SEMIRIGOROUS CALCULATION ALGORITHM FOR COMPLEX

FRACTIONATORS

By

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1956

Submitted to the faculty of the Graduate School
of the Oklahoma State University in partial
fulfillment of the requirements
for the degree of
MASTER OF SCIENCE
May, 1966

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PREFACE

A mathematical model has been developed to characterize a multicomponent distillation column. A fractionator with a maximum of three feeds and six products can be computed. The number of theoretical stages, the product rates and the product compositions are calculated. Feed entry and product withdrawal points are also computed. The input data required include the number of product streams and the ratio of light key split between products and the ratio of heavy key split between products. The method is programmed in FORTRAN for a digital computer. Results of comparison between the semirigorous method and the conventional rigorous tray-by-tray calculations demonstrate the reliability of the proposed model.

The author wishes to thank Dr. R. N. Maddox for his advice and encouragement; and Phillips Petroleum Company for their support.

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CHAPTER I

INTRODUCTION

This work develops and evaluates a mathematical model for complex fractionators. Fractionators are an economical method of effecting separation of liquids. Due to the vast number of industrial applications, engineers must be able to characterize a great variety of fractionators. The model developed will accept one through three multicomponent feeds with two through six product streams.

There are many algorithms to calculate multicomponent complex columns (i.e., multifeed and/or more than two product columns). Most tray-by-tray computer programs have difficulty in converging on complex tower configuations. The programs either do not converge or converge very slowly.

Separation programs are used as an integral part of the mathematical model for process plants. Each subroutine in such a process plant model must be accurate and fast. This is particularly true if: (1) the separation routine is in a convergence loop in the plant model; or (2) the plant model is optimized by the case study method or by nonlinear optimization techniques where many partial derivatives are numerically evaluated. It would be desirable to have a method of designing complex fractionators which is fast and accurate.

The intent of this work is to satisfy this need. The proposed mathematical model of complex fractionators is based on the relative operability approach. It is both fast and accurate. The method is useful for both hand and computer applications.

The model is limited by the following assumptions:

(1) The relative operability varies linearly across each section of the column.

(2) The feed streams enter the column at the plate where the ratio of the light and heavy key components is the same as in the feed.

(3) The side product streams are withdrawn as liquid streams.

CHAPTER II

LITERATURE SURVEY

The Literature Survey is divided into two parts, literature on rigorous fractionation methods and literature on short-cut procedures. The term rigorous is used to denote that the material balance, heat balance, and equilibrium relationships are met on each ideal equilibrium stage in the "rigorous" fractionation models.

2.1 Literature on Rigorous Fractionation Methods

The ideas of the theoretical stage, heat balance and material balance as applied first by Sorel (23) are quite old. The application of these ideas to solution of fractionation problems via computer algorithms is recent. The approach of Sorel as used by Lewis and Matheson (16) has been applied to computer solutions by Bonner (3), Maddox and Erbar (18), and Greenstadt (11). The method of Thiele and Geddes (24) is used by Lyster (17), Holland (13), and Hansen (12) for computer solutions. Amundsen and Pontinen (1) have developed a method using matrix techniques. Rose, et al (21) developed a relaxation technique. Ball (2) and Burman, et al (2a) reduced the convergence time by modifying the relaxation method.

The difficult problem in computer solution of rigorous equilibrium stage models is convergence. Friday (7) has analyzed the convergence problem and proposed solutions in certain general cases.

2.2 Literature on Short-cut Fractionation Methods

The literature abounds in references to short-cut solutions to fractionation problems. Edmister (4) uses absorption and stripping factors coupled with a sectional approach to describe fractionators. Fenske (6) or Winn (27) equations can be used to determine product split and number of trays at total reflux. Gilliland (8) or Underwood (25) equations can be used to determine minimum reflux. Knowing minimum reflux and minimum number of trays, the operating reflux can be calculated if the actual number of theoretical stages is known. A correlation such as proposed by Erbar and Maddox (5) is used to complete the calculation. This correlation relates reflux ratio (L_o/V_1) to the ratio of minimum theoretical stages divided by actual theoretical stages using the minimum reflux ratio as a parameter. Likewise, the actual number of theoretical stages can be calculated if the operating reflux is known.

Joyner et al (14) developed a computer program to describe a complex tower at total reflux.

The relative operability approach is semirigorous. The method is based on the work of Underwood (26) and Gilliland (9). Maddox and Takaoka (19) developed a computer program for multiproduct one feed columns using the relative operability method. The relative operability approach will be discussed in detail in Chapter III.

CHAPTER III

THEORY

To adequately cover the theoretical aspects of this work, the following items must be discussed: determination of the number of independent variables for complex fractionators, fractionator operation at total reflux, and the relative operability method of describing fractionators.

3.1 Determination of the Number of Independent Variables for Complex Fractionators

Gilliland and Reed (9), Kwauk (15), and Smith (22) discuss the determination of the number of independent variables in multistage separation equipment.

Appendix A gives the derivation of the number of independent variables which must be specified to define a complex fractionator. The number of independent variables in a simple fractionator, i.e., a one feed two product column, with a total condenser and a partial reboiler is $C + 2N + 9$. For each additional feed $C + 3$ independent variables are added. For each side product stream two additional independent variables are added. The total number of independent variables is calculated by the following formula:

$$N_i = C+2N+9 + (\text{No. Feed} - 1)(C+3) + (\text{No. Products} - 2)(2)$$

In this work the following independent variables are specified.

Specification	Number of Independent Variables		
Column pressure: the pressure on each tray, condenser, reflux divider		N	+2
No heat leak: each stage excluding reboiler, plus reflux divider		N	
Feed definition, composition, rate, temperature and pressure	C		+2
Reflux temperature, assumed to be at the bubble point			+1
Reflux rate			+1
Feed location: the feed enters where the ratio of heavy to light key in the feed is the same as the liquid from the tray above			+1
Product specification: the ratio of moles of light key in the top product to moles of light key in the product stream below			+1
Product specification: the ratio of moles of heavy key in the top product to moles of heavy key in the product stream below			+1
Sub Total: for simple fractionator	C	+2N	+9
Feed specification for each additional feed stream: composition, rate, temperature pressure	(No. Feeds - 1) (C + 2)		

Specification	Number of Independent Variables
Feed location for each additional feed: same criterion for feed tray location as above	(No. Feeds - 1)
Sub total: for additional feeds	(No. Feeds - 1) (C + 3)
Product specification: for each additional product stream (1) ratio moles of light key between adjacent product streams (2) ratio moles of heavy key between adjacent product streams	(No. Products - 2) 2
Sub total: for additional products	(No. Products - 2) 2
Total	C+2N+9 + (No. Feeds - 1) (C + 3) + (No. Products - 2) 2

If a partial condenser is assumed instead of a total condenser, the reflux divider is eliminated in this work. The number of independent variables for a tower is reduced by three. The specifications differ from those listed above by the elimination of the following three variables: (1) pressure of the reflux divider, (2) heat loss of the reflux divider, and (3) reflux temperature.

3.2 Fractionator Operation at Total Reflux

A fractionator operating at total reflux can be considered as a column with all the overhead product returned to the column as reflux and with no product withdrawn; or, the column may be considered as having an infinite reflux (thus an infinite diameter) with finite product rates. Inspection of a McCabe-Thiele diagram for binary separation at total reflux, shows that the column operation is independent of the feed location, feed composition, feed temperature, and feed pressure with the one obvious restriction that the feed entry must lie between the composition points of the distillate and bottoms.

The Fenske equation is used to describe fractionators operating at total reflux. The derivation of the Fenske equation is shown below. Writing a material balance around the top of a column gives:

$$V = L + D$$

At total reflux

$$V = L$$

And

$$v = \ell$$

Therefore

$$y_2 = x_1$$

By definition

$$y_1 = K_1 x_1$$

And

$$y_1' = K_1' x_1'$$

Dividing the above two equations and substituting in the total reflux identities

$$\frac{y_1}{y_1'} = \frac{K_1\ x_1}{K_1'\ x_1'} = \frac{K_1\ y_2}{K_1'\ y_1'}$$

Rearranging

$$\frac{y_2}{y_2'} = \frac{K_2\ x_2}{K_2'\ x_2'}$$

Therefore

$$\frac{y_1}{y_1'} = \frac{K_1\, y_2}{K_1'\, y_2'} = \frac{K_1\, K_2\, x_2}{K_1'\, K_2'\, x_2'}$$

By definition

$$\alpha = \frac{K}{K'}$$

Combining and extending the above two equations gives

$$\frac{y_1}{y_1'} = \alpha_1 \quad \alpha_2 \ldots \alpha_N \quad \frac{x_N}{x_N}$$

Assume

$$\alpha_1 = \alpha_2 = \alpha_3 = \quad \ldots \quad = \alpha_N$$

Therefore

$$\alpha^{S_m} = \alpha_1\, \alpha_2\, \alpha_3 \ldots \alpha_N$$

And

$$\frac{y_1}{y_1'} = (\alpha)^{S_m} \quad \frac{x_N}{x_N'}$$

Multiplying the above equation by

$$\frac{D}{D}\ \frac{y_1}{y_1'} = (\alpha)^{S_m} \quad \frac{x_N}{x_N'}\ \frac{B}{B}$$

Gives the equation in component rate form

$$\frac{d}{d'} = (\alpha)^{S_m} \qquad \frac{b}{b'}$$

Rearranging gives the Fenske equation expressed in terms of component rates

$$(\alpha)^{S_m} = \frac{d}{b}\ \frac{b'}{d'} \tag{3.2-1}$$

In the derivation of the Fenske equations, two assumptions are made; (1) the column is operating at total reflux, therefore passing streams have the same composition; and, (2) constant relative volatility, i.e.,

$$\alpha_1 = \alpha_2 = \alpha_3 = \dots = \alpha_N \quad \text{and thus}$$

$$\alpha^{S_m} = \alpha_1 \alpha_2 \alpha_3 \dots \alpha_N \quad \text{or} \quad (\alpha_{Av})^{S_m} = \alpha_1 \alpha_2 \alpha_3 \dots \alpha_N$$

The Fenske equation was originally intended to describe simple one feed two product columns. For columns with more than two products, the Fenske equations can be used if the fractionator is considered to be composed of sections defined by adjacent product streams. Edmister (4) successfully utilized the sectional concept for separation columns using absorption and stripping factors. A three product column operating at total reflux would be composed of two sections. The Fenske type equations can be written (as described by Joyner et al (14)) as follows:

For the top section

$$\alpha_{Av}^{S_{mI}} = \frac{d}{p} \quad \frac{p'}{d'}$$

For the bottom section

$$\alpha_{Av}^{S'_{mII}} = \frac{p}{b} \quad \frac{b'}{p'}$$

These equations do not consider the feed locations. As shown above, the feed location and feed condition are not relevant for a simple column operating at total reflux. By analogy this is true for a complex fractionator.

The Fenske equation is valid for a multiple section column with multiple feeds. Since the feed location and condition do not effect the column operation, all the feed may be summed up and treated as one feed for a fractionator operating at total reflux. The material balance

$$d + p_1 + p_2 + \ldots + p_N + b \;=\; f_1 + f_2 + \ldots + f_m = \sum_{i=1}^{m} f_i = f_T$$

is for a complex tower with "N" side products and "M" feeds. The feeds are assumed to enter the column at the proper location.

If the ratio of product split between adjacent products is specified for the light and heavy key components, the number of stages can be calculated for each section in a complex fractionator using the Fenske equation. For a two section column, the stages in each section are calculated as follows:

$$\alpha_{AvI}^{S_{mI}} = \left(\frac{d}{p_1}\right)_{LK}\left(\frac{p_1}{d}\right)_{HK}$$

Rearranging the above equation gives for the top section

$$S_{mI} = \frac{\ln\left[\left(\frac{d}{p_1}\right)_{LK}\left(\frac{p_1}{d}\right)_{HK}\right]}{\ln \alpha_{Av\,I}} \qquad (3.2\text{-}2)$$

Likewise for the bottom section

$$S_{mII} = \frac{\ln\left[\left(\frac{p_1}{b}\right)_{LK}\left(\frac{b}{p_1}\right)_{HK}\right]}{\ln \alpha_{AvII}} \qquad (3.2\text{-}3)$$

Knowing the stages in any section, the component distribution is calculated as follows:

Top section:

$$\left(\frac{d}{p_1}\right)_i = \alpha_{AvI}^{S_{mI}} \left(\frac{d}{p_1}\right)_{HK} \qquad (3.2\text{-}4)$$

Bottom section:

$$\left(\frac{p_1}{b}\right)_i = \alpha_{AvII}^{S_{mII}} \left(\frac{p_1}{b}\right)_{HK} \qquad (3.2\text{-}5)$$

The ratios $\frac{d}{p_1}$, $\frac{p_1}{p_2}$, $\frac{p_2}{p_3}$, $\frac{p_3}{p_4}$, $\frac{p_{N-1}}{p_N}$, $\frac{p_N}{b}$ can be computed for all sections and for all components as suggested from the above equations for a simple column. By material balance around the column $f_T = d + b + p_1 + p_2 + \ldots + p_N$ is calculated for each component.

Dividing both sides by p_1 or if there are no side products, dividing by d gives

$$\frac{f_T}{p_1} = 1 + \frac{d}{p_1} + \frac{b}{p_1} + \frac{p_2}{p_1} + \frac{p_3}{p_1} + \ldots + \frac{p_N}{p_1} \tag{3.2-6}$$

The ratios calculated above can be converted to the form of this equation:

$$\frac{p_2}{p_1} = 1\bigg/\left(\frac{p_1}{p_2}\right), \quad \frac{p_3}{p_1} = \frac{p_3}{p_2}\,\frac{p_2}{p_1} \quad \text{etc.}$$

Equation (3.2-6) can be rearranged:

$$p_1 = \frac{f_T}{1 + \frac{d}{p_1} + \frac{b}{p_1} + \frac{p_2}{p_1} + \frac{p_3}{p_1} + \ldots + \frac{p_N}{p_1}} \tag{3.2-7}$$

or

$$p_1 = \frac{f_T}{1 + \frac{d}{p_1} + \frac{p_2}{p_1} + \frac{p_2}{p_1}\,\frac{p_3}{p_2} + \ldots + \frac{p_N}{p_{N-1}}\,\frac{b}{p_N}} \tag{3.2-9}$$

and

$$d = \left(\frac{d}{p_1}\right) p_1, \quad p_2 = \left(\frac{p_2}{p_1}\right) p_1 \quad \text{etc.} \tag{3.2-9}$$

In the special case of a two product column

$$d = \frac{f_T}{1 + \frac{b}{d}} \qquad (3.2\text{-}10)$$

The above equations are used to estimate the number of trays and product splits in a complex fractionator. These estimates are then used as initial guesses in the relative operability method to improve the fractionator solution.

The relative operability solution requires estimates of composition and flow rates at the terminal of each section of a complex fractionator. The intent of the relative operability calculation is to solve the fractionator problem at a given operating reflux. Hence the feed locations must be considered. The column is therefore divided into sections bounded by adjacent inlet or outlet streams, either feed or product streams. A two feed three product column would be composed of four sections. By the total reflux method as discussed above and assuming constant molal overflow, the composition, flow rates, and trays per section are calculated for section terminals defined by product streams. The terminal conditions for sections defined by feed streams remain to be estimated.

To determine the liquid composition flowing into the feed zone and the liquid flow rates, some criterion must be established to determine the feed location and thus the number of stages in a feed section. Robinson and Gilliland (20) define an optimum intersection ratio. According to this criterion, a feed stream enters the column below the tray where the ratio of the light key to heavy key composition of the liquid from the tray is the same as the ratio in the feed stream. Using this criterion and the Fenske equation, the number of stages in a section whose bottom defining stream is a feed is calculated as follows:

$$\alpha_{LK}^{S_{mf}} = \left(\frac{d}{f}\right)_{LK}\left(\frac{f}{d}\right)_{HK} \tag{3.2-11}$$

$$\alpha_{LK}^{S_{mf}} = \frac{d_{LK}}{d_{HK}} \quad \frac{f_{HK}}{f_{LK}} \tag{3.2-12}$$

$$\alpha_{LK}^{S_{mf}} = \frac{x_{dLK}}{x_{dHK}} \quad \frac{Z_{fHK}}{Z_{fLK}} \tag{3.2-13}$$

The quantity S_{mf} is the minimum number of stages in the section between the distillate and the feed. Knowing the number of stages in this section, the composition of the liquid stream entering the feed zone can be calculated. This calculation is made via the Fenske equation as follows:

$$\frac{\ell_{Ni}}{\ell_{NHK}} = \frac{d_i}{d_{HK}} \; \alpha_i^{-S_{mf}} \tag{3.2-14}$$

The ratios ℓ_{Ni}/ℓ_{NHK} can be calculated for each component, i. The total liquid rate, L_N, can be estimated by assuming constant molar overflow. For a one feed two product column L_N = Reflux Rate. The sum of the ratios times the liquid rate of the heavy key is equal to the total flow rate, L_N.

$$\ell_{NHK} \sum_{i=1}^{N} \frac{\ell_{Ni}}{\ell_{NHK}} = L_N \tag{3.2-15}$$

Therefore

$$\ell_{NHK} = \frac{L_N}{\sum_{i=1}^{N} \frac{\ell_{Ni}}{\ell_{NHK}}} \tag{3.2-16}$$

Solving for ℓ_{NHK}, the flow rates for the other components are then computed:

$$\ell_{Ni} = \ell_{NHK} \frac{\ell_{Ni}}{\ell_{NHK}} \tag{3.2-17}$$

The composition of the liquid coming into the feed zone for all sections, whose terminal is defined by a feed stream, can be similarly calculated. Likewise, the number of stages in a feed section can be estimated.

The above calculated compositions, flow rates, and number of stages at total reflux conditions are used as initial estimates in the relative operability method to converge on a solution at a given finite reflux.

3.3 The Relative Operability Method Of Calculating Fractionators

The fractionator is divided into sections defined as the trays between adjacent feed streams or product streams (see Figure 3.3-0). Each section of trays is described by the same equation.

The derivation of the equation defining any section follows.

$$y_1 V_1 + L_N x_N = V_{N+1} y_{N+1} + L_o x_o \tag{3.3-1}$$

Equation (3.3-1) is a material balance for any component around a section whose top tray is 1 and bottom tray is N. Equation (3.3-1) is rearranged as follows:

$$y_{N+1} V_{N+1} = y_1 V_1 + L_N x_N - L_o x_o \tag{3.3-2}$$

Dividing by V_{N+1}

$$y_{N+1} = \frac{y_1 V_1 + L_N x_N - L_o x_o}{V_{N+1}} \tag{3.3-3}$$

Equation (3.3-3) for any component, i, is divided by equation (3.3-3)

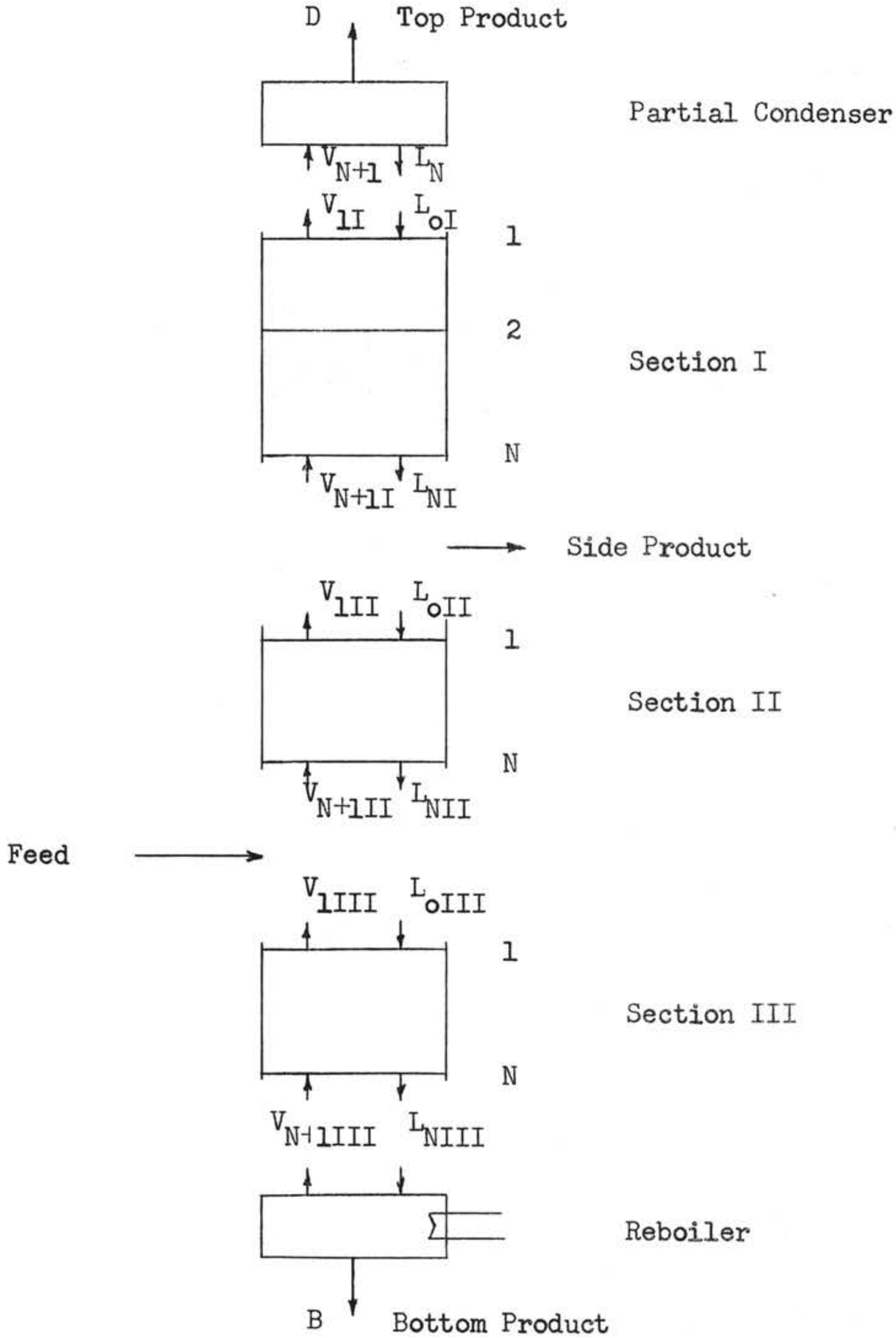

Figure 3.3-0. Typical Column Nomenclature

for the heavy key.

$$\frac{y_{N+1i}}{y_{N+1HK}} = \frac{\dfrac{y_{1i}V_1 + x_{Ni}L_N - x_{oi}L_o}{V_{N+1}}}{\dfrac{y_{1\,HK}V_1 + x_{NHK}L_N - x_{oHK}L_o}{V_{N+1}}} \tag{3.3-4}$$

The quantity V_{N+1} is cancelled

$$\frac{y_{N+1i}}{y_{N+1HK}} = \frac{y_{1i}V_1 + x_{Ni}L_N - x_{oi}L_o}{y_{1HK}V_1 + x_{NHK}L_N - x_{oHK}L_o} \tag{3.3-5}$$

By algebraic manipulation the equation becomes

$$\frac{y_{N+1i}}{y_{N+1HK}} = \frac{x_{Ni}\left(1 + \dfrac{y_{1i}V_1}{x_{Ni}L_N} - \dfrac{x_{oi}L_o}{x_{Ni}L_N}\right)}{x_{NHK}\left(1 + \dfrac{y_{1HK}V_1}{x_{NHK}L_N} - \dfrac{x_{oHK}L_o}{x_{NHK}L_N}\right)} \tag{3.3-6}$$

Define

$$\beta_{N+1} = \frac{1 + \dfrac{y_{1i}V_1}{x_{Ni}L_N} - \dfrac{x_{oi}L_o}{x_{Ni}L_N}}{1 + \dfrac{y_{1HK}V_1}{x_{NHK}L_N} - \dfrac{x_{oHK}L_o}{x_{NHK}L_N}} \tag{3.3-7}$$

Substituting equation (3.3-7) into equation (3.3-6) gives

$$\frac{y_{N+1i}}{y_{N+1HK}} = \frac{x_{Ni}}{x_{NHK}}\,\beta_{N+1} \tag{3.3-8}$$

By the definition of K

$$\frac{y_{N+1i}}{y_{N+1HK}} = \frac{K_{N+1i}}{K_{N+1HK}}\,\frac{x_{N+1i}}{x_{N+1HK}} \tag{3.3-9}$$

And

$$\alpha_{N+1i} = \frac{K_{N+1i}}{K_{N+1HK}} \tag{3.3-10}$$

Therefore

$$\frac{y_{N+1i}}{y_{N+1HK}} = \alpha_{N+1i} \frac{x_{N+1i}}{x_{N+1HK}} \tag{3.3-11}$$

Using equations (3.3-8) and (3.3-11), an expression is developed which relates the terminal streams for any section of a complex fractionator.

$$\frac{y_1}{y_1'} = \frac{x_o}{x_o'} \beta_1 \tag{3.3-12}$$

$$\frac{y_1}{y_1'} = \alpha_1 \frac{x_1}{x_1'} \tag{3.3-13}$$

Therefore, combining equation (3.3-12) and (3.3-13)

$$\frac{x_1}{x_1'} = \left(\frac{\beta}{\alpha}\right)_1 \frac{x_o}{x_o'} \tag{3.3-14}$$

Likewise

$$\frac{y_2}{y_2'} = \frac{x_1}{x_1'} \beta_2 \tag{3.3-15}$$

And

$$\frac{y_2}{y_2'} = \alpha_2 \frac{x_2}{x_2'} \tag{3.3-16}$$

Combining equations (3.3-15) and (3.3-16)

$$\frac{x_2}{x_2'} = \left(\frac{\beta}{\alpha}\right)_2 \frac{x_1}{x_1'} \tag{3.3-17}$$

Combining equations (3.3-14) and (3.3-17)

$$\frac{x_2}{x_2'} = \left(\frac{\beta}{\alpha}\right)_1 \left(\frac{\beta}{\alpha}\right)_2 \frac{x_o}{x_o'} \tag{3.3-18}$$

The expression for N trays is

$$\frac{x_N}{x'_N} = \left(\frac{\beta}{\alpha}\right)_1 \left(\frac{\beta}{\alpha}\right)_2 \left(\frac{\beta}{\alpha}\right)_3 \cdots \left(\frac{\beta}{\alpha}\right)_{N-1} \left(\frac{\beta}{\alpha}\right)_N \frac{x_o}{x'_o} \qquad (3.3\text{-}19)$$

The assumption is made that

$$\frac{x_N}{x'_N} = \left(\frac{\beta}{\alpha}\right)_{Av}^N \frac{x_o}{x'_o} \qquad (3.3\text{-}20)$$

Where

$$\left(\frac{\beta}{\alpha}\right)_{Av} = \left\{ \left(\frac{\beta}{\alpha}\right)_1 \left[\frac{\left(\frac{\beta}{\alpha}\right)_2 + \left(\frac{\beta}{\alpha}\right)_N}{2}\right]^{N-1} \right\}^{1/N} \qquad (3.3\text{-}21)$$

Therefore, any section can be represented by equation (3.3-20). If β in equation (3.3-20) is equal to 1.0, then the equation reduces to the Fenske equation shown below.

$$\left(\frac{\alpha}{\beta}\right)_{Av}^N = \frac{x_o}{x_N} \frac{x'_N}{x'_o} \qquad (3.3\text{-}22)$$

If $\beta_{Av} = 1.0$

$$(\alpha)^N = \frac{x_o}{x_N} \frac{x'_N}{x'_o} \qquad (3.3\text{-}23)$$

If β_1, β_2, and β_N and thus β_{Av} can be evaluated for any section, then that section can be characterized by equation (3.3-20). Using formula (3.3-7) the terms in $(\beta/\alpha)_{Av}$ are calculated as shown below.

$$\left(\frac{\beta}{\alpha}\right)_1 = \frac{\left(\dfrac{1 + \dfrac{y_1 V_1}{x_o L_o} - \dfrac{x_o L_o}{x_o L_o}}{1 + \dfrac{y'_1 V_1}{x'_o L_o} - \dfrac{x'_o L_o}{x'_o L_o}}\right)}{\alpha_1} \qquad (3.3\text{-}24.1)$$

$$\left(\frac{\beta}{\alpha}\right)_2 = \frac{\left(\dfrac{1 + \dfrac{y_1 V_1}{x_1 L_1} - \dfrac{x_o L_o}{x_1 L_1}}{1 + \dfrac{y_1' V_1}{x_1' L_1} - \dfrac{x_o' L_o}{x_1' L_1}}\right)}{\alpha_2} \qquad (3.3\text{-}24.2)$$

$$\left(\frac{\beta}{\alpha}\right)_N = \frac{\left(\dfrac{1 + \dfrac{y_1 V_1}{x_{N-1} L_{N-1}} - \dfrac{x_o L_o}{x_{N-1} L_{N-1}}}{1 + \dfrac{y_1' V_1}{x_{N-1}' L_{N-1}} - \dfrac{x_o' L_o}{x_{N-1}' L_{N-1}}}\right)}{\alpha_N} \qquad (3.3\text{-}24.3)$$

Equation (3.3-20) can be expressed as moles rather than mole fraction. Multiplying the left side of equation (3.3-20) by L_N/L_N and the right side by L_o/L_o

$$\frac{\ell_N}{\ell_N'} = \left(\frac{\beta}{\alpha}\right)_{Av}^{N} \frac{\ell_o}{\ell_o'} \qquad (3.3\text{-}25)$$

The partial reboiler is related to the bottom section by the equation

$$\frac{x_{N+1}}{x_{N+1}'} = \left(\frac{\beta}{\alpha}\right)_{N+1} \frac{x_N}{x_N'} \qquad (3.3\text{-}26)$$

Or

$$\frac{b}{b'} = \left(\frac{\beta}{\alpha}\right)_{N+1} \frac{\ell_N}{\ell_N'} \qquad (3.3\text{-}27)$$

Where ℓ_N is the component flow rate from the bottom section. Condensers are treated in a similar manner. The equation relating a partial condenser to the top section is as follows:

$$\frac{x_o}{x_o'} = \frac{1}{\alpha_o}\frac{y_o}{y_o'} \tag{3.3-28}$$

Or

$$\frac{\ell_o}{\ell_o'} = \frac{d}{\alpha_o \; d'} \tag{3.3-29}$$

The above equation follows from the definition of the equilibrium ratio. In equation (3.3-29) ℓ_o represents the liquid component flow to the first section — the reflux. For a total condenser

$$\frac{x_o}{x_o'} = \frac{y_o}{y_o'}$$

since the reflux and distillate have the same composition. Therefore,

$$\frac{\ell_o}{\ell_o'} = \frac{d}{d'} \tag{3.3-30}$$

which is the analogous equation to equation (3.3-27) for a total condenser.

The various sections of a column can be related as described below. The sections of a complex column are defined by a feed stream entering, or a product stream leaving. For a feed stream entering the column, the liquid stream from the tray above the feed entry point can be related to the liquid stream entering the tray below the feed entry point by the following equation (see figure 3.3-1).

$$\ell_{NI} + FZ_{\ell} = \ell_{oII} \tag{3.3-31}$$

The vapor streams above and below the feed point can be related as follows:

$$v_{N+1I} - FZ_v = v_{1II} \tag{3.3-32}$$

The liquid stream from the tray above a product exit point (see

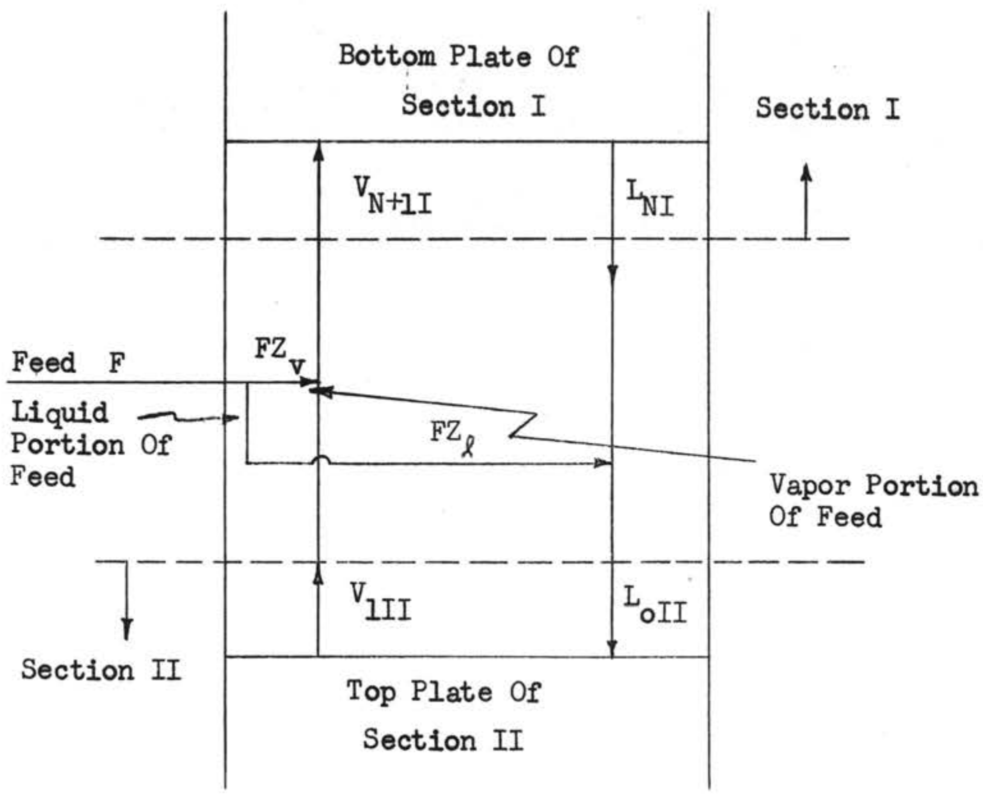

Figure 3.3-1. Feed Entry Point

figure 3.3-2) has the same composition as the product stream.

$$x_p = x_{NI} \tag{3.3-33}$$

The liquid stream above and below the product exit point are related as shown below.

$$\ell_{NI} - Px_p = \ell_{oII} \tag{3.3-34}$$

The vapor streams are related as follows:

$$v_{N+1I} = v_{1II} \tag{3.3-35}$$

The above equation development enables us to describe all the sections in a complex column and also to describe the relationship among streams between each section. These equations can be used to describe a complete column. Starting with the values generated from the total reflux calculation, the $(\beta/\alpha)_{Av}$ for each section is calculated. The compositions at the section terminals for the light and heavy keys are known from the total reflux calculations. Therefore, equation (3.3-25) can be rearranged and the number of trays in each section can be computed.

$$N = \frac{\ln\left(\dfrac{\ell_N}{\ell_N'} \; \dfrac{\ell_o'}{\ell_o}\right)}{\ln\left(\dfrac{\beta}{\alpha}\right)_{Av}} \tag{3.3-36}$$

The component distribution is then computed for each section.

The temperatures at all section terminals are computed by bubble point and dew point calculations based on the new compositions. Using the new compositions and new temperatures, a heat balance is made on each section beginning with section one. The liquid flow rate from section one is corrected to bring that section in heat balance. The

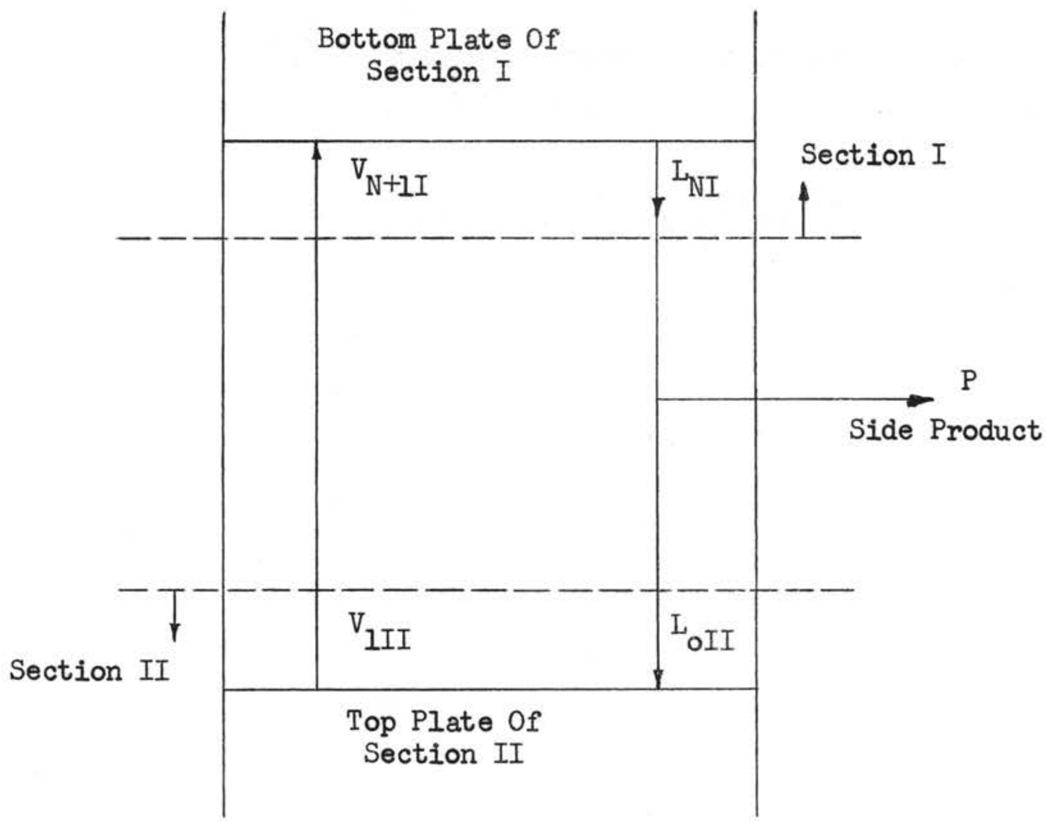

Figure 3.3-2. Side Exit Point

following formula is used.

$$L_N = L_N \left[1 - \frac{Q_{in} - Q_{out}}{Q_{out}}\right] \qquad (3.3\text{-}37)$$

where

$$Q_{in} = V_{N+1}H \qquad (3.3\text{-}38)$$

and

$$Q_{out} = L_N h + \text{Condenser Duty} + DH \qquad (3.3\text{-}39)$$

After correcting the liquid flow rate, the vapor stream to the section, V_{N+1}, is corrected by material balance. All sections are brought into heat balance in this manner.

Next, new β's are calculated based on the new compositions, temperatures, and flow rates. The process is repeated until the model has converged within given tolerances on the temperatures and heat balance. The discussion of the calculation procedure follows in Chapter IV.

CHAPTER IV

CALCULATIONAL PROCEDURE

The computer solution of engineering problems involves expressing the problem in mathematical terms and then writing a step-by-step procedure for solving the various mathematical expressions.

The first step in the calculational procedure is an analyst flow sheet outlinning the basic blocks of logic. Figure 4.0-1 represents the basic logical blocks. These blocks are (1) the feed flashes and feed enthalpy calculations, (2) total reflux calculations, and (3) finite reflux calculations. An outline of the logic in each basic block is shown in Figures 4.1-1, 4.2-1 and 4.3-1.

4.1 Outline Of Feed Flashes And Feed Enthalpy Calculations (see Figure 4.1-1)

If the specified feed pressure is less than the column pressure a diagnostic is printed stating this condition. The feed is then flashed at column pressure and feed temperature. Next the enthalpy of the liquid and vapor portions of the feed are computed (assuming ideal enthalpy) and summed. If the feed pressure is greater than the column pressure an adiabatic flash is made on the feed stream at the calculated enthalpy and column pressure. The calculation is repeated for all feeds. The feed enthalpy, and moles of liquid and vapor from the feed flashes are used in the calculations that follow.

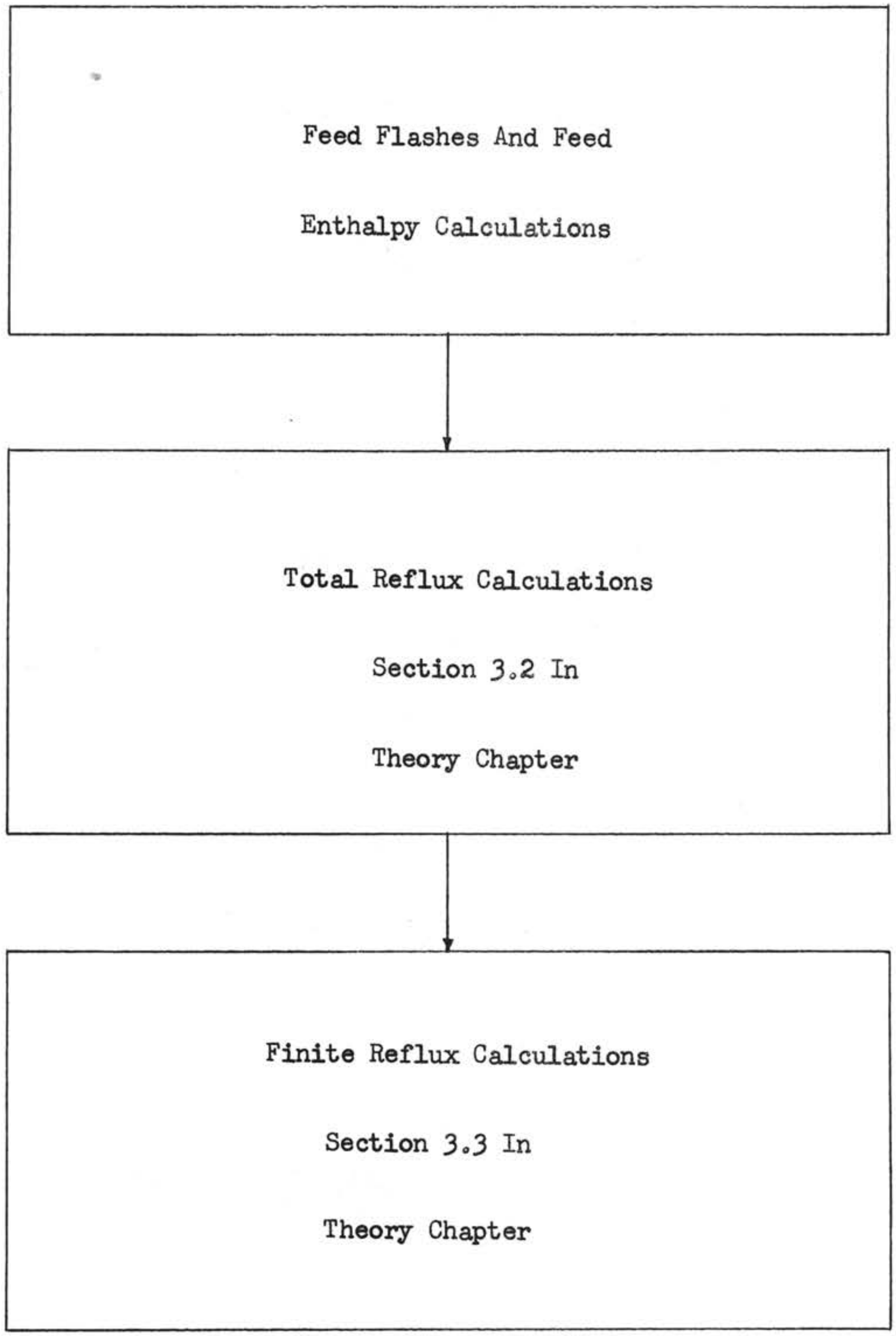

Figure 4.0-1. Basic Logic Blocks In Calculational Procedure

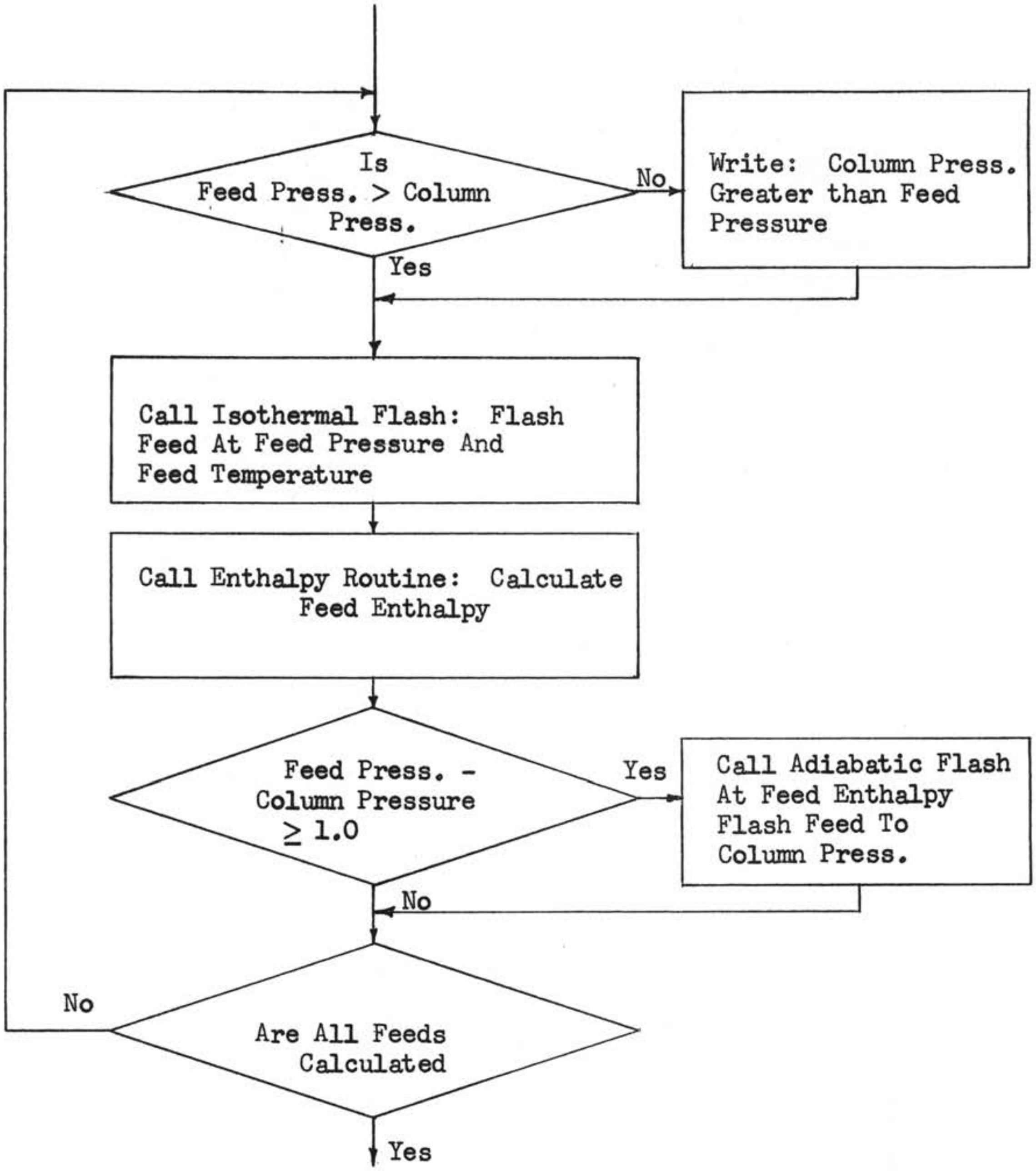

Figure 4.1-1. Outline Of Logic In Basic Block I Feed Flashes And Feed Enthalpy Calculation

4.2 Outline Of Calculational Procedure In Total Reflux Calculations (see Figure 4.3-1)

The number of stages in each section defined by product streams is calculated. The Fenske equation (3.2-2) is used for the top section. Similar equations are used for each section. The number of stages as calculated by the Fenske equation is based on the specified split between the light and heavy key.

Next the distribution ratio for each component is calculated by equation (3.2-4) for the section. Similar equations are used to calculate the distribution ratio for each component in each section. The first side product stream is then calculated using equation (3.2-8). The other product streams are then calculated using equation (3.2-9).

The feed stream locations are calculated next. First the feed streams are ordered. The first feed being the one with the largest ratio of moles of light to heavy key. The other feeds follow in decreasing order. Each feed is then placed in the proper section of the column. This calculation is accomplished by finding the section whose top product stream has a larger ratio of light to heavy key than the feed and whose bottom product has a lower ratio of light to heavy key. If it is determined that a section has a feed stream entering, the trays between the top product of the section and the feed entry point are computed. Equation (3.2-12) is used to compute these trays. If two or three feeds enter the same section each feed is located by the number of trays the feed is from the top product. Equations similar to equation (3.2-12) are used. The section is thus divided into other sections by the feed streams. The number of stages in each of these

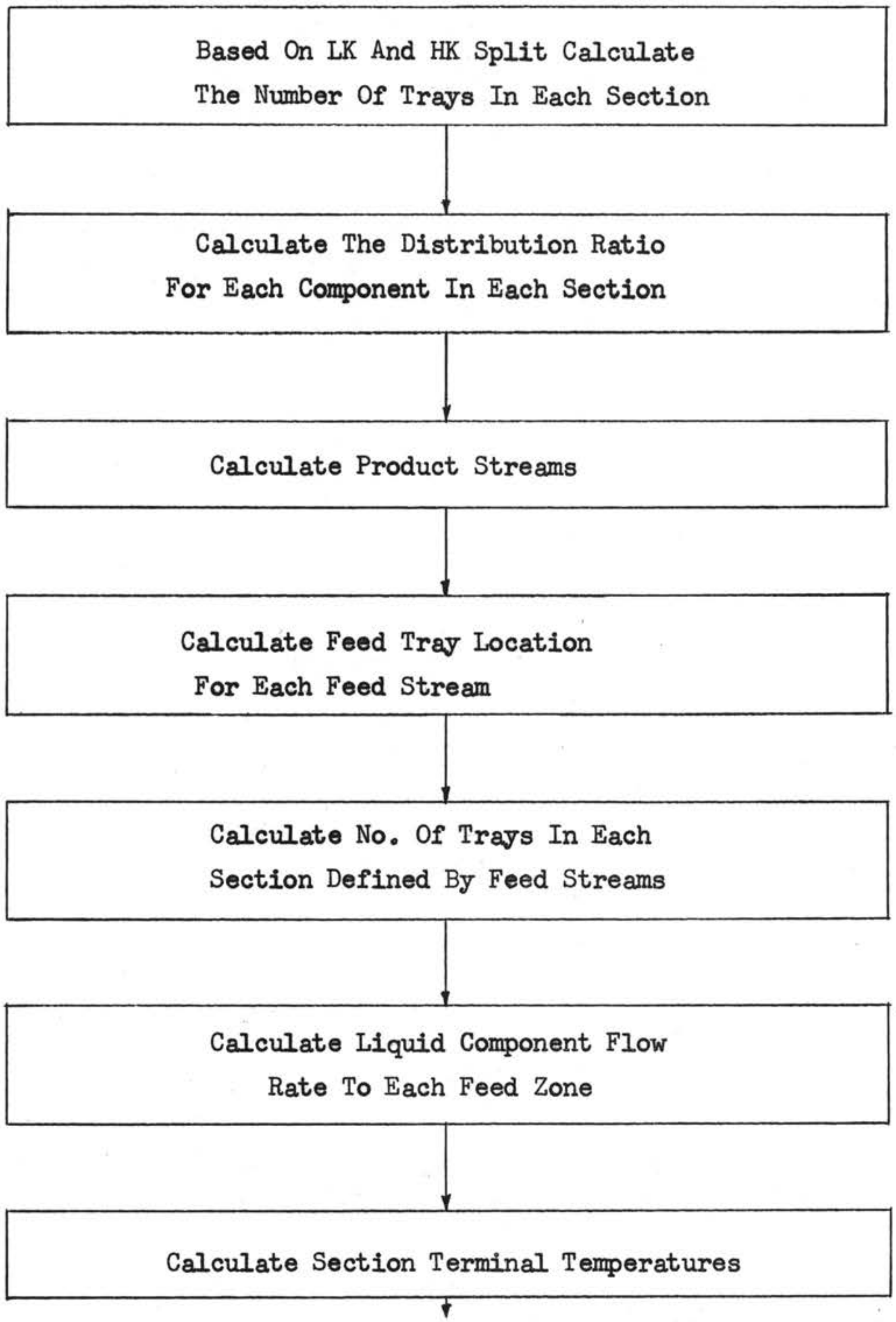

Figure 4.2-1. Outline Of Logic In Basic Block II Total Reflux Calculations

sections is computed simply by knowing the feed location with respect to the top product stream.

The composition of the liquid streams are known for the terminals of each section defined by a product stream (they have the same compositions as the product streams). For sections whose bottom defining stream is a feed inlet we must compute the component flow rates entering the feed zone. The ratio of light key to heavy key in the liquid entering the feed zone is equal to the ratio in the feed (this is the criterion used to locate the feed). The component rates can then be computed via equations (3.2-14), (3.2-15), (3.2-16), and (3.2-17).

The liquid leaving the feed zone is simply the liquid entering the zone plus the liquid portion of the feed. Likewise the vapor entering the feed zone is equal to the vapor leaving the feed zone minus the vapor portion of the feed. The same material balance is made between sections separated by a product stream. The vapor entering the product zone is equal to the vapor leaving the product zone since no vapor is removed. The liquid leaving the product zone is equal to the liquid entering minus the side product. Thus all the component rates can be calculated for the section terminals. The number of trays in each section is also known.

The temperature of all section terminals is calculated by bubble point or dew point calculations.

4.3 Outline Of Calculational Procedure In Finite Reflux Calculations (see Figure 4.3-1)

The first step in solving the fractionator at finite reflux is to compute β/α for the top section and then the sections below based

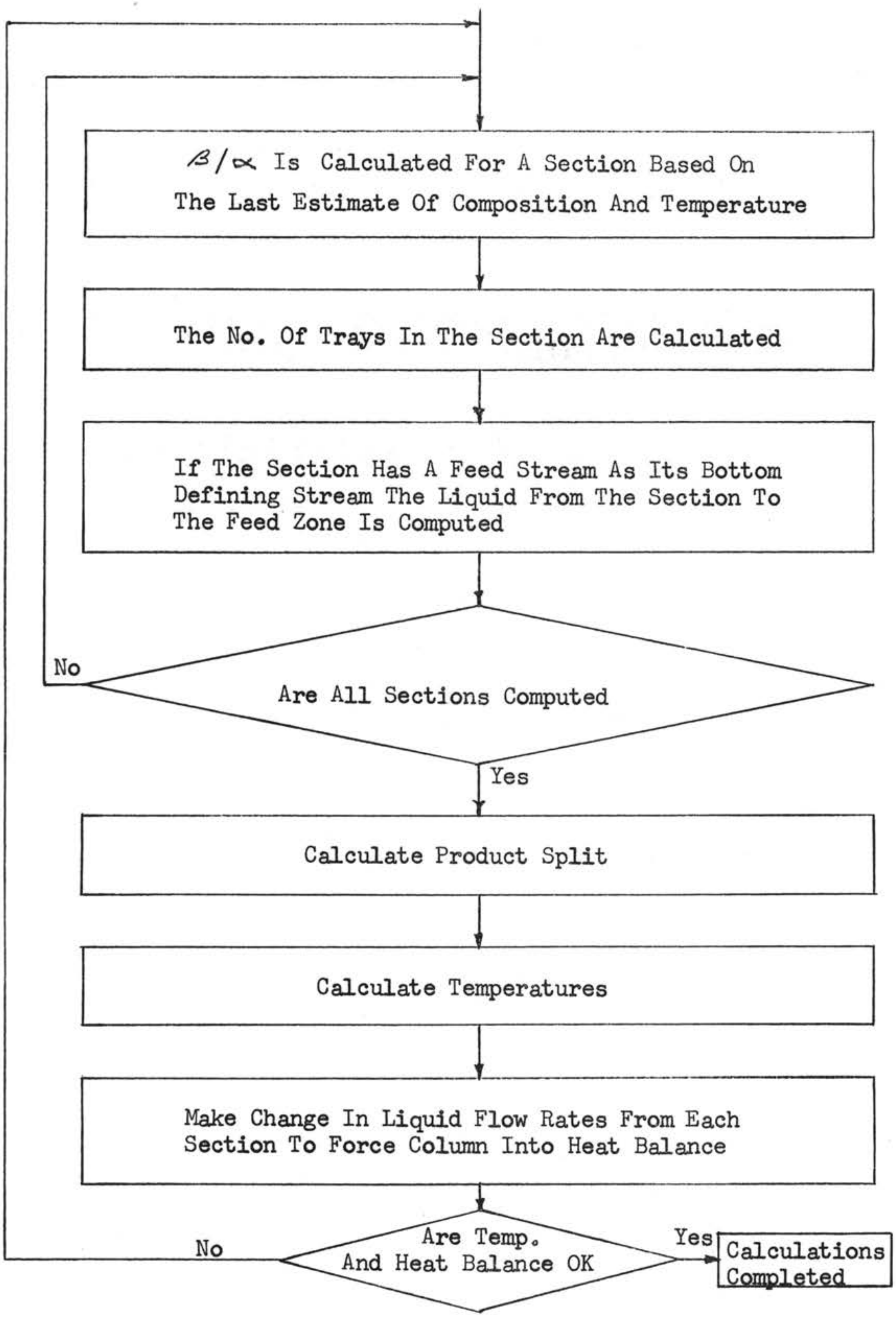

Figure 4.3-1. Outline Of Logic In Basic Block III Finite Reflux Calculations

on the compositions and temperatures calculated at total reflux. Equation (3.3-24) is used for this purpose. Knowing the β/α 's the number of trays in each section can be computed by equation (3.3-36).

If a section contains a feed stream as the bottom defining stream the liquid from the section to the feed zone is computed. This computation is similar to the analogous calculation at total reflux. At total reflux equations (3.3-16) and (3.3-17) are used. At finite reflux the same equations are calculated using finite reflux equations. Equation (3.3-25) is used for this purpose. The $(\beta/\alpha)^N_{Av}$ is known and the ℓ_o/ℓ'_o is known from the last composition calculations. Thus ℓ_N/ℓ'_N can be calculated using equation (3.3-25). These results are substituted into equation (3.3-16) to solve for ℓ_{NHK}. The other component flow rates are then computed using equation (3.3-17).

The product splits are computed next by equations (3.2-8) and (3.2-9).

$$\frac{\ell_N}{\ell'_N} = \left(\frac{\beta}{\alpha}\right)^N_{Av} \frac{\ell_o}{\ell'_o}$$

And equation (3.3-29) for a partial condenser

$$\frac{\ell_o}{\ell'_o} = \frac{1}{\alpha_o} \frac{d}{d'}$$

Combining the above equations to describe section I:

$$\frac{\ell_{NI}}{\ell'_{NI}} = \left(\frac{\beta}{\alpha}\right)^N_{AvI} \frac{1}{\alpha_o} \frac{d}{d'} \qquad (4.3\text{-}1)$$

From equation (3.3-31)

$$\ell_{NI} + FZ_\ell = \ell_{oII} \qquad (4.3\text{-}2)$$

Also from equation (3.3-25)

$$\frac{p_1}{p_1'} = \left(\frac{\beta}{\alpha}\right)^N_{AvII} \frac{\ell_{oII}}{\ell'_{oII}} \tag{4.3-3}$$

Multiplying the left side of equation (4.3-1) and equation (4.3-3) and setting the result equal to the product of the right hand side of the same two equations gives

$$\frac{p_1}{p_1'} \frac{\ell_{NI}}{\ell'_{NI}} = \left(\frac{\beta}{\alpha}\right)^N_{AvI} \frac{1}{\alpha_o} \frac{d}{d'} \left(\frac{\beta}{\alpha}\right)^N_{AvII} \frac{\ell_{oII}}{\ell'_{oII}} \tag{4.3-4}$$

Rearranging and substituting in equation (4.3-2) gives

$$\frac{d}{p_1} = \left(\frac{\beta}{\alpha}\right)^{-N}_{AvI} \alpha_o \left(\frac{\beta}{\alpha}\right)^{-N}_{AvII} \frac{d'}{p'} \frac{\ell_{NI}}{\ell_{NI} + \ell_{FI}} \frac{\ell'_{NI} + \ell'_{FI}}{\ell'_{NI}} \tag{4.3-5}$$

All the values on the right hand side of equation (4.3-5) have been estimated. Similarly for two feeds between products.

$$\frac{d}{p_1} = \left(\frac{\beta}{\alpha}\right)^{-N}_{AvI} \alpha_o \frac{d'}{p_1'} \left(\frac{\beta}{\alpha}\right)^{-N}_{AvII} \left(\frac{\beta}{\alpha}\right)^{-N}_{AvIII} \frac{\ell_{NI}}{\ell_{NI} + \ell_{FI}} \cdot \frac{\ell_{NII}}{\ell_{NII} + \ell_{FII}} \frac{\ell'_{NI} + \ell'_{FI}}{\ell'_{NI}} \frac{\ell'_{NII} + \ell'_{FII}}{\ell'_{NII}} \tag{4.3-6}$$

A similar equation can be written for three feeds between adjacent product streams.

The temperatures are computed for the terminals of each section by bubble point and dew point calculations based on the last composition calculations.

Heat balance corrections are made by equation (3.3-37). If the heat balances are within 1% for every section and if the temperatures calculated on this pass are within 1/2 degree of the temperatures calculated on the last pass the algorithm has converged. If the algorithm has not converged calculations revert to the beginning of the finite reflux calculation.

4.4 Forcing Techniques

The fractionator calculation converges in most cases without the use of forcing techniques. However, when the calculations do not converge, the following procedure is used.

1. The heat balance correction is limited. For the first five passes no heat balance correction is made (the column operates at constant molal overflow). For the next three passes the liquid flow rate is limited to a maximum change of 10%. For the next three passes the liquid flow rate is limited to a maximum change of 5%, then 2% for the next three passes, then 1% for the next three passes, and finally .5% for the last three passes. After twenty passes a message is printed stating that the Beta method did not converge. Results for the total reflux calculations are printed.
2. For components whose K's are larger than K_{HK}, the (β/α)'s are restrained to be equal to or less than one. If in the initial passes the (β/α)'s are greater than one for these components, they are set equal to one. Similarly, for components heavier than the heavy key, the β/α 's are restrained to be equal to or greater than one. The β/α for the heavy key is equal to one by definition.

CHAPTER V

RESULTS AND CONCLUSIONS

5.1 Statement Of Problem

A mathematical model was developed to characterize a multicomponent distillation column. The model will accept a maximum of three multicomponent feeds and distribute the feeds into a maximum of six product streams. The number of theoretical stages, the product rates and the product compositions are calculated. Feed entry and product withdrawal points are also computed. The input data required include the number of product streams and the ratio of light key split between adjacent products and the ratio of heavy key split between adjacent products. The method is programmed in FORTRAN II for a IBM 7094 computer. The following assumptions are made: (1) The relative operability varies linearly across each section of the column, (2) The feed streams enter the column at the plate where the ratio of the light and heavy key components is the same as in the feed, and (3) The side products are withdrawn as liquid streams.

5.2 Important Findings

The proposed method gives reliable answers for problems which converge. However, there are fractionator problems which do not converge using this program. Table I shows the converged solution to a simple column (one feed, two products). The table shows the solution at total reflux, at the given finite reflux but at constant molal overflow using the proposed method, at the given finite reflux using the proposed method and at the given finite reflux using a rigorous program. The product splits computed by all the methods compare favorably with the rigorous method. The total number of trays required as computed by the rigorous program is 12.0. The number computed by the proposed method is 11.6 and 10.6 at constant molal overflow. The minimum number of stages is 9.0. Thus the number of trays computed by the proposed method compares very well with the rigorous method.

The results for a two feed three product column are shown in Table II. The results look reasonable. The fractionator problems presented in Table I and Table II were solved using the physical data coefficients given in Appendix B.

A fractionator problem with a feed identical to the simple column feed shown in Table I and six product streams was run. The problem did not converge because negative flow rates for the heavier components were computed below the feed entry. The total reflux solution is the inital guess at the finite reflux solution. However, the total reflux solution is independent of feed location. Therefore using this estimate sometimes causes negative flow rates to occur in the column. A negative vapor rate was computed to the section below the feed entry in the one feed six product column. The program shut down because the dew point could not be found of the stream containing the negative flow rates.

Several procedures were developed to avoid the problem of negative flow rates. One method was to start at a finite reflux one-hundred times larger than the specified finite reflux. The reflux was then decreased each pass or two until the column was operating at the specified reflux. The intent of the approach was to make a smooth transition from the total or infinite reflux approximation to the finite reflux calculation. This approach did not eliminate the problem. Another method developed in an attempt to prevent negative flow rates was to consider the side product compositions below the feed entrance to be vapor rather than liquid. Passing streams at total reflux have the same composition. Therefore this approach was theoretically sound. However, this method did not produce all positive streams. No procedure was found that would produce positive streams in all problems.

5.3 Conclusions

The proposed calculational procedure solved fractionation columns with multifeed and multiproduct streams. The solutions appeared reasonable. The solution of a simple column by the proposed method compared favorably with a rigorous run. The method does not always converge. However, for those problems which converge the solutions are good.

5.4 Future Work

Another approach to the problem of complex fractionation towers is proposed for future work. This is a matrix technique. A brief sketch of the idea follows:

1. Specify all feeds, trays in each section (as defined by product or feed streams), reflux rate and all product rates.

2. Assume a linear V/L ratio and temperature profile between

the top and bottom of each section. Characterize each section by absorption and stripping factors based on these linear estimates.

3. Treat the following parts of the column as ideal stages: the partial condenser if one is specified, the top tray in the column, feed trays, and the reboiler.

4. Construct a component matrix from the material balance and equilibrium relationships for each component. The independent variables are the liquid flow rates for each component from each section and each ideal stage.

5. Solve the set of equations for the independent variables.

6. Using the liquid rates for each component solve for the vapor rates.

7. Compute temperatures of the section terminals by bubble or dew point calculations.

8. Write a heat balance around each ideal tray and section. Solve for the total flow rates.

9. Using these total flow rates estimate new V/L ratios. Using the new V/L ratios and the new temperatures (calculated in step 7), new component matrices are set up (step 4).

10. The above procedure is continued until the V/L's and the temperatures are converged.

The procedure is similar to that proposed by Friday and Smith (7). However, the above method treats the sections as a series of stripping and absorption factors instead of making tray-by-tray calculations.

TABLE I

RESULTS FOR A ONE FEED TWO PRODUCT COLUMN

Feed Composition (moles)

C_1	1.0
C_2	15.0
C_3	9.6
iC_4	2.8
NC_4	5.6
iC_5	2.4
NC_5	5.8

Feed Temperature 150.5^{o} F

Column Pressure 450 PSIA

Distribution Ratio, Light Key 20.0

Distribution Ratio, Heavy Key .05

The light key is C_2 and the heavy key is C_3

Reflux rate 75 moles

Condenser Type: Partial

Distillate

Comp.	Total Reflux	Beta at Constant Molal Overflow	Beta	Rigorous
C_1	1.0	1.0	1.0	1.0
C_2	14.2857	14.2857	14.2857	14.29
C_3	.4571	.4571	.4571	.4570
iC_4	$.3833\times10^{-2}$	$.3060\times10^{-2}$	$.3067\times10^{-2}$	.1117
NC_4	$.1493\times10^{-2}$	$.9765\times10^{-3}$	$.8944\times10^{-3}$	$.7716\times10^{-2}$
iC_5	$.1252\times10^{-4}$	$.1857\times10^{-5}$	$.1535\times10^{-5}$	$.3193\times10^{-3}$
NC_5	$.6581\times10^{-5}$	$.4709\times10^{-6}$	$.3784\times10^{-6}$	$.2736\times10^{-3}$

TABLE I (continued)

RESULTS FOR A ONE FEED TWO PRODUCT COLUMN

Bottom Product

Comp.	Total Reflux	Beta at Constant Molal Overflow	Beta	Rigorous
C_1	$.2860 \times 10^{-6}$	$.1773 \times 10^{-4}$	$.8886 \times 10^{-5}$	$.2426 \times 10^{-6}$
C_2	.7143	.7143	.7143	.7100
C_3	9.143	9.143	9.143	9.143
iC_4	2.796	2.797	2.797	2.789
NC_4	5.599	5.599	5.599	5.592
iC_5	2.400	2.400	2.400	2.400
NC_5	5.800	5.800	5.800	5.800
Trays				
Partial Condenser	1.0	1.0	1.0	1.0
Section I	3.2	3.8	3.9	2.0
Section II	3.8	4.8	5.7	8.0
Partial Reboiler	1.0	1.0	1.0	1.0
TOTAL	9.0	10.6	11.6	12.0
Temperatures				
Condenser	65.8	65.7	65.7	66.5
Top Section I	78.8	81.5	81.5	84.8
Bt. Section I	121.6	121.8	122.7	103.3
Top Section II	152.4	138.4	136.5	131.4
Bt. Section II	239.2	219.7	223.5	220.8
Reboiler	245.8	245.8	245.8	245.9

TABLE II

RESULTS FOR A TWO FEED THREE PRODUCT COLUMN

Feed Composition (moles)

	Top Feed	Bottom Feed
C_1	1.0	1.0
C_2	15.0	5.0
C_3	9.6	9.6
iC_4	2.8	2.8
NC_4	5.6	5.6
iC_5	2.4	2.4
NC_5	5.8	5.8

Top Feed Temperature 150.5° F

Bottom Feed Temperature 180.6° F

Column Pressure 450 PSIA

Distribution Ratios:

Between Top and Middle Products, Light Key	=	2.0
Between Middle and Bottom Products, Light Key	=	10.0
Between Top and Middle Products, Heavy Key	=	0.5
Between Middle and Bottom Products, Heavy Key	=	0.1

The light key is C_2 and the heavy key is C_3

Condenser Type: Partial

Reflux Rate 75 moles

TABLE II (continued)

RESULTS FOR A TWO FEED THREE PRODUCT COLUMN

Distillate

Components	Total Reflux	Beta at Constant Molal Overflow	Beta
C_1	1.947	1.917	1.917
C_2	12.90	12.900	12.90
C_3	.8348	.8348	.8348
iC_4	$.1273 \times 10^{-1}$	$.7321 \times 10^{-2}$	$.9047 \times 10^{-2}$
NC_4	$.7406 \times 10^{-2}$	$.3455 \times 10^{-3}$	$.4603 \times 10^{-3}$
iC_5	$.1455 \times 10^{-3}$	$.6212 \times 10^{-13}$	$.3176 \times 10^{-14}$
NC_5	$.1211 \times 10^{-3}$	$.6286 \times 10^{-16}$	$.3633 \times 10^{-27}$

Side Product

Components	Total Reflux	Beta at Constant Molal Overflow	Beta
C_1	$.5325 \times 10^{-1}$	$.8266 \times 10^{-1}$	$.8304 \times 10^{-1}$
C_2	6.452	6.452	6.452
C_3	1.670	1.670	1.670
iC_4	$.6939 \times 10^{-1}$	$.4209 \times 10^{-1}$	$.5205 \times 10^{-1}$
NC_4	$.6364 \times 10^{-1}$	$.3199 \times 10^{-2}$	$.4267 \times 10^{-2}$
iC_5	$.3504 \times 10^{-2}$	$.1674 \times 10^{-11}$	$.8577 \times 10^{-13}$
NC_5	$.4658 \times 10^{-2}$	$.2805 \times 10^{-14}$	$.1625 \times 10^{-25}$

TABLE II (continued)

RESULTS FOR A TWO FEED THREE PRODUCT COLUMN

Bottom Product

Components	Total Reflux	Beta at Constant Molal Overflow	Beta
C_1	$.5010 \times 10^{-4}$	$.1685 \times 10^{-3}$	$.2500 \times 10^{-4}$
C_2	.6452	.6452	.6452
C_3	16.70	16.70	16.70
iC_4	5.518	5.551	5.539
NC_4	11.13	11.20	11.20
iC_5	4.796	4.800	4.800
NC_5	11.60	11.60	11.60

Ordering of Feed and Product Streams

Stream 1, Distillate

Stream 2, Side Product

Stream 3, Top Feed

Stream 4, Bottom Feed

Stream 5, Bottom Product

Trays	Total Reflux	Beta at Constant Molal Overflow	Beta
Partial Condenser	1.00	1.00	1.00
Section I	0.90	0.80	0.80
Section II	1.40	1.70	1.70
Section III	1.40	2.80	3.30
Section IV	2.10	4.80	7.30
Partial Reboiler	1.00	1.00	1.00
TOTAL TRAYS	7.8	12.10	15.10

TABLE II (continued)

RESULTS FOR A TWO FEED THREE PRODUCT COLUMN

Temperatures:

	Total Reflux	Beta at Constant Molal Overflow	Beta
Condenser	63.1	62.7	62.7
Top Section I	78.0	90.3*	90.5*
Bt. Section I	91.0	86.0*	86.2*
Top Section II	113.7	103.7	103.8
Bt. Section II	122.0	113.7	114.5
Top Section III	213.9	125.6	124.9
Bt. Section III	249.4	186.8	189.8
Top Section IV	250.7	218.2	212.7
Bt. Section IV	252.0	234.3	238.4
Reboiler	253.3	253.3	253.3

*These temperatures are inverted because there is less than one tray in the section. Therefore the liquid and vapor from the section are not in equilibrium. Hence the bubble point gives a lower temperature for the liquid stream than the dew point on the vapor stream coming from the section even though the liquid stream is heavier than the vapor stream.

LIST OF NOMENCLATURE

b - component bottom product rate, moles

B - bottom product, moles

C - number of components

d - component distillate rate, moles

D - distillate, moles

f - component feed rate, moles

h - enthalpy of liquid, BTU per mole

H - enthalpy of vapor, BTU per mole

K - equilibrium ratio

ℓ - component liquid rate, moles

L - total liquid rate, moles

N - number of trays

N_c - number of constraints

N_i - number of independent variables

N_v - number of variables

p - side product component liquid rate, moles

P - side product total liquid rate, moles

S - number of stages

v - component vapor rate, moles

V - total vapor rate, moles

x - mole fraction in liquid phase

y - mole fraction in vapor phase

Z - mole fraction of a component in the feed

Greek Symbols

α - relative volativity, K_i/K_{HK}

β - relative operability defined by equation (3.3-7)

Subscripts

Av - average

d - refers to the distillate

f - refers to the feed

F - refers to the feed

HK - refers to heavy key

i - refers to any component, i

ℓ - refers to liquid phase

LK - refers to light key

m - minimum trays

M - minimum trays or the last tray in a section

N - last tray in a section

p - refers to product stream

T - total

v - refers to vapor phase

Superscripts

' - refers to heavy key

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APPENDIX A

CALCULATION OF THE NUMBER OF INDEPENDENT VARIABLES IN COMPLEX FRACTIONATORS

SIMPLE TOWER: One feed, two products (see Figure A-1)

Elements	Number of Variables	
Total Condenser	C	+4
Divider (Reflux)	C	+5
(N-1)-(M+1) Simple Equilibrium Stages	2C+2(N-1-M-1)	+5
Feed Stage	3C	+8
M Simple Equilibrium Stages	2C+2M	+5
Partial Reboiler	C	+4
Total (N_v^u)	10C + 2N	+ 27

Nine interstreams are created by the combination of elements.

Therefore, $N_v^u = 9(C+2) = 9C+18$

The number of independent variables is the following:

$N_i^u = N_v^u - N_c^u = (10C + 2N + 27) - (9C + 18) = C + 2N + 9$

Specifications:	Number of Variables	
Pressure in Each Stage (including reboiler)	N	
Pressure in Condenser		1
Pressure in Reflux Divider		1
Heat Leak in Each Stage, (excluding reboiler)	N	-1
Heat Leak in Reflux Divider		1
Feed Definition	C	2
Reflux Temperature		2
Reflux Rate		1
Feed Location		1

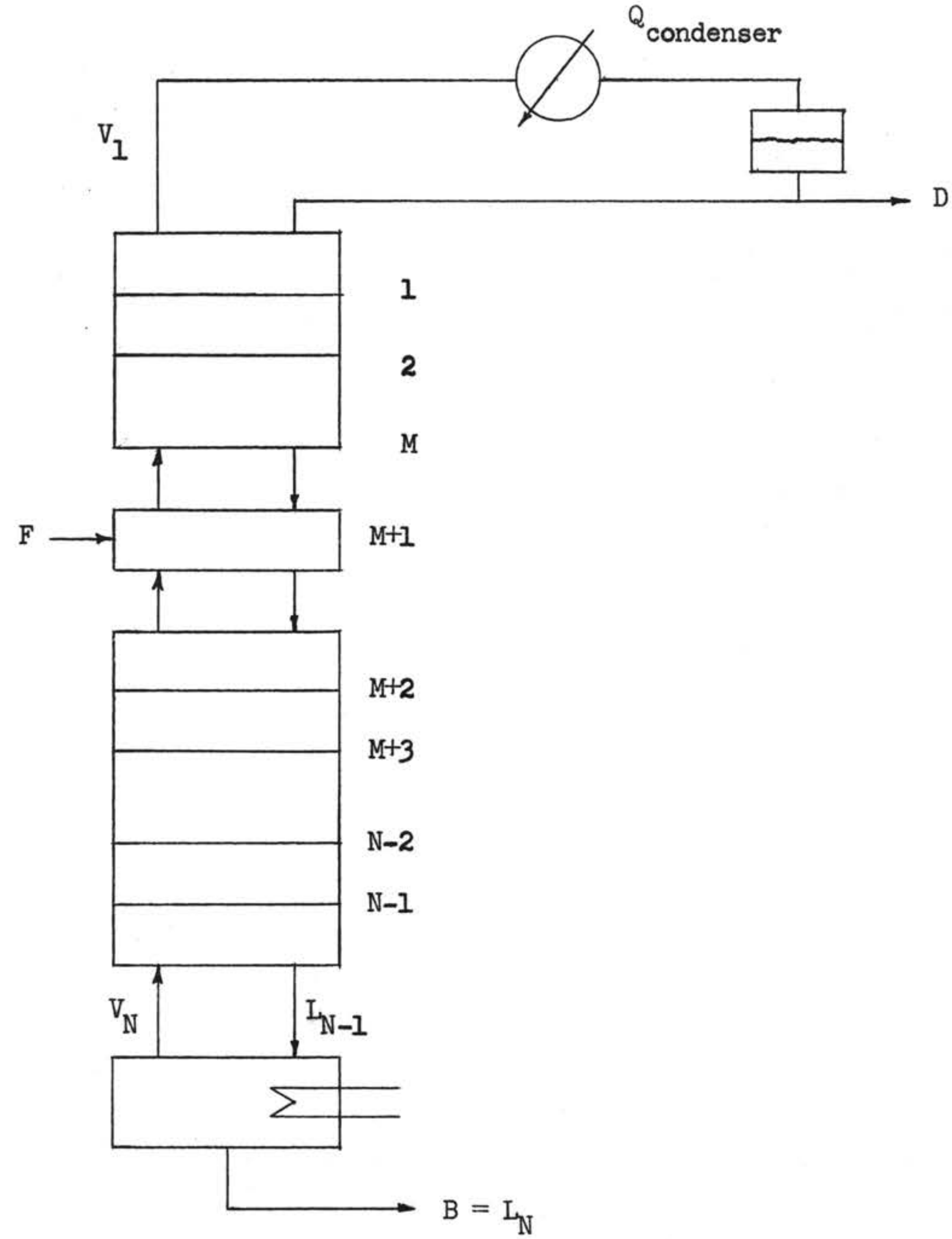

Figure A-1. Distillation Column With One Feed, Total Condenser, And Partial Reboiler

Product Specification:		
Ratio of Moles Light Key in D to Light Key in B		1
Product Specification:		
Ratio of Moles of Heavy Key in D to Heavy Key in B		1
Total	C+2N	+9

SIMPLE TOWER: One feed, two products (see figure A-2)

Elements	Number of Variables	
Partial Condenser	C	+4
(N-1)-(M+1) Simple Equilibrium Stages	2C+2(N-2-M)	+5
Feed Stage	3C	+8
M Simple Equilibrium Stages	2C+2M	+5
Partial Reboiler	C	+4
Total	9C+2N	+22

Eight interstreams are created by the combination of elements.

Therefore, $N_c^u = 8(C+2) = 8C+16$

$N_i^u = N_v^u - N_c^u = (9C+2N+22) - (8C+16) = C+2N+6$

Specifications:	Number of Variables	
Pressure in Each Stage (including reboiler)	N	
Pressure in Condenser		1
Heat Leak in Each Stage (excluding reboiler)	N	-1
Feed Definition	C	+2
Reflux Rate		1
Feed Location		1

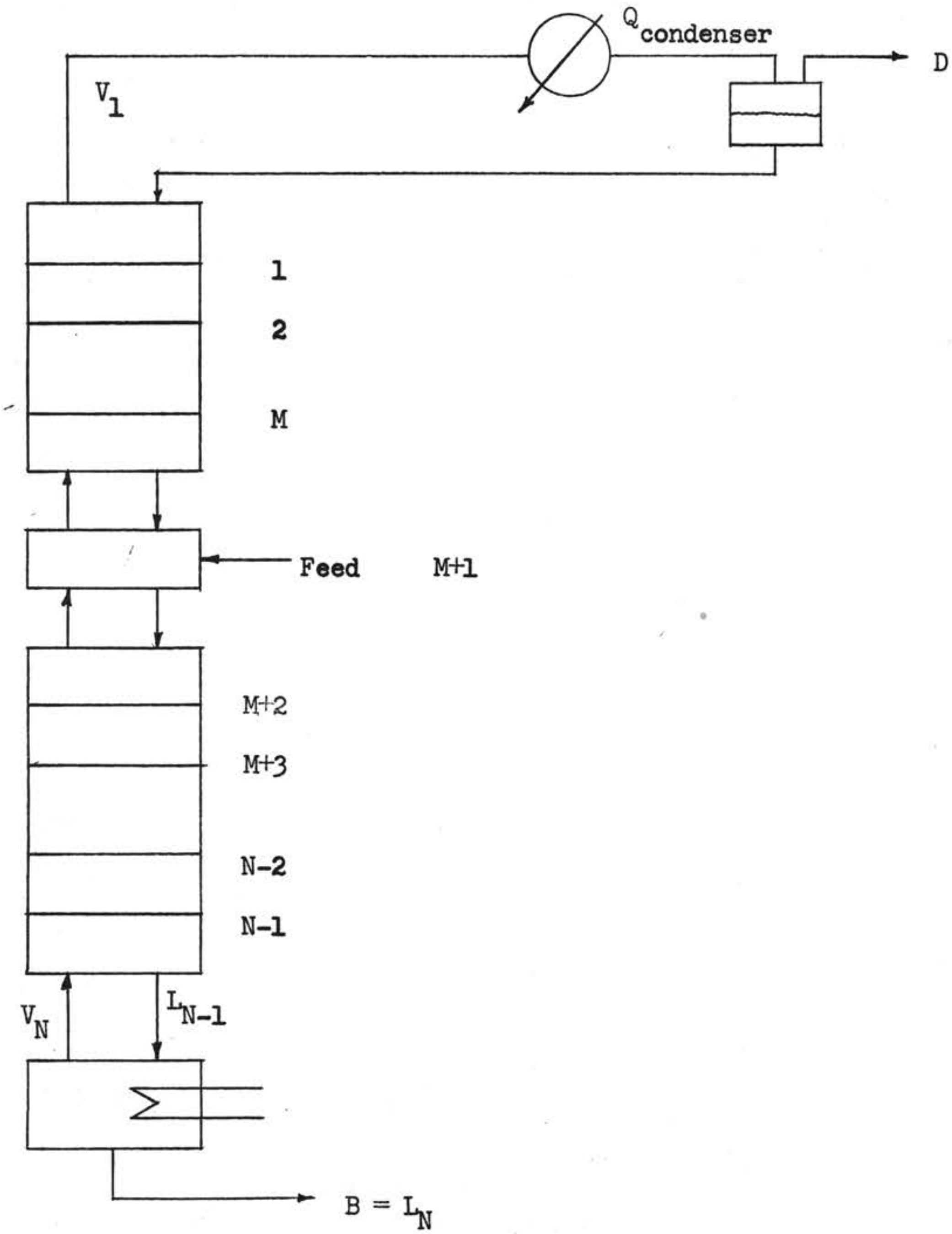

Figure A-2. Distillation Column With One Feed, Partial Condenser, And Partial Reboiler

Product Specification:

Ratio of Moles Light Key in D to Light Key in B	1

Product Specification:

Ratio of Moles Heavy Key in D to Heavy Key in B	1
Total	C + 2N + 6

COMPLEX TOWER: **Two feeds, two products (see Figure A-3)**

Elements	Number of Variables
Total Condenser	C +4
Divider (reflux)	C +5
(N-1)-M Simple Equilibrium Stages	2C + 2(N-1-M) +5
Feed Stage	3C +8
(M-1)-S Simple Equilibrium Stages	2C + 2(M-1-S) +5
Feed Stage	3C +8
(S-1) Simple Equilibrium Stages	2C + 2(S-1) +5
Partial Reboiler	C +4
Total, N_v^u	15C + 2N + 38

Thirteen interstreams are created by the combination of elements. Therefore, $N_c^u = 13(C+2) = 13C+26$

Therefore the number of independent variables is the following:

$N_i^u = N_v^u - N_c^u = (15C+2N+38) - (13C+26) = 2C+2N+12$

The number of independent variables is increased by C+3 over the simple tower by the addition of each feed stream. The independent variables specified are the additional feed stream definition, C+2 independent variables, plus the feed location.

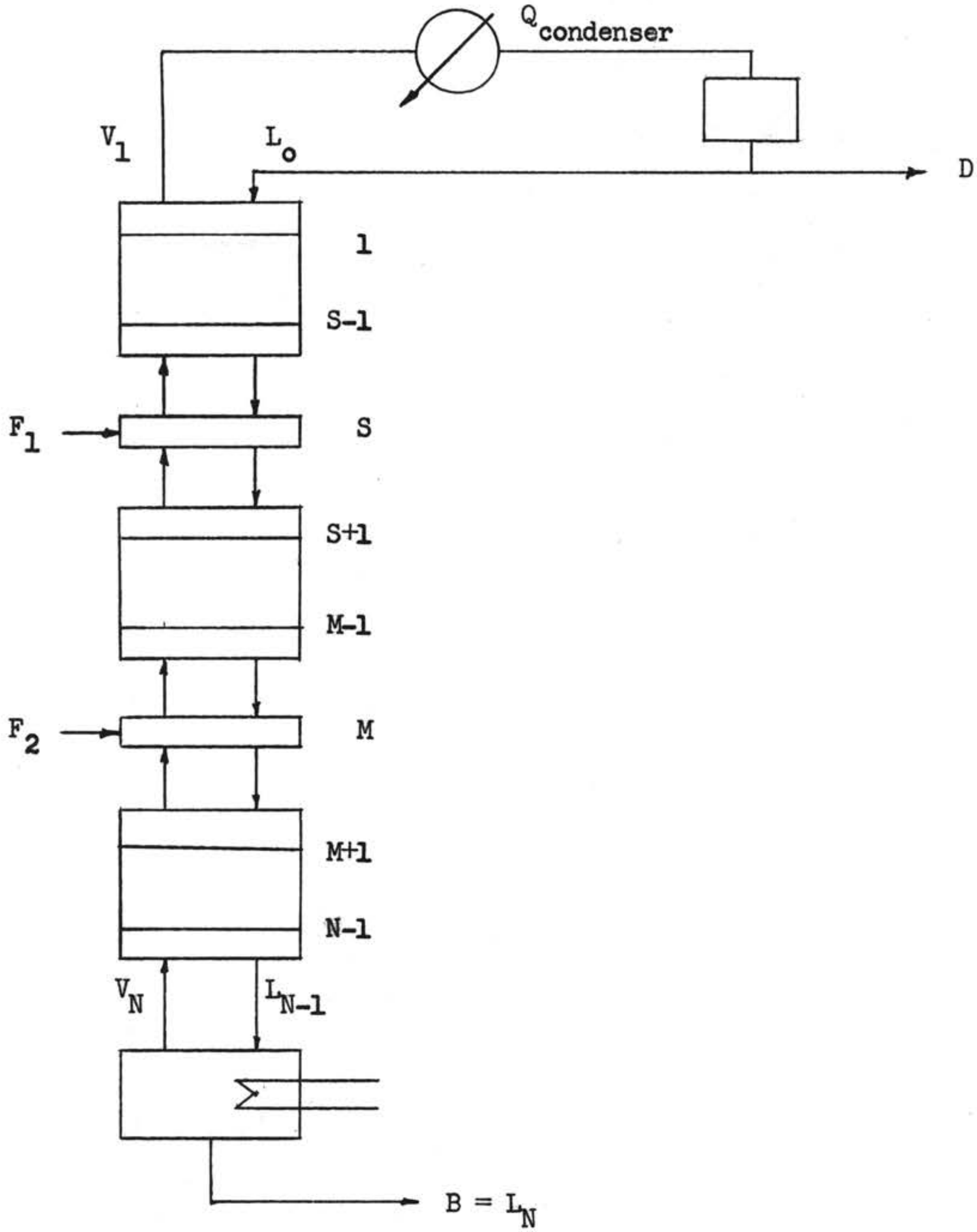

Figure A-3. Distillation Column With Two Feeds, A Total Condenser, And A Partial Reboiler

COMPLEX TOWER: One feed, three products (see figure A-4)

Elements	Number of Variables	
Total Condenser	C	+4
Divider (Reflux)	C	+5
(S-1) Simple Equilibrium Stages	2C+2(S-1)	+5
Side Stream Stage	2C	+7
M-(S+1) Simple Equilibrium Stages	2C+2(M-S-1)	+5
Feed Stage	3C	+8
N-(M+1) Simple Equilibrium Stages	2C+2(N-M-1)	+5
Partial Reboiler	C	+4
Total, N_v^u	14C + 2N	+ 37

Thirteen interstreams give $N_c^u = 13(C+2) = 13C + 26$. Therefore the number of independent variables is as follows:

$$N_i^u = N_v^u - N_c^u = (14C+2N+37) - (13C+26) = C+2N+11$$

For each side product stream the number of independent variables is increased by two. The two additional independent variable specifications are the ratio of moles of light key in the adjacent product streams and the ratio of moles of heavy key in the adjacent product streams.

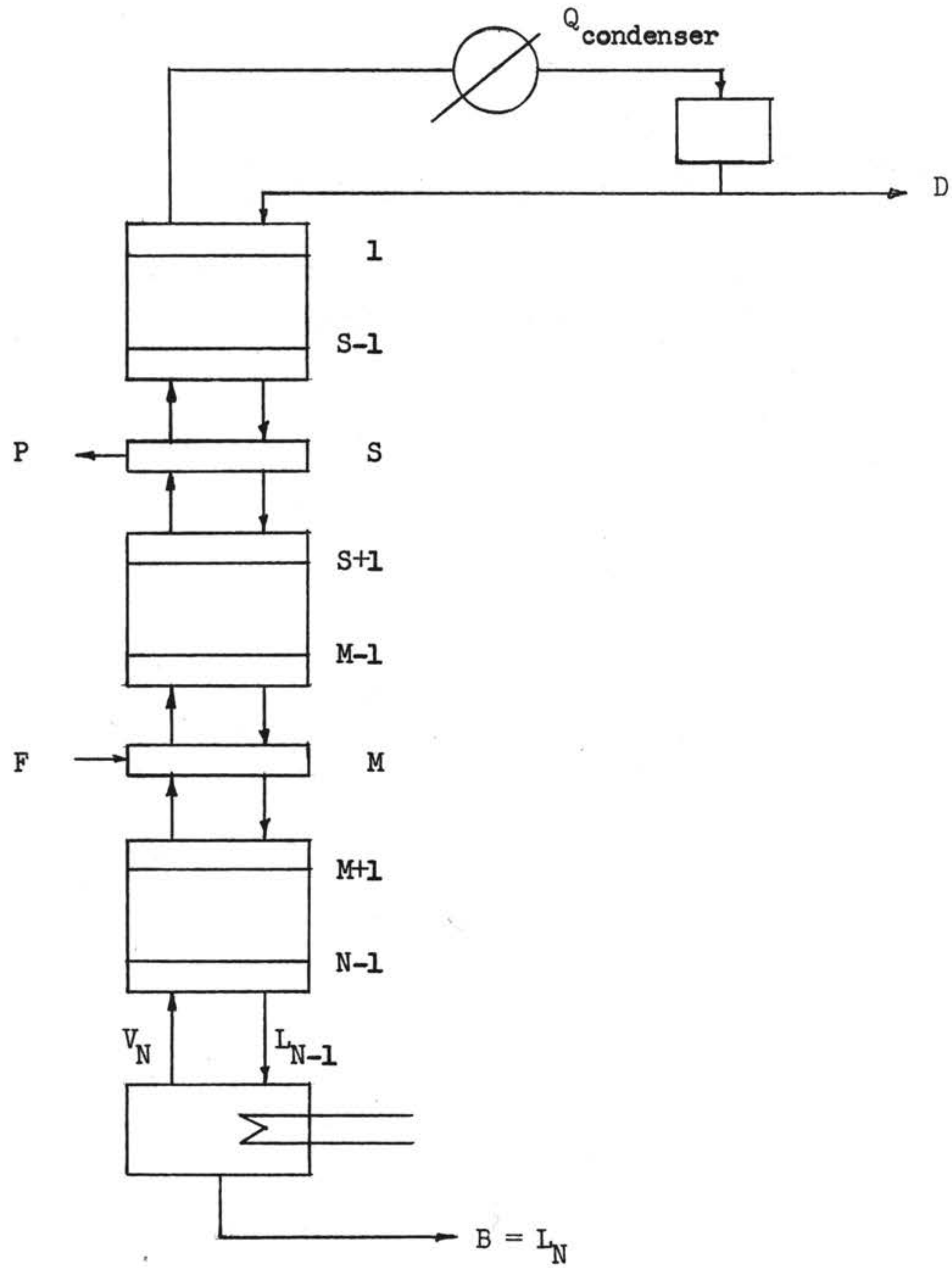

Figure A-4. Distillation Column With One Feed, One Side Stream, A Total Condenser, And A Partial Reboiler

APPENDIX B

PHYSICAL DATA

Vapor Liquid Equilibrium Ratio

$$\ln K P = A + B/(T+460) + C/(T+460)^2 + D/(T+460)^3$$

P = 450 PSIA

T = Degree F.

Component	A	B	C	D
Methane	$.5499378 \times 10^{1}$	$.4663469 \times 10^{4}$	$-.2551307 \times 10^{7}$	$.3696128 \times 10^{9}$
Ethane	$.2984046 \times 10^{2}$	$-.3313591 \times 10^{5}$	$.1576587 \times 10^{8}$	$-.2580009 \times 10^{10}$
Propane	$.1517222 \times 10^{2}$	$-.1156195 \times 10^{5}$	$.5156270 \times 10^{7}$	$-.9560957 \times 10^{9}$
IsoButane	$.8398354 \times 10^{1}$	$-.6608265 \times 10^{3}$	$-.6951510 \times 10^{6}$	0
N Butane	$.7720158 \times 10^{1}$	$.4959718 \times 10^{3}$	$-.1385131 \times 10^{7}$	$.1009837 \times 10^{9}$
i-Pentane	$.5478247 \times 10^{1}$	$.4194846 \times 10^{4}$	$-.3569396 \times 10^{7}$	$.4629868 \times 10^{9}$
N Pentane	$.4787024 \times 10^{1}$	$.5648353 \times 10^{4}$	$-.4535553 \times 10^{7}$	$.6268509 \times 10^{9}$

Liquid Enthalpy

$$H = A + B\,T + C\,T^2 + D\,T^3$$

T = Degree F. + 460

Component	A	B	C	D
Methane	$.1235649 \times 10^{4}$	$.8369604 \times 10^{1}$	$.2240656 \times 10^{-2}$	$.1190588 \times 10^{-5}$
Ethane	$.1522972 \times 10^{4}$	$.1819285 \times 10^{2}$	$-.1376706 \times 10^{-1}$	$.2048111 \times 10^{-4}$
Propane	$.1076967 \times 10^{4}$	$.2991379 \times 10^{2}$	$-.4357376 \times 10^{-2}$	0
i-Butane	$.4472884 \times 10^{4}$	$.2740840 \times 10^{2}$	$.2831585 \times 10^{-1}$	$-.2784634 \times 10^{-4}$
N Butane	$.1820311 \times 10^{4}$	$.3295338 \times 10^{2}$	$.2992319 \times 10^{-1}$	$-.3689593 \times 10^{-4}$
i-Pentane	$.2863586 \times 10^{4}$	$.3293703 \times 10^{2}$	$.6040724 \times 10^{-1}$	$-.5838273 \times 10^{-4}$
N Pentane	$.3158600 \times 10^{4}$	$.3410701 \times 10^{2}$	$.5718648 \times 10^{-1}$	$-.5547083 \times 10^{-4}$

PHYSICAL DATA (continued)

Vapor Enthalpy

$H = A + B\,T + C\,T^2 + D\,T^3$

T = Degrees F. + 460

Component	A	B	C	D
Methane	$.3706007 \times 10^{4}$	$.9947516 \times 10^{1}$	$-.1933666 \times 10^{-2}$	$.4960991 \times 10^{-5}$
Ethane	$.5423173 \times 10^{4}$	$.1366153 \times 10^{2}$	$.1079270 \times 10^{-1}$	$-.6788551 \times 10^{-5}$
Propane	$.7323896 \times 10^{4}$	$.1628828 \times 10^{2}$	$.2951619 \times 10^{-1}$	$-.2211021 \times 10^{-4}$
i-Butane	$.9793049 \times 10^{4}$	$.2025555 \times 10^{2}$	$.3398501 \times 10^{-1}$	$-.1844284 \times 10^{-4}$
N Butane	$.9672688 \times 10^{4}$	$.2183363 \times 10^{2}$	$.2143613 \times 10^{-1}$	0
i-Pentane	$.1111833 \times 10^{5}$	$.2386870 \times 10^{2}$	$.3219549 \times 10^{-1}$	0
N Pentane	$.1176631 \times 10^{5}$	$.2570043 \times 10^{2}$	$.2619305 \times 10^{-1}$	$.4324608 \times 10^{-5}$

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