    MNR22100
C                                                                       MNR22120
      COMMON  / SHRTCT /                                                MNR22140
     A   AA(100),        AB(100),        AC(100),        AD(100),       MNR22160
     B   B(50),          BDI(50),        BFLOW,          BN(50),        MNR22180
     C   D(50),          DCALC,          DCON,           DELBAR(100),   MNR22200
     D   DELF(100),      DL,             DLS(50),        DLST,          MNR22220
     E   DN(50),         DSPEC,          DV,             DVS,           MNR22240
     F   DVX(50),        DVXT,           ENTH,           ER,            MNR22260
     G   FACT(100),      FEND(50,6),     FFLOW,          FL(50),        MNR22280
     H   FLTOT,          FMAXA,          FMAXS,          FMINA,         MNR22300
     I   FMINS,          FP,             FRVAP,          FT,            MNR22320
     J   FTOT(50),       FV(50),         FVTOT,          ICON,          MNR22340
     K   ID,             IP,             ISEC,           MTRY,          MNR22360
     L   ISTAGE,         KODE(10),       KSEC,           LFD(50),       MNR22380
     M   LFFX(50),       LV(6),          NABSR,          NCOMP,         MNR22400
     N   NFSTG,          NITER,          NS(5),          NSTRP,         MNR22420
     O   P(6),           R,              S2(50),         S3(50),        MNR22440
     P   S4(50),         S5(50),         T(6),           THETA,         MNR22460
     Q   VFB(50),        VFFX(50),    NTRY,    IHK,    ILK              MNR22480
C                                                                       MNR22500
      REAL LFD                                                          MNR22520
C                                                                       MNR22540
C     KSEC = 1   STRIPPING SECTION                                      MNR22560
C     KSEC = 2   RECTIFYING SECTION                                     MNR22580
C                                                                       MNR22600
C                                                                       MNR22620
      GO TO ( 10, 20 ), KSEC                                            MNR22640
C                                                                       MNR22660
C     STRIPPING SECTION                                                 MNR22680
C                                                                       MNR22700
   10 LU = 2                                                            MNR22720
      LL = 3                                                            MNR22740
C                                                                       MNR22760
      GO TO 30                                                          MNR22780
C                                                                       MNR22800
C     RECTIFYING SECTION                                                MNR22820
C                                                                       MNR22840
   20 LU = 5                                                            MNR22860
      LL = 4                                                            MNR22880
C                                                                       MNR22900
C     TEST FOR COMPONENTS TO BE CALCULATED                              MNR22920
C                                                                       MNR22940
   30 IF ( ICOMP.EQ.0 ) GO TO 32                                        MNR22960
```

```
C                                                                       MNR22980
      GO TO ( 101, 102, 103, 104 ), LOCA                                MNR23000
C                                                                       MNR23020
  101 I1 = ICOMP                                                        MNR23040
      I2 = ICOMP                                                        MNR23060
      GO TO 34                                                          MNR23080
C                                                                       MNR23100
  102 GO TO 101                                                         MNR23120
C                                                                       MNR23140
  103 I1 = 1                                                            MNR23160
      I2 = ICOMP                                                        MNR23180
      GO TO 34                                                          MNR23200
C                                                                       MNR23220
  104 I1 = ICOMP                                                        MNR23240
      I2 = NCOMP                                                        MNR23260
      GO TO 34                                                          MNR23280
C                                                                       MNR23300
   32 I1 = 1                                                            MNR23320
      I2 = NCOMP                                                        MNR23340
C                                                                       MNR23360
   34 DO 100 I = I1,I2                                                  MNR23380
C                                                                       MNR23400
C     INITIALIZE LINEAR MODEL                                           MNR23420
C                                                                       MNR23440
      IF(( LOCA .EQ. 3 ) .OR. ( LOCA .EQ. 4 ))  GO TO 35                MNR23460
C                                                                       MNR23480
C     INITIALIZE FOR LOCA = 1 OR 2.  THIS IS USED FOR THE DISTRIBUTED   MNR23500
C     COMPONENTS AND GENERATES THE SERIES FROM THE COMPONENT FACTORS    MNR23520
C                                                                       MNR23540
C                                                                       MNR23560
      ASA = FEND(I,LL)                                                  MNR23580
      DEL = ( FEND(I,LU) - ASA ) / XNM                                  MNR23600
      GO TO 36                                                          MNR23620
C                                                                       MNR23640
C     INITIALIZE FOR LOCA = 3 OR 4.  THIS IS USED FOR THE SEPARATED     MNR23660
C     COMPONENTS AND REQUIRES THE RECIPROCAL OF THE COMPONENT FACTORS   MNR23680
C                                                                       MNR23700
C                                                                       MNR23720
   35 ASA = 1. / FEND(I,LL)                                             MNR23740
      DEL =  (( 1. / FEND(I,LU) ) - ASA ) / XNM                         MNR23760
C                                                                       MNR23780
C     INITIALIZE FOR LOCA = 1 OR 2 OR 3 OR 4                            MNR23800
C                                                                       MNR23820
   36 CSA = ASA                                                         MNR23840
      FLSA = ASA                                                        MNR23860
      IDO = IFIX (XNM)                                                  MNR23880
C                                                                       MNR23900
C     CALCULATE FACTORS, PRODUCTS, AND SUMS FOR TRUNCATED INTERGER      MNR23920
C     NUMBER OF TRAYS                                                   MNR23940
C                                                                       MNR23960
      IF ( IDO .LE. 0 ) GO TO 42                                        MNR23980
C                                                                       MNR24000
      DO 40 J = 1,IDO                                                   MNR24020
```

```
      FLSA = FLSA + DEL                                                 MNR24040
      ASA = ASA * FLSA                                                  MNR24060
      CSA = CSA + ASA                                                   MNR24080
   40 CONTINUE                                                          MNR24100
C                                                                       MNR24120
C                                                                       MNR24140
C     CALCULATED FACTORS, PRODUCTS, AND SUMS FOR NEXT INTERGER          MNR24160
C     NUMBER OF TRAYS                                                   MNR24180
C                                                                       MNR24200
   42 FLSA = FLSA + DEL                                                 MNR24220
      ASA1 = ASA * FLSA                                                 MNR24240
      CSA1 = CSA + ASA1                                                 MNR24260
C                                                                       MNR24280
   44 CONTINUE                                                          MNR24300
C                                                                       MNR24320
C                                                                       MNR24340
C     BRANCH PER LOCA                                                   MNR24360
C                                                                       MNR24380
      GO TO ( 1000, 2000, 3000, 4000 ),  LOCA                           MNR24400
C                                                                       MNR24420
C     CALCULATE RATIOS ON FEED TRAY FROM RATIOS AT STRIPPING PINCH ZONE MNR24440
C                                                                       MNR24460
 1000 IF ( IDO ) 1010, 1010, 1020                                       MNR24480
C                                                                       MNR24500
 1010 FN = SVFB(I)                                                      MNR24520
      GO TO 1030                                                        MNR24540
 1020 FN = ASA * SVFB(I) + CSA                                          MNR24560
 1030 F1 = ASA1 * SVFB(I) + CSA1                                        MNR24580
      RIDO = IDO                                                        MNR24600
      VFB(I) = FN + ( F1 - FN ) * ( XNM - RIDO )                        MNR24620
C                                                                       MNR24640
C                                                                       MNR24660
      GO TO 100                                                         MNR24680
C                                                                       MNR24700
C     CALCULATE RATIOS ON TRAY ABOVE FEED FROM RATIOS AT RECTIFYING     MNR24720
C     PINCH ZONE                                                        MNR24740
C                                                                       MNR24760
 2000 IF ( IDO ) 2010, 2010, 2020                                       MNR24780
 2010 FN = SLFD(I)                                                      MNR24800
      GO TO 2030                                                        MNR24820
 2020 FN = ASA * SLFD(I) + CSA                                          MNR24840
 2030 F1 = ASA1 * SLFD(I) + CSA1                                        MNR24860
      RIDO = IDO                                                        MNR24880
      LFD(I) = FN + ( F1 - FN ) * ( XNM - RIDO )                        MNR24900
C                                                                       MNR24920
C                                                                       MNR24940
      GO TO 100                                                         MNR24960
C                                                                       MNR24980
C     CALCULATE FLOW OF LIGHT SEPARATED COMPONENTS AT STRIPPING PINCH   MNR25000
C                                                                       MNR25020
 3000 IF ( IDO ) 3010, 3010, 3020                                       MNR25040
C                                                                       MNR25060
 3010 FN = S3(I)                                                        MNR25080
```

```
      GO TO 3030                                                        MNR25100
 3020 FN = ASA * S3(I)                                                  MNR25120
 3030 F1 = ASA1 * S3(I)                                                 MNR25140
      RIDO = IDO                                                        MNR25160
      S2(I) = FN + ( F1 - FN ) * ( XNM - RIDO )                         MNR25180
C                                                                       MNR25200
C                                                                       MNR25220
      GO TO 100                                                         MNR25240
C                                                                       MNR25260
C     CALCULATE FLOW OF HEAVY SEPARATED COMPONENTS AT RECTIFYING PINCH  MNR25280
C                                                                       MNR25300
 4000 IF ( IDO ) 4010, 4010, 4020                                       MNR25320
C                                                                       MNR25340
 4010 FN = S4(I)                                                        MNR25360
      GO TO 4030                                                        MNR25380
 4020 FN = ASA * S4(I)                                                  MNR25400
 4030 F1 = ASA1 * S4(I)                                                 MNR25420
      RIDO = IDO                                                        MNR25440
      S5(I) = FN + ( F1 - FN ) * ( XNM - RIDO )                         MNR25460
C                                                                       MNR25480
C                                                                       MNR25500
  100 CONTINUE                                                          MNR25520
C                                                                       MNR25540
      RETURN                                                            MNR25560
C                                                                       MNR25580
C                                                                       MNR25600
      END                                                               MNR25620
```

LINEAR

```
*OPTIONS IN EFFECT*  ID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP
*OPTIONS IN EFFECT*  NAME = LINEAR  , LINECNT =       55
*STATISTICS*    SOURCE STATEMENTS =        80,PROGRAM SIZE =      1906
*STATISTICS*  NO DIAGNOSTICS GENERATED
```

PROGRAM 7. MINIMUM REFLUX CALCULATIONS

```
      SUBROUTINE MINR
C
      COMMON / LINMIN /   SLFD, SVFB
C
      COMMON / FNSKOP /  IREF,            REFRCL,         FNM,
     1    REFRCH,        DEST,
     2    LRSTAR,        FNAME(3),        DUMDUM(100)
C
      COMMON /KVALUE/ AK(50),             DK(50),          DDK(50)
C
      COMMON    / SHRTCT /
     A    AA(100),       AB(100),         AC(100),         AD(100),
     B    B(50),         BDI(50),         BFLOW,           BN(50),
     C    D(50),         DCALC,           DCON,            DELBAR(100),
     D    DELF(100),     DL,              DLS(50),         DLST,
     E    DN(50),        DSPEC,           DV,              DVS,
     F    DVX(50),       DVXT,            ENTH,            ER,
     G    FACT(100),     FEND(50,6),      FFLOW,           FL(50),
     H    FLTOT,         FMAXA,           FMAXS,           FMINA,
     I    FMINS,         FP,              FRVAP,           FT,
     J    FTOT(50),      FV(50),          FVTOT,           ICON,
     K    ID,            IP,              ISEC,      MTRY,
     L    ISTAGE,        KODE(10),        KSEC,            LFD(50),
     M    LFFX(50),      LV(6),           NABSR,           NCOMP,
     N    NFSTG,         NITER,           NS(5),           NSTRP,
     O    P(6),          R,               S2(50),          S3(50),
     P    S4(50),        S5(50),          T(6),            THETA,
     Q    VFB(50),       VFFX(50),    NTRY,    IHK,    ILK
C
      DIMENSION LVRAT(6),TEMP(6),SLFD(50),SVFB(50),AAHK(50),SALK(50)
      REAL LRSTAR,KRSTAR,LSSTAR,LVRAT,KSSTAR,KSTAR,LFD,LFFX,LV,MULT,
     1     LFDTRY,LRSTR1,LRSTR2
C
 7777 CONTINUE
C
C
C     INITIALIZE TEMPERATURES
      DO 10 I = 1,6
   10 TEMP(I) = T(I)
C
C     CALCULATE FRACTION RECOVERIES AND B/D'S FOR LIGHT AND HEAVY KEY
      FRCL = REFRCL / 100
      FRCH = REFRCH / 100.
      BDI(ILK) = ( 1.0 - FRCL ) / FRCL
      BDI(IHK) = FRCH / ( 1.0 - FRCH )
C
C     SET COUNTERS FOR NUMBER OF ITERATIONS. ITRY IS FOR ITERATIONS AT
C     CONSTANT VALUE OF LRSTAR. JLK OR JHK IS FOR ITERATIONS ON LRSTAR.
      ITRY = 0
      JTRY = 1
      JLK = 0
      JHK = 0
C
```

```
      STGM = 5.
      STGN = 5.
C
      IF ( DEST ) 110,110,120
C
C     CALCULATE DEFAULT ESTIMATE ON DISTILLATE ASSUMING IDEAL SPLIT OF
C     LIGHTER THAN LIGHT KEY AND SPECIFIED SPLIT OF LIGHT AND HEAVY KEY
C
  110 IDO = ILK - 1
      DEST = 0.0
      DO 115 I=1,IDO
      DEST = DEST + FTOT(I)
  115 CONTINUE
      IDO = IHK - 1
      DO 116 I=ILK,IDO
  116 DEST = DEST + (FTOT(I) * FRCL)
      DEST = DEST + FTOT(IHK) * (1.0 - FRCH)
  120 IF (LRSTAR .GT. 0.) GO TO 200
C
C     INITIAL DEFAULT ESTIMATE ON LRSTAR IS TO ASSUME A TYPE ONE SYSTEM
C     IN TOP AND BOTTOM AND USE UNDERWOOD EQUATION METHOD NOT PRESENTLY
C     PROGRAMMED
C
      STOP
  200 CONTINUE
C     THIS IS RETURN POINT FOR MAJOR EXTERNAL LOOP.
      ITRY = ITRY + 1
      ICONV = 0
C
C
C     CALCULATE INTERNAL FLOW RATES AND L/V RATIOS FOR LOCATIONS 2 TO 5
C
C
      VRSTAR = LRSTAR + DEST
      LSSTAR = LRSTAR + FLTOT
      VSSTAR = VRSTAR - FVTOT
      BEST   = FFLOW - DEST
C
C
      LVRAT(5) = LRSTAR / VRSTAR
      LVRAT(4) = LVRAT(5)
      LVRAT(2) = LSSTAR/ VSSTAR
      LVRAT(3) = LVRAT(2)
C
C     INITIAL DEFAULT ESTIMATE ON STAR TEMPERATURES BY ASSUMING FACTORS
C     EQUAL 0.9 FOR LIGHT AND HEAVY KEY.
  300 IF (TEMP(2) .NE. 0. .AND. TEMP(5) .NE. 0.) GO TO 400
  310 KRSTAR = LVRAT(5) / 0.9
      KSSTAR = LVRAT(2) * 0.9
      TSTART = FT
      KKEY = 1
      KSTAR = KSSTAR
      IK = ILK
```

```
C     EVALUATE POLYNOMIAL AND DERIVATIVES                               MNR27760
C                                                                       MNR27780
  320 DO 330 I=1,50                                                     MNR27800
      FCN = AA(IK) + TSTART * (AB(IK) + TSTART * (AC(IK) + AD(IK) *     MNR27820
     1    TSTART))                                                      MNR27840
      DFN = AB(IK) + TSTART * (2.*AC(IK) + TSTART * 3. * AD(IK))        MNR27860
      FFT  = ((TSTART + 460.) * FCN **3) - KSTAR                        MNR27880
      DFFT = (FCN ** 2) * (FCN + 3.0 * (TSTART + 460.) * DFN )          MNR27900
      IF (ABS (FFT) .LT. 1.0 E-04)  GO TO 340                           MNR27920
      TSTART = TSTART - ( FFT / DFFT)                                   MNR27940
  330 CONTINUE                                                          MNR27960
      PRINT 335                                                         MNR27980
  335 FORMAT ('0',5X,'**** NEWTON''S METHOD FAILED TO GENERATE A NEW TEMMNR28000
     1PERATURE IN 50 ITERATIONS. ****' )                                MNR28020
      STOP                                                              MNR28040
  340 GO TO (350,360), KKEY                                             MNR28060
  350 TEMP(2) = TSTART                                                  MNR28080
      TSTART = FT                                                       MNR28100
      KKEY = 2                                                          MNR28120
      KSTAR = KRSTAR                                                    MNR28140
      IK = IHK                                                          MNR28160
      GO TO 320                                                         MNR28180
  360 TEMP(5) = TSTART                                                  MNR28200
C                                                                       MNR28220
C                                                                       MNR28240
C     CALCULATE ABSORPTION AND STRIPPING FACTORS FOR ALL COMPONENTS AT  MNR28260
C     KEY LOCATIONS                                                     MNR28280
C                                                                       MNR28300
  400 DO 410 J=2,5                                                      MNR28320
      DO 409 I=1,NCOMP                                                  MNR28340
      FCN = AA(I) + TEMP(J) * (AB(I) + TEMP(J) * (AC(I) + AD(I) *       MNR28360
     1    TEMP(J) ) )                                                   MNR28380
      A   = (FCN ** 3) * (TEMP(J) + 460.)                               MNR28400
      IF(J.EQ.2.OR.J.EQ.3) FEND(I,J) = A / LVRAT(J)                     MNR28420
      IF(J.EQ.4.OR.J.EQ.5) FEND(I,J) = LVRAT(J) / A                     MNR28440
C                                                                       MNR28460
C                                                                       MNR28480
C                                                                       MNR28500
  409 CONTINUE                                                          MNR28520
  410 CONTINUE                                                          MNR28540
C                                                                       MNR28560
C     CALCULATE TYPE OF SEPARATION IN TOP AND BOTTOM SECTIONS           MNR28580
C                                                                       MNR28600
C                                                                       MNR28620
C     START WITH FIRST COMPONENT HEAVIER THAN HEAVY KEY AND CHECK IF    MNR28640
C     ABSORPTION FACTOR AT TOP PINCH IS GREATER THAN ONE.IF NOT CONTINUEMNR28660
C     THROUGH HEAVY COMPONENTS. FIRST COMPONENT WITH ABSORPTION FACTOR  MNR28680
C     GREATER THAN ONE SETS INDEX FOR HEAVY SEPARATED COMPONENTS AND    MNR28700
C     SETS TOP SECTION AS TYPE TWO. IF ALL COMPONENTS HAVE ABSORPTION   MNR28720
C     FACTORS LESS THAN ONE THE TOP IS TYPE ONE.                        MNR28740
      IDO = IHK + 1                                                     MNR28760
      DO  440   I=IDO,NCOMP                                             MNR28780
      IF (FEND(I,5) .LE. 1.0) GO TO 440                                 MNR28800
```

```
      ITR = 2
      IHS = I
C
      IF (STGN) 432, 432, 450
  432 STGN = 5.0
      GO TO 450
  440 CONTINUE
      STGN = 0.0
  442 ITR = 1
      IHS = NCOMP + 1
  450 CONTINUE
C     START WITH FIRST COMPONENT LIGHTER THAN LIGHT KEY AND CHECK IF
C     STRIPPING FACTOR AT BOTTOM PINCH IS GREATER THAN ONE. IF NOT
C     CONTINUE UP THROUGH LIGHT COMPONENTS, FIRST COMPONENT WITH
C     STRIPPING FACTOR GREATER THAN ONE SETS INDEX FOR LIGHT SEPARATED
C     COMPONENTS AND SETS BOTTOM SECTION AS TYPE TWO. IF ALL COMPONENTS
C     HAVE STRIPPING FACTORS LESS THAN ONE THE BOTTOM IS TYPE ONE.
      IDO = ILK - 1
      J = IDO
      DO  460 I = 1,IDO
      J = J + 1 - I
      IF (FEND(J,2) .LE. 1.0)  GO TO 460
      ITS =  2
      ILS = J
      IF (STGM) 452, 452, 464
  452 STGM = 5.0
      GO TO 464
  460 CONTINUE
      STGM = 0.0
  462 ITS = 1
      ILS = 0
  464 CONTINUE
C     BRANCH FOR CALCULATION ON N AND M DEPENDING ON TYPE OF SYSTEM
C
      IF ( ITR .EQ. 1 )  GO TO 550
      IF ( ITS .EQ. 2 )  GO TO 580
C     CONTINUE FOR TYPE TWO TOP AND TYPE ONE BOTTOM.
C
C     CALCULATE NUMBER OF STAGES (N)
C     LOCA=2 IS FOR DISTRIBUTED COMPS IN THE RECTIFYING SECTION
C     KSEC=2 IS FOR THE RECTIFYING SECTION
      LOCA = 2
      KSEC = 2
C
  504 SLFD(IHK) = FEND(IHK,5) / (1.0 - FEND(IHK,5))
      VFB(IHK)  = FEND(IHK,2) / (1.0 - FEND(IHK,2))
      DIV = VFB(IHK) + VFFX(IHK)
C
C     INITIALIZE FOR N = 0. TRANSFER OUT IF B/D EQUALS OR EXCEEDS SPEC.
C     HOWEVER RECOGNIZE INCONSISTANCY OF N = 0 AND TYPE TWO TOP.
C
C
      BDHK=  (SLFD(IHK) + LFFX(IHK)) / DIV
```

```
C
      DELBD1 = BDI(IHK) - BDHK
      IF ( DELBD1 .LT. 0.0 )  GO TO 505
C
      STGN = 0.0
      GO TO 530
C
  505 CONTINUE
C     CONVERGE ON N BY LINEAR INTERPOLATION WITH B/D CALC. AND B/D SPEC.
      STGN1 = 0.0
      STGN2 = STGN
C
      DO 520 I = 1,25
      CALL LINEAR ( STGN, LOCA, IHK )
      BDHK= (LFD(IHK) + LFFX(IHK)) / DIV
      DELBD2 = BDI(IHK) - BDHK
      IF ( ABS ( DELBD2 ) .LT. .00001 )  GO TO 530
      STGN = ( STGN1 * DELBD2 - STGN2 * DELBD1 ) / ( DELBD2 - DELBD1 )
C
C     IF STGN HAS EXCEEDED 50, PROGRAM WILL USE 50. FOR THIS TRIAL
C
C
      IF ( STGN .GT. 50. )  GO TO 522
      IF ( STGN .LE. 0.0 )  GO TO 526
      STGN1 = STGN2
      STGN2 = STGN
      DELBD1 = DELBD2
      DELBD1 = DELBD2
  520 CONTINUE
C
      PRINT 525
  525 FORMAT ('0',5X,'**** HEAVY KEY B/D SPEC AND B/D CALC HAVE NOT CONV
     1ERGED IN 25 ITERATIONS. ****' )
      GO TO 530
  522 STGN = 50.
      PRINT 523
  523 FORMAT ( '0', 5X, '**** N EXCEEDS 50.  PROGRAM WILL USE 50. FOR',
     1  ' THIS TRIAL. ****' )
C
      GO TO 530
  526 STGN = 0.0001
C
  530 CONTINUE
C
  550 IF ( ITS.EQ.1 ) GO TO 600
C
C     CONTINUE FOR TYPE ONE TOP AND TYPE TWO BOTTOM.
C     CALCULATE NUMBER OF STAGES (M)
C
C     LOCA = 1 IS FOR DISTRIBUTED COMPS IN THE STRIPPING SECTION
C     KSEC = 1 IS FOR THE STRIPPING SECTION
      LOCA = 1
      KSEC = 1
```

```
  554 SVFB(IREF) = FEND(IREF,2)  /  (1.0 - FEND(IREF,2))
      LFD(IREF)  = FEND(IREF,5)  /  (1.0 - FEND(IREF,5))
      MULT =  LFD(IREF) + LFFX(IREF)
C
C     INITIALIZE FOR M = 0. TRANSFER OUT IF B/D EQUALS OR EXCEEDS SPEC.
C     HOWEVER RECOGNIZE INCONSISTANCY OF M = 0 AND TYPE TWO BOTTOM.
      BDLK= MULT/ (SVFB(ILK) + VFFX(ILK))
      DELBD1 = BDI(ILK) - BDLK
      IF ( DELBD1 .GT. 0.0 )  GO TO 565
C
      STGM = 0.0
      GO TO 574
C
  565 CONTINUE
C     CONVERGE ON M BY LINEAR INTERPOLATION WITH B/D CALC. AND B/D SPEC.
      STGM1 = 0.0
      STGM2 = STGM
      DO 570 I = 1,25
      CALL LINEAR ( STGM, LOCA, ILK )
      BDLK= MULT / ( VFB(ILK)+VFFX(ILK))
      DELBD2 = BDI(ILK) - BDLK
      IF (ABS(DELBD2).LT. .00001 ) GO TO 578
      STGM = ( STGM1*DELBD2 - STGM2*DELBD1) / ( DELBD2 - DELBD1 )
C
C     IF STGM HAS EXCEEDED 50, PROGRAM WILL USE 50. FOR THIS TRIAL
C
      IF ( STGM .GT. 50. )  GO TO 572
C
      IF ( STGM .LE.  0.0 ) GO TO 574
      STGM1 = STGM2
      STGM2 = STGM
      DELBD1 = DELBD2
  570 CONTINUE
      PRINT 575
  575 FORMAT ('0',5X,'**** LIGHT KEY B/D SPEC AND B/D CALC HAVE NOT CONV
     1ERGED IN 25 ITERATIONS. ****' )
      GO TO 574
  572 STGM = 50.
      PRINT 573
  573 FORMAT ( '0', 5X, '**** M EXCEEDS 50.  PROGRAM WILL USE 50. FOR',
     1  ' THIS TRIAL' )
      GO TO 578
  574 STGM = 0.0001
  578 CONTINUE
      GO TO 600
  580 CONTINUE
C
C     CALCULATE NUMBER OF STAGES FOR TYPE TWO BOTTOM AND TYPE TWO TOP
C
C
      SVFB(ILK) = FEND(ILK,2) / (1.0 - FEND(ILK,2))
      SLFD(ILK) = FEND(ILK,5) / (1.0 - FEND(ILK,5))
      SVFB(IHK) = FEND(IHK,2) / (1.0 - FEND(IHK,2))
```

```
      SLFD(IHK) = FEND(IHK,5) / (1.0 - FEND(IHK,5))
C     INITIALIZE FOR N AND M = 0
C     TRANSFER OUT IF B/D'S EQUAL OR EXCEED SPEC. HOWEVER RECOGNIZE
C     INCONSISTANCY OF M=0 AND N=0 FOR TYPE TWO TOP AND BOTTOM
      BDHK = (SLFD(IHK) + LFFX(IHK)) / (SVFB(IHK) + VFFX(IHK))
      BDLK = (SLFD(ILK) + LFFX(ILK)) / (SVFB(ILK) + VFFX(ILK))
      DBDHK1 = BDI(IHK) - BDHK
      DBDLK1 = BDI(ILK) - BDLK
      IF ((DBDHK1.LT.0.).OR.(DBDLK1.GT.0.)) GO TO 582
      STGN = 0.0
      STGM = 0.0
      GO TO 585
  582 CONTINUE
C     CONVERGE ON N AND M BY LINEAR INTERPOLATION WITH B/D CALC.
C     AND B/D SPEC.
      STGN1 = 0.0
      STGM1 = 0.0
      STGN2 = STGN
      STGM2 = STGM
      DO 584 I = 1, 25
      LOCA = 2
      KSEC = 2
      CALL LINEAR (STGN, LOCA, IHK)
      CALL LINEAR (STGN, LOCA, ILK)
      LOCA = 1
      KSEC = 1
      CALL LINEAR (STGM, LOCA, IHK)
      CALL LINEAR (STGM, LOCA, ILK)
C
      BDHK = (LFD(IHK) + LFFX(IHK)) / (VFB(IHK) + VFFX(IHK))
      BDLK = (LFD(ILK) + LFFX(ILK)) / (VFB(ILK) + VFFX(ILK))
      DBDHK2 = BDI(IHK) - BDHK
      DBDLK2 = BDI(ILK) - BDLK
      IF ((ABS(DBDHK2).LT.0.00001).AND.(ABS(DBDLK2).LT.0.00001))
     1   GO TO 590
      STGN = (STGN1*DBDHK2 - STGN2*DBDHK1) / (DBDHK2 - DBDHK1)
      IF (STGN.LE.0.0) STGN = 0.0001
      IF ( STGN .GT. 50. )  STGN = 50.
      STGN1 = STGN2
      STGN2 = STGN
      DBDHK1 = DBDHK2
      STGM = (STGM1*DBDLK2 - STGM2*DBDLK1) / (DBDLK2 - DBDLK1)
      IF ( STGM .GT. 50. )  STGM = 50.
      IF (STGM.LE.0.0) STGM = 0.0001
      STGM1 = STGM2
      STGM2 = STGM
      DBDLK1 = DBDLK2
      IF(STGM.EQ.50..AND.STGN.EQ.50.) GO TO 585
      IF(STGM.EQ.0.0001.AND.STGN.EQ.0.0001) GO TO 590
  584 CONTINUE
      PRINT 525
      PRINT 575
      GO TO 590
```

```
  585 PRINT 523                                                          MNR33060
      PRINT 573                                                          MNR33080
  590 CONTINUE                                                           MNR33100
  600 IF ( ITR.EQ.2 ) GO TO 620                                          MNR33120
C                                                                        MNR33140
C     MATERIAL BALANCE FOR TYPE ONE RECTIFYING SECTION                   MNR33160
C                                                                        MNR33180
      DO 610 I = 1,NCOMP                                                 MNR33200
      LFD(I) = FEND(I,5) / ( 1.0 - FEND(I,5) )                           MNR33220
  609 SLFD(I) = LFD(I)                                                   MNR33240
  610 CONTINUE                                                           MNR33260
C                                                                        MNR33280
      GO TO 640                                                          MNR33300
C                                                                        MNR33320
C     MATERIAL BALANCE FOR TYPE TWO RECTIFYING SECTION                   MNR33340
C                                                                        MNR33360
  620 IDO = IHS - 1                                                      MNR33380
      KSEC = 2                                                           MNR33400
      LOCA = 2                                                           MNR33420
C                                                                        MNR33440
      DO 625 I = 1,IDO                                                   MNR33460
  625 SLFD(I) = FEND(I,5) / ( 1.0 - FEND(I,5) )                          MNR33480
      IF ( STGN )  628, 628, 630                                         MNR33500
  628 DO 629 I = 1,IDO                                                   MNR33520
  629 LFD(I) = SLFD(I)                                                   MNR33540
      GO TO 640                                                          MNR33560
C                                                                        MNR33580
  630 CALL LINEAR ( STGN, LOCA, 0 )                                      MNR33600
  640 CONTINUE                                                           MNR33620
C                                                                        MNR33640
      IF ( ITS.EQ.2 ) GO TO 660                                          MNR33660
C                                                                        MNR33680
C     MATERIAL BALANCE FOR TYPE ONE STRIPPING SCTION                     MNR33700
C                                                                        MNR33720
      DO 650 I = 1,NCOMP                                                 MNR33740
      VFB(I) = FEND(I,2) / ( 1.0 - FEND(I,2) )                           MNR33760
  649 SVFB(I) = VFB(I)                                                   MNR33780
  650 CONTINUE                                                           MNR33800
C                                                                        MNR33820
      GO TO 680                                                          MNR33840
C                                                                        MNR33860
C     MATERIAL BALANCE FOR TYPE TWO STRIPPING SECTION                    MNR33880
C                                                                        MNR33900
  660 IDO = ILS + 1                                                      MNR33920
C                                                                        MNR33940
      KSEC = 1                                                           MNR33960
      LOCA = 1                                                           MNR33980
C                                                                        MNR34000
C                                                                        MNR34020
      DO 665 I = IDO,NCOMP                                               MNR34040
  665 SVFB(I) = FEND(I,2) / ( 1.0 - FEND(I,2) )                          MNR34060
C                                                                        MNR34080
      IF ( STGM ) 668,668,670                                            MNR34100
```

```
  668 DO 669 I= IDO,NCOMP                                                MNR34120
  669 VFB(I) = SVFB(I)                                                   MNR34140
      GO TO 680                                                          MNR34160
C                                                                        MNR34180
  670 CALL LINEAR ( STGM, LOCA, 0 )                                      MNR34200
  680 CONTINUE                                                           MNR34220
C     OVERALL MATERIAL BALANCE AND DISTILLATE RATE                       MNR34240
C                                                                        MNR34260
      I1 = ILS + 1                                                       MNR34280
      I2 = IHS - 1                                                       MNR34300
      DTRIAL = 0.0                                                       MNR34320
      THETLK = 1.0                                                       MNR34340
      THETHK = 1.0                                                       MNR34360
C                                                                        MNR34380
      BDHK = ( LFD(IHK) + LFFX(IHK) ) / ( VFB(IHK) +  VFFX(IHK) )        MNR34400
      THETHK = BDI(IHK) / BDHK                                           MNR34420
C                                                                        MNR34440
      BDLK = ( LFD(ILK) + LFFX(ILK) ) / ( VFB(ILK) + VFFX(ILK) )         MNR34460
      THETLK = BDI(ILK) / BDLK                                           MNR34480
      PRINT 6868, THETLK, THETHK                                         MNR34500
 6868 FORMAT(/5X,'THETA LIGHT KEY =',F9.3,/5X,'THETA HEAVY KEY =',F9.3/)MNR34520
      IF ( ITS .EQ. 1 ) GO TO 684                                        MNR34540
C                                                                        MNR34560
C     CALCULATE DISTILLATE RATE FOR LIGHT SEPARATED COMPONENTS           MNR34580
C                                                                        MNR34600
      DO 682 I = 1,ILS                                                   MNR34620
      D(I) = FTOT(I)                                                     MNR34640
      B(I) = 0.0                                                         MNR34660
  682 DTRIAL = DTRIAL + D(I)                                             MNR34680
      CONTINUE                                                           MNR34700
C                                                                        MNR34720
C     CALCULATE DISTILLATE RATE FOR DISTRIBUTED COMPONENTS               MNR34740
C                                                                        MNR34760
  684 DO 698 I = I1,I2                                                   MNR34780
      BDI(I) = ( LFD(I) + LFFX(I) ) /   ( VFB(I) + VFFX(I) )             MNR34800
      IF ( I .EQ. IHK ) GO TO 686                                        MNR34820
      IF ( I .EQ. ILK )  GO TO 685                                       MNR34840
      GO TO 688                                                          MNR34860
  685 BDI(I) = THETLK * BDI(I)                                           MNR34880
      GO TO 688                                                          MNR34900
  686 BDI(I) = THETHK * BDI(I)                                           MNR34920
 688  D(I) = FTOT(I) / ( 1. + BDI(I) )                                   MNR34940
 697  B(I) = BDI(I) * D(I)                                               MNR34960
      DTRIAL = DTRIAL + D(I)                                             MNR34980
 698  CONTINUE                                                           MNR35000
  700 IF ( ITR.EQ.1 ) GO TO 710                                          MNR35020
C                                                                        MNR35040
C     CALCULATE DISTILLATE RATE FOR HEAVY SEPARATED COMPONENTS           MNR35060
C                                                                        MNR35080
      DO 702 I = IHS,NCOMP                                               MNR35100
      D(I) = 0.0                                                         MNR35120
      B(I) = FTOT(I)                                                     MNR35140
  702 CONTINUE                                                           MNR35160
```

```
  710 CONTINUE
C
C     FIRST CONVERSION CHECK: CHANGE IN DISTILLATE RATE
C
      IF ( ABS(DTRIAL - DEST).LE.(0.001*DEST) ) ICONV = 1
      DEST = DTRIAL
      BEST = FFLOW - DEST
C
C     CALC LR(STAR) FOR TRIAL.
      TRYLFS = 0.0
      TRYLRS = 0.0
      IDO = IHS - 1
C
      DO 720 I = 1,IDO
      S5(I) = SLFD(I) * D(I)
      TRYLRS = TRYLRS + S5(I)
      S4(I) = LFD(I) * D(I)
      TRYLFS = TRYLFS + S4(I)
  720 CONTINUE
C
      IF ( ITR.EQ.1 ) GO TO 730
C
      DO 722 I = IHS,NCOMP
      S4(I) = VFB(I) * B(I) + FV(I)
      TRYLFS = TRYLFS + S4(I)
  722 CONTINUE
      IF ( STGN )  723, 723, 726
  723 DO 724 I = IHS,NCOMP
  724 S5(I) = S4(I)
      GO TO 727
  726 KSEC = 2
      LOCA = 4
      CALL LINEAR ( STGN, LOCA,IHS)
  727 DO 728 I = IHS,NCOMP
  728 TRYLRS = TRYLRS + S5(I)
C
  730 CONTINUE
C
C
C     CALC VS(STAR) FOR TRIAL
C
      TRYVSS = 0.0
      TRYVFS = 0.0
      IDO = ILS + 1
C
      DO 740 I = IDO,NCOMP
      S3(I) = VFB(I) * B(I)
      S2(I) = SVFB(I) * B(I)
      TRYVSS = TRYVSS + S2(I)
      TRYVFS = TRYVFS + S3(I)
  740 CONTINUE
C
      IF ( ITS.EQ.1 ) GO TO 750
```

```
C
      DO 742 I = 1,ILS
      S3(I) = S4(I) + FL(I)
      TRYVFS = TRYVFS + S3(I)
  742 CONTINUE
C
      IF ( STGM ) 743,743,746
  743 DO 744 I = 1,ILS
  744 S2(I) = S3(I)
      GO TO 747
C
  746 KSEC = 1
      LOCA = 3
      CALL LINEAR ( STGM, LOCA,ILS)
  747 DO 748 I = 1,ILS
  748 TRYVSS = TRYVSS + S2(I)
C
  750 KSEC = 2
C
C
C     THE FOLLOWING IS INTENDED FOR TYPE ONE IN TOP AND BOTTOM SECTIONS.
C     USES THE CALCULATED LRSTAR AS MINIMUM REFLUX ON THE NEXT TRIAL.
C
      IF (( ITR .EQ. 2 ) .OR. ( ITS .EQ. 2 ))  GO TO 759
C
      LRSTAR = TRYLRS
  759 CONTINUE
C     TEMPERATURE OF RECTIFYING PINCH ZONE. SECOND CONVERGENCE CHECK.
C     USE AVERAGE TEMPERATURE FOR NEXT TRIAL IF OSCILLATION DEVELOPING.
C
C
C     TEMPERATURE OF RECTIFYING PINCH ZONE
C
      TEMP5 = TEMP(5)
      CALL BUB ( P(5), TEMP(5), S5 )
C
      DELT = ABS ( TEMP5 - TEMP(5) )
      IF ( DELT - 0.1 ) 760, 760, 762
  760 ICONV = ICONV + 1
      GO TO 767
  762 DELTR1 = TEMP(5) - TEMP5
      IF ( ITRY - 1 )  768, 768, 764
  764 IF ( DELTR1 / DELTR2 )  766, 766, 768
  766 TEMP(5) = ((( TEMP(5) + TEM5 ) / 2. ) + TEMP5 ) / 2.
  767 DELTR1 = TEMP(5) - TEMP5
  768 DELTR2 = DELTR1
      TEM5 = TEMP5
C     TEMPERATURE OF STAGE ABOVE FEED
C
  769 CALL BUB ( P(4), TEMP(4), S4 )
C
C     TEMPERATURE OF DISTILLATE (LIQUID)
C
```

```
      CALL BUB ( P(6), TEMP(6), D )
C
C
      KSEC = 1
C
C     TEMPERATURE OF STRIPPING PINCH ZONE.  THIRD CONVERGENCE CHECK.
C     USE AVERAGE TEMPERATURE FOR NEXT TRIAL IF OSCILLATION DEVELOPING.
      TEMP2 = TEMP(2)
C
      CALL DEW ( P(2), TEMP(2), S2 )
C
      DELT = ABS ( TEMP2 - TEMP(2) )
      IF ( DELT - 0.1 )  770, 770, 772
  770 ICONV = ICONV + 1
C
      GO TO 777
C
  772 DELTS1 = TEMP(2) - TEMP2
      IF ( ITRY - 1 )  778, 778, 774
  774 IF ( DELTS1 / DELTS2 )  776, 776, 778
  776 TEMP(2) = ((( TEMP(2) + TEM2 ) / 2. ) + TEMP2 ) / 2.
  777 DELTS1 = TEMP(2) - TEMP2
  778 DELTS2 = DELTS1
      TEM2 = TEMP2
C     TEMPERATURE OF FEED STAGE
C
  779 CALL DEW ( P(3), TEMP(3), S3 )
C
C     TEMPERATURE OF BOTTOMS
      CALL BUB ( P(1), TEMP(1), B )
C
C
      IF ( ICONV.EQ.3 ) GO TO 1010
C
      IF ( ITRY - NTRY ) 200,1010,1010
 1000 CONTINUE
C
C     NO CONVERGENCE ON LRSTAR FOR TYPE ONE IN TOP AND BOTTOM.
 8888 CONTINUE
C
 1010 IF ((ITR.EQ.1).AND.(ITS.EQ.1)) GO TO 1196
C     USES THETA LK OR THETA HK FOR CONVERGENCE ADJUSTMENT ON LRSTAR.
      LRSTR1 = LRSTAR
      DTHL1 = THETLK - 1.0
      DTHH1 = THETHK - 1.0
C     CHECK FOR TYPE TWO TOP AND TYPE ONE BOTTOM. CONTINUE FOR THIS
C     CASE AND CONVERGE ON DEVIATION OF THETA LK FROM 1.0. IF THETA LK
C     IS WITHIN TOLERANCE THE CALCULATION IS FINISHED.
      IF (ITS .EQ. 2) GO TO 1100
      ADTHLK = ABS (DTHL1 - 0.001)
      IF (ADTHLK) 1200, 1200, 1020
C     IF THIS IS SECOND TRIAL OR GREATER GO TO INTERPOLATION FOR LRSTAR.
C     IF THIS IS FIRST TRIAL USE ARBITRARY FACTORS TO ADJUST LRSTAR BUT
```

```
C     FIRST CHECK TO SEE IF JHK IS GREATER THAN ZERO. THIS WOULD MEAN
C     TYPE SYSTEM HAS CHANGED AND CALCULATION IS STOPPED.
 1020 IF (JLK .GT. 0) GO TO 1080
 1030 IF (JHK .EQ. 0) GO TO 1050
 1040 PRINT 1045
 1045 FORMAT ('0',5X,'**** CONVERGENCE PATH ON LRSTAR HAS SWITCHED FROM
     1THETA HK TO THETA LK ****' )
      STOP
 1050 IF (DTHL1) 1060, 1200, 1070
 1060 LRSTAR = LRSTAR * 0.95
      GO TO 1090
 1070 LRSTAR = LRSTAR * 1.05
      GO TO 1090
 1080 LRSTAR = (LRSTR1*DTHL2 - LRSTR2*DTHL1) / (DTHL2 - DTHL1)
 1090 JLK = JLK + 1
      GO TO 1195
C     CHECK FOR TYPE TWO TOP AND BOTTOM. TEMPOARY STOP FOR THIS CASE.
 1100 IF (ITR.EQ.2) GO TO 1200
C     CONTINUE FOR TYPE ONE TOP AND TYPE TWO BOTTOM AND CONVERGE ON
C     DEVIATION OF THETA HK FROM 1.0. IF THETA HK IS WITHIN TOLERANCE
C     THE CALCULATION IS FINISHED.
      ADTHHK = ABS(DTHH1 - 0.001)
      IF (ADTHHK) 1200, 1200, 1120
C     IF THIS IS SECOND TRIAL OR GREATER GO TO INTERPOLATION FOR LRSTAR.
C     IF THIS IS FIRST TRIAL USE ARBITRARY FACTORS TO ADJUST LRSTAR BUT
C     FIRST CHECK TO SEE IF JLK IS GREATER THAN ZERO, THIS WOULD MEAN
C     TYPE SYSTEM HAS CHANGED AND CALCULATION IS STOPPED.
C     INITALIZE N AND M AT FIVE.
 1120 IF (JHK .GT. 0) GO TO 1180
 1130 IF (JLK .EQ. 0) GO TO 1150
 1140 PRINT 1145
 1145 FORMAT ('0',5X,'**** CONVERGENCE PATH ON LRSTAR HAS SWITCHED FROM
     1THETA LK TO THETA HK ****' )
      STOP
 1150 IF (DTHH1) 1160, 1200, 1170
 1160 LRSTAR = LRSTAR * 0.95
      GO TO 1190
 1170 LRSTAR = LRSTAR * 1.05
      GO TO 1190
 1180 LRSTAR = (LRSTR1*DTHH2 - LRSTR2*DTHH1) / (DTHH2 - DTHH1)
 1190 JHK = JHK + 1
 1195 LRSTR2 = LRSTR1
      DTHL2 = DTHL1
      DTHH2= DTHH1
      ITRY = 1
 1196 JTRY = JTRY + 1
      IF (MTRY - JTRY) 1200, 1200, 200
 1200 STOP
C
C
C
      END
```

MINR

```
*OPTIONS IN EFFECT*  ID,EBCDIC,SOURCE,NOLIST,NODECK,LOAD,NOMAP
*OPTIONS IN EFFECT*  NAME = MINR     , LINECNT =       55
*STATISTICS*    SOURCE STATEMENTS =       432,PROGRAM SIZE =     9836
*STATISTICS*  NO DIAGNOSTICS GENERATED

*STATISTICS*  NO DIAGNOSTICS THIS STEP 2
```

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