

MINIMUM REFLUX FOR MULTICOMPONENT DISTILLATION SYSTEMS

By

RUTH CAMPBELL ERBAR

Bachelor of Science

Oklahoma State University

Stillwater, Oklahoma

1958

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, 1960

SEP 1 1960

MINIMUM REFLUX FOR MULTICOMPONENT DISTILLATION SYSTEMS

Thesis Approved:

R. N. Maddox

Thesis Adviser

W. C. Edmister

John W. Maudslayi

Dean of the Graduate School

452711

PREFACE

A theoretically rigorous method for the calculation of minimum reflux in multicomponent distillation systems is presented in this thesis. I have attempted to explain the differences between this method and other calculation methods.

A comparison of the results using this new method was made with the results of techniques.

I sincerely appreciate the advice and constructive criticism given by Dr. Robert N. Maddox.

I wish to thank the Dow Chemical Company for its fellowship grant which made this work possible.

TABLE OF CONTENTS

Chapter	Page
I. INTRODUCTION	1
II. GENERAL CHARACTERISTICS OF A COLUMN OPERATING AT MINIMUM REFLUX	3
III. SURVEY OF THE LITERATURE - DISCUSSION OF METHODS	10
IV. DISCUSSION AND EXPLANATION OF NEW METHOD	24
V. COMPARISON OF NEW METHOD WITH OTHER METHODS	34
Discussion of Calculation Procedures	34
Discussion of Results of Calculations	35
VI. CONCLUSIONS	46
LIST OF NOMENCLATURE	48
A SELECTED BIBLIOGRAPHY	50
APPENDIX A - OUTLINE OF BACHELOR'S METHOD OF CALCULATING MINIMUM REFLUX	52
APPENDIX B - OUTLINE OF J. ERBAR'S MINIMUM REFLUX CALCULATION PROCEDURE	64
APPENDIX C	72
APPENDIX D - PERCENT DEVIATION OF APPROXIMATE METHODS FROM RIGOROUS CALCULATION RESULTS	75
APPENDIX E - BLOCK DIAGRAM OF RIGOROUS METHOD	77

LIST OF TABLES

Table	Page
I. Feed Compositions	38
II. Minimum Reflux Rate, Feed Composition 1, BP Liq., Distillate Rate 25.113	39
III. Minimum Reflux Rate, Feed Composition 1, BP Liq., Distillate Rate 25.766	39
IV. Minimum Reflux Rate, Feed Composition 1, BP Liq., Distillate Rate 25.964	39
V. Minimum Reflux Rate, Feed Composition 1, BP Liq., Distillate Rate 50.005	39
VI. Minimum Reflux Rate, Feed Composition 1, BP Liq., Distillate Rate 50.003	39
VII. Minimum Reflux Rate, Feed Composition 1, BP Liq., Distillate Rate 50.004	39
VIII. Minimum Reflux Rate, Feed Composition 1, BP Liq., Distillate Rate 49.999	39
IX. Minimum Reflux Rate, Feed Composition 2, BP Liq., Distillate Rate 19.840	39
X. Minimum Reflux Rate, Feed Composition 2, BP Liq., Distillate Rate 20.051	40
XI. Minimum Reflux Rate, Feed Composition 2, BP Liq., Distillate Rate 20.020	40
XII. Minimum Reflux Rate, Feed Composition 2, BP Liq., Distillate Rate 39.737	40
XIII. Minimum Reflux Rate, Feed Composition 2, BP Liq., Distillate Rate 39.614	40
XIV. Minimum Reflux Rate, Feed Composition 2, BP Liq., Distillate Rate 39.677	40
XV. Minimum Reflux Rate, Feed Composition 2, BP Liq., Distillate Rate 60.394	40
XVI. Minimum Reflux Rate, Feed Composition 2, BP Liq., Distillate Rate 60.160	40
XVII. Minimum Reflux Rate, Feed Composition 2, BP Liq., Distillate Rate 60.251	40

LIST OF TABLES (Continued)

Table	Page
XVIII. Minimum Reflux Rate, Feed Composition 3, BP Liq., Distillate Rate 29.985	41
XIX. Minimum Reflux Rate, Feed Composition 3, BP Liq., Distillate Rate 29.853	41
XX. Minimum Reflux Rate, Feed Composition 3, BP Liq., Distillate Rate 50.384	41
XXI. Minimum Reflux Rate, Feed Composition 3, BP Liq., Distillate Rate 50.377	41
XXII. Minimum Reflux Rate, Feed Composition 4, BP Liq., Distillate Rate 24.331	41
XXIII. Minimum Reflux Rate, Feed Composition 4, BP Liq., Distillate Rate 24.340	41
XXIV. Minimum Reflux Rate, Feed Composition 4, BP Liq., Distillate Rate 39.932	41
XXV. Minimum Reflux Rate, Feed Composition 4, BP Liq., Distillate Rate 39.998	41
XXVI. Minimum Reflux Rate, Feed Composition 4, BP Liq., Distillate Rate 55.280	42
XXVII. Minimum Reflux Rate, Feed Composition 4, BP Liq., Distillate Rate 55.477	42
XXVIII. Minimum Reflux Rate, Feed Composition 5, BP Liq., Distillate Rate 29.848	42
XXIX. Minimum Reflux Rate, Feed Composition 5, BP Liq., Distillate Rate 29.956	42
XXX. Minimum Reflux Rate, Feed Composition 5, BP Liq., Distillate Rate 60.030	42
XXXI. Minimum Reflux Rate, Feed Composition 5, BP Liq., Distillate Rate 60.033	42
XXXII. Minimum Reflux Rate, Feed Composition 7, BP Liq., Distillate Rate 20.610	42
XXXIII. Minimum Reflux Rate, Feed Composition 7, BP Liq., Distillate Rate 21.364	42

LIST OF TABLES (Continued)

Table		Page
XXXIV.	Minimum Reflux Rate, Feed Composition 7, BP Liq., Distillate Rate 40.166	43
XXXV.	Minimum Reflux Rate, Feed Composition 7, BP Liq., Distillate Rate 40.191	43
XXXVI.	Minimum Reflux Rate, Feed Composition 3, BP Liq., Distillate Rate 14.904	44
XXXVII.	Minimum Reflux Rate, Feed Composition 3, BP Liq., Distillate Rate 16.170	44
XXXVIII.	Minimum Reflux Rate, Feed Composition 3, BP Liq., Distillate Rate 15.046	44
XXXIX.	Minimum Reflux Rate, Feed Composition 3, BP Liq., Distillate Rate 15.788	44
XL.	Minimum Reflux Rate, Feed Composition 4, BP Liq., Distillate Rate 7.666	44
XLI.	Minimum Reflux Rate, Feed Composition 4, BP Liq., Distillate Rate 8.403	44
XLII.	Minimum Reflux Rate, Feed Composition 4, BP Liq., Distillate Rate 7.727	44
XLIII.	Minimum Reflux Rate, Feed Composition 4, BP Liq., Distillate Rate 9.159	44
XLIV.	Minimum Reflux Rate, Feed Composition 1, BP Liq., Distillate Rate 26.549	45
XLV.	Minimum Reflux Rate, Feed Composition 1, 50% Liq., Distillate Rate 26.549	45
XLVI.	Minimum Reflux Rate, Feed Composition 1, DP Vap., Distillate Rate 26.549	45

LIST OF FIGURES

Figure	Page
1. Column at Minimum Reflux	4
2. McCabe-Thiele Diagram	7
3. Feed Zones	13
4. L/K_iV , VK_i/L As Functions of Tray Numbers	25
5. Column at Minimum Reflux - Bachelor's Method	55
6. Column at Minimum Reflux - J. Erbar's Method	69
7. Effective Absorption Factors	71

CHAPTER I

INTRODUCTION

The problem of determining minimum reflux for multicomponent systems has received attention from a large number of investigators since the concept was first presented. All of the previous investigators, with two exceptions, have made one or more limiting assumptions which cause the results of their methods to be questionable for the majority of actual problems.

In 1955 Bachelor (1) presented and later published (2) a method for calculating the minimum reflux ratio. This method was not based on the classic assumptions of constant molal overflow, constant or linear relative volatility, perfect or very sharp product splits, pseudo-binary is equivalent to a multicomponent system, or that actual products are the same as products at the minimum reflux.

The purpose of this work was to develop a reliable and accurate method for calculating the minimum reflux ratio. Because of the complexity of the calculational procedure, the IBM 650 computer was used for making all calculations.

Bachelor presented his method as an accurate, but short cut, calculation suitable for hand solution. However, due to the methods used to simplify the method for hand calculation, it was not readily adaptable for machine computation. These simplifying assumptions

greatly reduce the time required for hand calculation, but merely serve to compound the problem and introduce unnecessary limitations for machine calculation.

For these reasons, a new method was developed and programmed. This method makes none of the earlier mentioned assumptions and is theoretically rigorous in those areas where Bachelor's is approximate.

Material and equilibrium relationships developed by Bachelor and other investigators are used in conjunction with plate to plate calculations for an iterative solution to the problem of minimum reflux. Since heat and material balances are made around each plate and the equilibrium relationships are always satisfied, the method at no time forces the assumption of constant molal overflow. Product compositions are computed at the conditions of minimum reflux, so there is no need to assume that actual operating products will suffice. This allows the products to be either completely distributed or to contain nondistributed components, whichever the key splits and other conditions indicate.

This method is not a short cut procedure nor is it recommended for hand calculation due to the enormous number of plate calculations which must be made, approximately 2000 in an average problem.

CHAPTER II

GENERAL CHARACTERISTICS OF A COLUMN

OPERATING AT MINIMUM REFLUX

A distillation column operating at the conditions of minimum reflux to separate a single feed into two products may be said to consist of seven zones. These zones are defined as: the feed zone, the rectifying zone, the rectifying pinch zone, the distillate specification zone, the stripping zone, the stripping pinch zone, and the bottom product zone. The schematic diagram of a column operating at minimum reflux, shown in Figure 1, shows these seven zones and their physical location with respect to each other. The function of these zones and their relationship to each other will be brought out in the discussion that follows.

The feed zone is between the two plates on either side of the point at which the feed is introduced. In the feed zone, the feed is flashed and combined with the liquid and vapor streams entering from adjacent sections. The resulting liquid and vapor streams are the feeds to the rectifying and stripping sections of the column.

The rectifying zone begins above the upper feed plate and extends to the plate at which all components not appearing in the distillate have been fractionated to zero. If any component is fractionated to zero, an infinite number of plates is required. However, temperatures and compositions do change from plate to plate in the

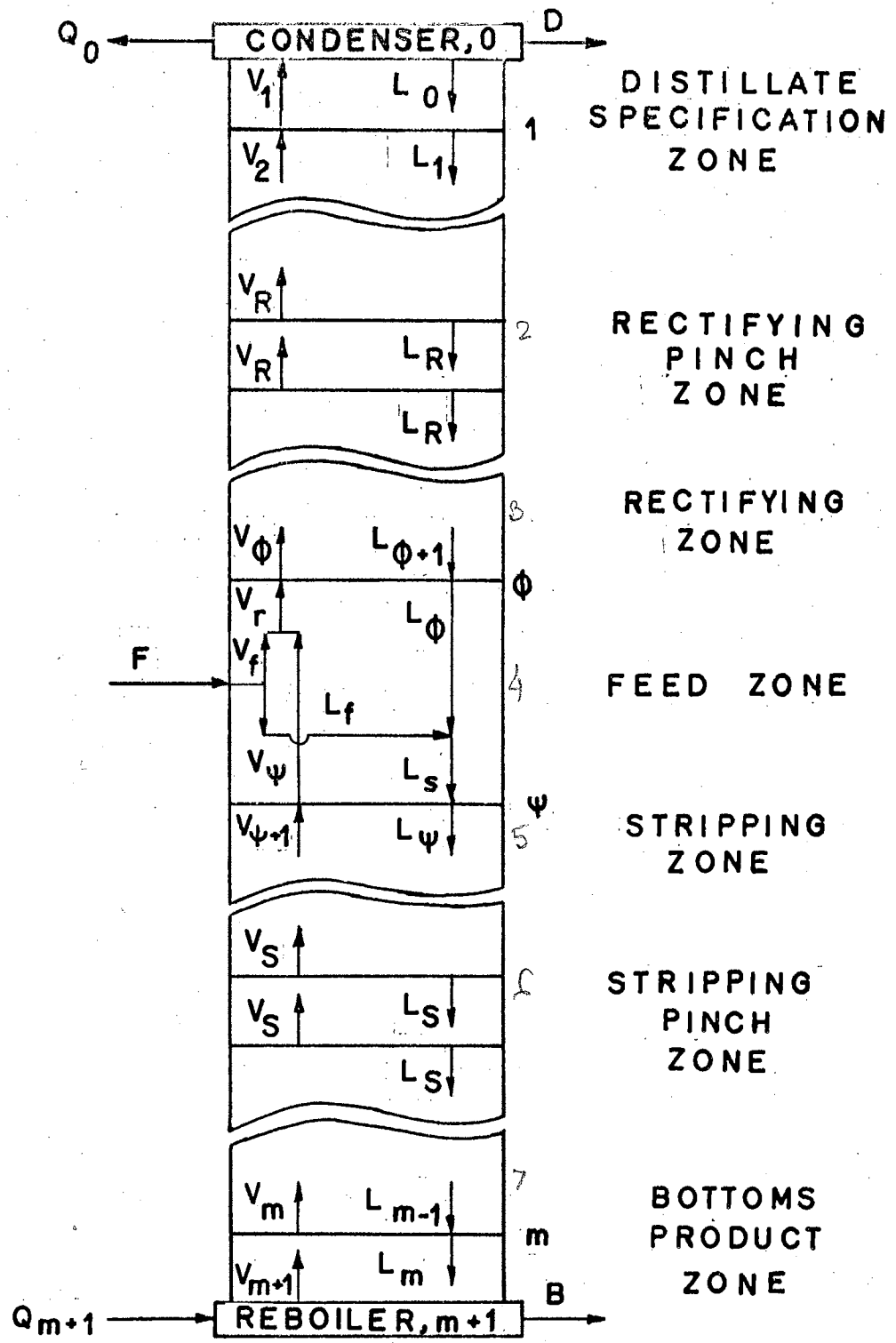


FIGURE 1

COLUMN AT MINIMUM REFLUX

rectifying zone and in this way, its behavior differs from that normally associated with a zone of infinite plates.

The rectifying pinch zone extends from the plate on which temperature and compositions have become constant. All components not appearing in the distillate (nondistributed components) have been fractionated to zero. Since there is no composition or temperature change from plate to plate, the rectifying pinch zone extends for an infinite number of plates. Because of the constancy of temperatures and compositions, passing streams are in equilibrium with each other. The rectifying pinch zone extends outward in the column until a change in temperature and composition would occur on the next plate.

The distillate specification zone extends from the plate above the rectifying pinch zone to the top of the tower. The first plate in the distillate specification zone is the plate on which temperatures and compositions differ from those of the rectifying pinch zone. The purpose of the distillate specification zone is to fractionate from the pinch zone composition to the composition of the desired overhead product.

Conditions in the stripping section of the column are similar to those in the rectifying section. The functions of the stripping zone, the stripping pinch zone, and the bottom product zone are analogous to those of their individual counterparts in the rectifying section of the column.

The foregoing discussion applies to a column with nondistributed components in both products. A nondistributed component is defined as a feed constituent which appears in only one product of the column at minimum reflux. If the distillation column at minimum reflux is

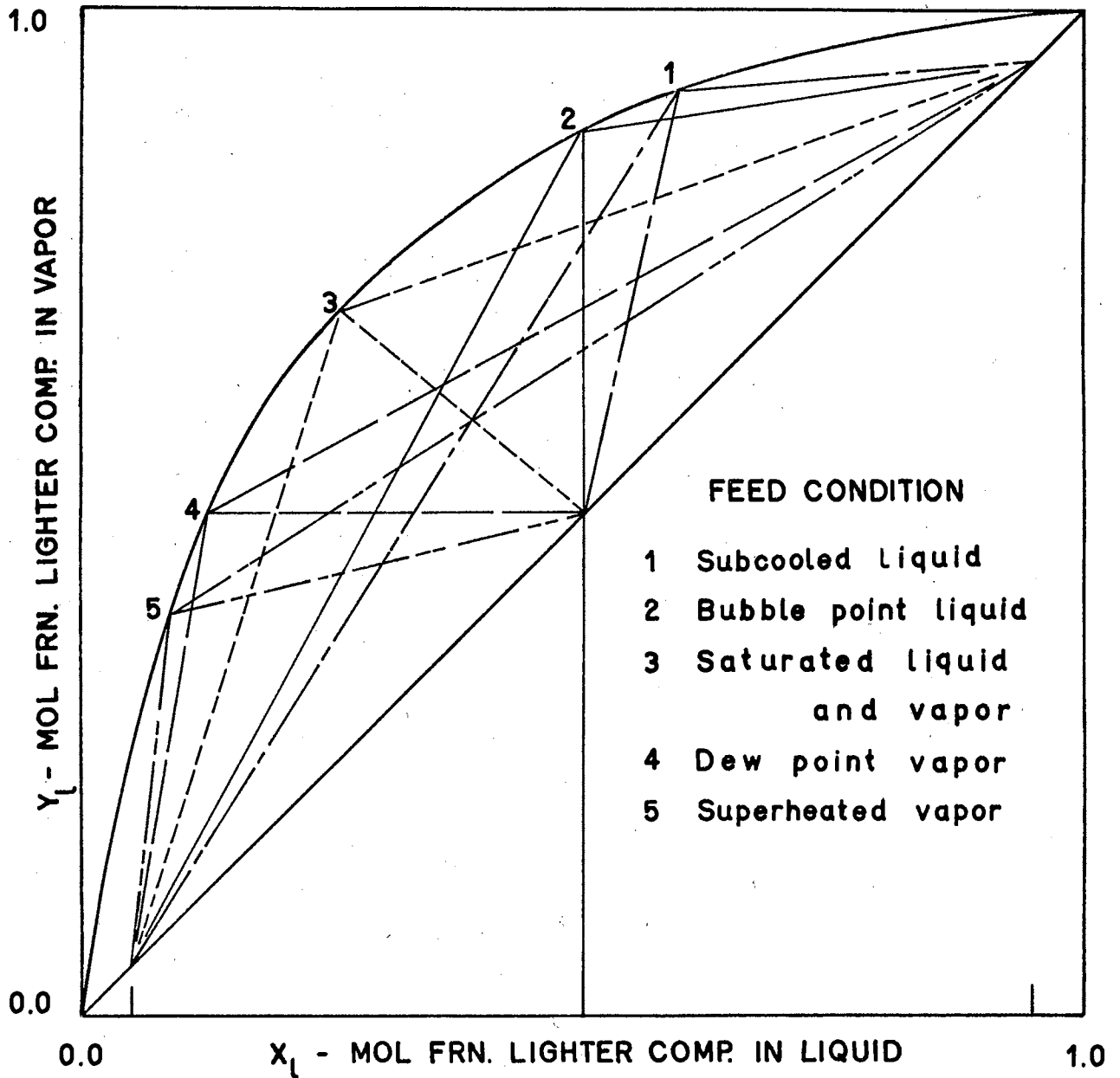
to contain all seven zones, there must be at least one nondistributed component in the rectifying section and one in the stripping section. Only in this case will the column operation be as described above.

If both products contain all components, the products are said to be completely distributed. When there are no nondistributed components, several of the zones discussed are absent from the system. Under conditions of complete distribution for all components, there is no need to fractionate any component to zero. Consequently the stripping zone and the rectifying zone disappear from the column and the two pinch zones extend from the feed zone to the product specification zones.

For the case of complete distribution, the pinch zone compositions are those of the equilibrium feed liquid and vapor. For this case, the pinch zones cross the feed and merge with each other. Temperatures and stream compositions are the same in both pinch zones. Total stream quantities, however, are different because of the addition of the feed stream in the feed zone.

Pinch zone compositions are the same as the feed compositions only if the feed is saturated liquid and/or saturated vapor. If the feed is either superheated or subcooled, the pinch zone compositions will be removed from the feed composition. This effect is most easily seen by use of a McCabe-Thiele (24) diagram as shown in Figure 2.

The operation of a multicomponent column with complete distribution of all components is analogous to the operation of a binary column. Figure 2 shows a McCabe-Thiele diagram for the conditions of minimum reflux. The operating line for the rectifying section of



MINIMUM REFLUX AT VARIOUS FEED CONDITIONS

FIGURE 2

McCABE-THIELE DIAGRAM

the column extends through the intersection of the q line with the equilibrium curve. The intersection occurs at the feed composition for any saturated feed, but is removed for either a subcooled liquid or superheated vapor feed. The operating line for the stripping section of the column behaves in a similar manner.

A third possibility for column operation at minimum reflux is nondistribution of only one product. For simplicity, a column operating with components missing in the distillate only will be discussed. Performance for a column operating with components equal to zero in the bottoms product is analogous.

If the column is operating with nondistributed components being removed in the rectifying section, all three zones (rectifying zone, rectifying pinch zone, and the distillate specification zone) will appear in the rectifying section. The function of these zones will be the same as described for both products containing nondistributed components.

The stripping section of the column, however, will operate as though both products were completely distributed. The stripping pinch zone will begin next to the feed zone and extend to the bottom product zone. The stripping pinch zone, however, will not have the compositions of the equilibrium feed.

A number of investigators (5,8,16,18) have discussed the column at minimum reflux, considering five zones to be present. Gilliland (16) presents this treatment very clearly.

Bachelor (1,2) and Edmister (9) have discussed the column at minimum reflux, using seven zones, but these zones are considered in a somewhat different manner than in this thesis. They both consider

the rectifying and stripping zones to have a finite number of plates, the pinch zones to have an infinite number of plates, and the product zones to have an infinite number of plates.

CHAPTER III

SURVEY OF THE LITERATURE - DISCUSSION OF METHODS

Investigators have been working on the problem of minimum reflux for a great many years, but only recently have methods been presented which are close to being theoretically rigorous for multicomponent systems with nondistributed components. With the exception of the methods of Bachelor and of J. Erbar (14), all of these methods are based on one or more severely limiting assumptions. Some of the more common limitations are the assumptions of constant molal overflow, constant or linear relative volatility, actual products identical to those at the minimum reflux, sharp product splits, and the resolution of multicomponent systems to pseudo-binary systems. These assumptions, while good for any system wherein the effect of these assumptions is negligible, are inadequate for the vast majority of actual problems.

The assumption of constant molal overflow implies that the interstage liquid and vapor rates remain constant in each section of the column. This condition would be present if the latent heats of vaporization for all components in the system were equal and constant for all temperatures and pressures in the tower. Even the rather approximate enthalpy data available shows how very inaccurate this assumption is for many systems. The condition of constant molal overflow could also occur if the changes in temperature, pressure

Constant Molal
Overflow

and composition from plate to plate were exactly compensating. This is possible to a limited extent for a few trays in some systems, but highly improbable over the infinite plates at minimum reflux for any system.

The assumption of constant relative volatility is only as good as the estimate of it. There is some "average" value of relative volatility for each component that, if used throughout the system, would give the same products as the use of the more correct values would. There is yet to be determined, a method of predicting such an "average" value. For an actual system to display constant relative volatility, only a very small temperature or pressure range could be used. This small range is not adequate for the range covered by an actual column, much less that covered at minimum reflux.

When actual products are assumed to be the same as the products at minimum reflux, one has fixed too many variables for the system. Even in actual operation it is well known that, if the plates and reflux are both changed, only two components can still be split in the same ratios and that the total of each product will be different, or that the total of each product and only one component can remain unchanged. Often it has been assumed that the percentage composition of two components in the distillate can be fixed. This effectively fixes the relationship of the total distillate to each of these components just as the fixing of the quantities of these two components and the total would do. This error has been made in those equations for minimum reflux which have been presented in the form $(L/D)_{\min} = f(X_{d1}, X_{dh})$ which is valid for binaries only. Underwood (32) and Fenske (15) have presented equations for minimum

reflux which, within the limits of their assumptions, would be exact for multicomponent systems if the equations were rearranged in the form $L_{\min} = f(d_l, d_h)$.

This can be easily seen if one applies the phase rule in combination with the first and second laws of thermodynamics to a distillation column. This was first done by Gilliland and Reed (17) and later presented again by Kwauk (19).

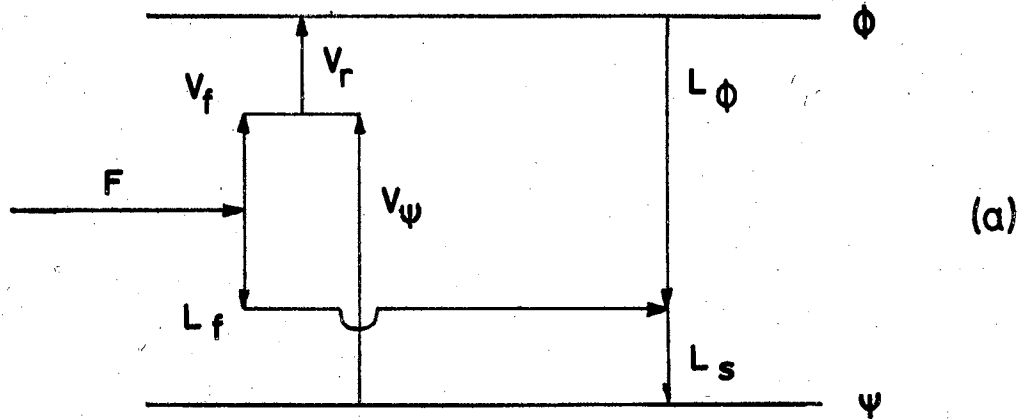
If a column is operating under the following conditions:

1. With reflux, either a partial or total condenser
2. With boilup, either a partial or total reboiler
3. With feed plate treated as in either Figure 3a or 3b
4. With single feed and two products

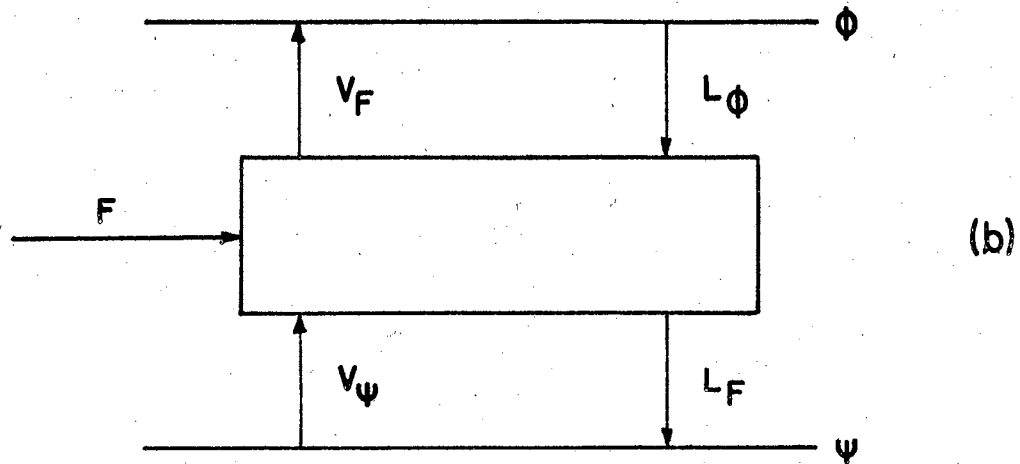
the following number of variables must be fixed if the column operation is to be described completely.

$$\text{Number of variables} = C + 2m + 2n + 10 \quad (17,19).$$

<u>SPECIFYING</u>	<u>FIXES VARIABLES</u>
1. Feed rate	1
2. Feed conditions (temperature, pressure, etc.)	2
3. Feed composition	C-1
4. Total plates, m+n (equal to infinity for column at minimum reflux)	1
5. Pressure on each plate	m+n
6. Pressure of feed flash or feed plate	1
7. Pressure of condenser and reboiler	2
8. Heat loss or gain on each plate (usually considered equal to zero for adiabatic operation)	m+n
9. Heat loss or gain in feed flash or on feed plate (usually adiabatic)	1
10. Condenser load (minimum for column at minimum reflux)	1
	<hr style="width: 100%;"/>
	C + 2m + 2n + 8



FEED ZONE USED IN RIGOROUS METHOD
AND BACHELORS' METHOD



FEED ZONE USED IN J. ERBAR'S METHOD

FIGURE 3

FEED ZONES

There remain two variables which must be fixed to completely describe the column operation. At the minimum reflux these can be either the total distillate and the amount of one component in the distillate, or the product split of two components. The individual components which are specified must be present in both products.

The assumption of sharp product splits immediately limits the use of a method containing this assumption. All components outside the keys are neglected in one section of the tower or the other. This means the heavier components are neglected in determining the reflux rate and condenser load and that the lighter components are neglected in determining the boilup rate and reboiler load. The possibilities for error are obvious.

The resolution of a multicomponent system to a pseudo-binary contains the possibility for a number of errors. It is not yet possible to describe the properties of a single composition at various conditions of temperature and pressure by assuming it is made up of one or two pseudo-components. Therefore, it is hardly probable that one can define the mixture in terms of two pseudo-components that describe a number of compositions at a number of temperatures and pressures with any degree of accuracy. This assumption often is used as a means of effectively neglecting all components except the keys.

The first methods of solution for the problem of minimum reflux were presented in the 1920's. McCabe and Thiele (24), Ponchon (25), and Savarit (26) presented methods which are quite easy to use and show graphically the conditions existing in the column at minimum reflux. The McCabe-Thiele method is limited to binary mixtures

whose components have identical latent heats of vaporization at all temperatures and pressures in the column, that is, constant molal overflow is assumed. The Ponchon-Savarit method takes into consideration enthalpy variations for different components with temperature and pressure, but is also limited to two component systems.

Souders and Brown (7) have published material balance and equilibrium relationships that apply at the pinch zones. These equations were the first to be presented which were valid for multicomponent systems.

$$v_{Ri} = \frac{d_i}{1 - (L/KV)_{Ri}} \quad \begin{array}{l} \text{V Rectifying pinch zone} \\ (1) \end{array}$$

$$l_{Si} = \frac{b_i}{1 - (VK/L)_{Si}} \quad \begin{array}{l} \text{L Stripping pinch zone} \\ (2) \end{array}$$

These equations are rigorous for all multicomponent distillation systems at minimum reflux. They are easily applied for a distributed system which has the feed zone included in the pinch zones (a saturated liquid and/or vapor feed). Since neither the products nor the pinch zone compositions could be predicted for nondistributed systems when these equations were presented, it was difficult to apply the equations usefully. Later however, several investigators (1,2,8,14) found these equations quite useful as prediction and correction equations when combined with other relationships.

In 1932, Fenske (15) and Underwood (32) each published methods for the determination of minimum reflux for multicomponent systems. Underwood's equation applies at all feed conditions and Fenske's

equation applies specifically to bubble point feeds.

$$\text{Fenske} \quad (L/D)_R = \frac{1}{\alpha_R - 1} \left[\frac{X_{d1}}{X_{R1}} - \alpha_R \frac{X_{dh}}{X_{Rh}} \right] \quad (3)$$

$$\text{Underwood} \quad \alpha_R \frac{(L/D)_R + 1}{(L/d)_R + 1} \frac{X_{R1} - (1+q)X_{d1}}{X_{Rh} - (1+q)X_{dh}} = \frac{X_{R1}(L/D)_R - qX_{d1}}{X_{Rh}(L/D)_R - qX_{dh}} \quad (4)$$

If the Underwood equation is applied to a bubble point feed, it reduces to that of Fenske. These equations are based on the assumptions of constant molal overflow and constant relative volatility. They are also based on the presumption that the distillate composition and the pinch compositions are known. The equations are rigorous for distributed products if relative volatilities at the feed temperature are used, and if they are slightly rearranged. For example, Fenske's equation is rigorous at the above conditions if in the following form.

$$L_R = \frac{1}{\alpha_R - 1} \left[\frac{d_1}{X_{R1}} - \alpha_R \frac{d_h}{X_{Rh}} \right] \quad (5)$$

The compositions of the rectifying pinch are those of the equilibrium feed liquid and vapor and the result is the liquid rate in the pinch. Since the two keys are known in the distillate, one can find the correct distillate composition for the other components by material balances. Then the usual methods may be used to find the reflux without assuming constant molal overflow.

In 1939, Jenny (18) published the first method that used plate to plate calculations. This method assumes that distillate compositions

are known. The problems solved for publication using this method were based on constant molal overflow due to the tedious nature of the method, although this assumption is not necessary. The pinch temperatures are estimated by the criterion that $(L/KV)_{Ri} \geq 1$ for all components that are not in the distillate, and by a similar relationship in the stripping section of the column. A reflux is assumed and stepwise component calculations are made to determine the feed plate compositions. The results of the trial and error solution are checked by plate to plate calculations from the feed. This was the first multicomponent method that did not force the assumption of constant relative volatility or constant molal overflow for nondistributed products. The method did not, however, include a means of predicting the composition of these products. Publication of this method added a great deal to the understanding of the conditions at minimum reflux and, for the first time, used plate to plate calculations to some advantage.

Brown and Holcomb (5) were the first to propose a method that used plate to plate calculations for the entire solution of a column operating at minimum reflux. This method still had the very common assumption that the products at the minimum were known. They suggested that the first assumption of the reflux rate be made by some short cut method, either their approximate method (4) or some other. Plate to plate calculations by the Thiele-Geddes (29) method are made from the products to the pinch zones. At the pinch zone, a small amount of the lightest nondistributed component not appearing in the distillate is added to the streams. Several plates are calculated and the next heavier component is introduced. In this manner

calculations are made in the rectifying pinch to the feed zone. A similar procedure is followed in the stripping section of the column. The matching of the components at the feed plate is tested and, if in error for any other than the keys and other distributed components, the calculations are repeated from the pinch zones with the nondistributed components being introduced on different trays. When the feed plate mesh is within the desired degree of accuracy on the nondistributed components, the distributed components are checked. If they mesh properly, the reflux chosen was the correct minimum reflux. If not, a new reflux rate must be chosen and the calculations resumed at the beginning. This method forces only the assumption that the distillate at the minimum reflux is known from actual operation or can be estimated accurately. This can be done easily for binary systems.

For multicomponent systems, the distillate can be found by several methods. These methods are all combined with other minimum reflux calculations. There is no reason to use Brown and Holcomb's method after solving the problem and predicting the distillate composition by some other method.

Gilliland (12) presented a trial and error short cut technique in 1940. This method takes into consideration those components other than the keys and their effect on the minimum reflux. Using this method, the minimum reflux can be bracketed within limits and a conservative value might be used. The assumptions of constant molal overflow, constant relative volatility, and products known are included. This method was an improvement over other short cut methods in that the effect of non-key components was recognized. However,

this improvement is somewhat negated by the tremendous increase in complexity.

Maxwell (22) later modified Gilliland's method. This modified method is considerably easier to use, but does retain the basic assumptions.

Using the results of Jenny's method as a basis, Colburn (8) developed an empirical method of determining the minimum reflux which was easier to use than Jenny's method and which gave comparable results. The problems used to develop this method and which were used to judge its validity were based on the assumption of constant molal overflow. Colburn's method, therefore, indirectly contains this assumption even though he does provide a means of partially correcting this error when desired.

Later, Underwood (31) developed a second method based on rigorous equations for the plates in a column. He reduced these equations to a simple set to solve for the minimum reflux. However, these equations are based on the assumptions of constant molal overflow and constant relative volatility. Therefore, only under these conditions are the equations strictly valid. They are good for both distributed and nondistributed products. Still later, Underwood (30) showed how these equations might be used to determine the compositions of components between the key components. They also can be used to determine the amount of any other components in the distillate.

$$v_f = \sum \frac{d_j f_i}{\alpha_i - \theta_j} \quad (6)$$

There are $n-1$ values of θ_j , one between each adjacent pair of values of relative volatility for the components in the system. For example, if there are four components in the system whose volatilities are 0.5, 1.0, 2.0, and 2.5, there are three values of θ . These values are between 0.5 and 1.0, 1.0 and 2.0, 2.0 and 2.5.

If all values of θ are found for the system, one can then substitute them into the following equation and solve for the product composition.

$$V_{\min} = \sum \frac{\alpha_i d_i}{\alpha_i - \theta_j} \quad (7)$$

Since quantities of the key components in the distillate are fixed, there remain $n-2$ compositions to find and the total V_{\min} . These variables may be found by solving simultaneously the $n-1$ independent equations formed by using a different value of θ in each one.

The distillate composition variables must be checked after solution. If unrealistic values were calculated, nondistributed components are indicated (28). For example, any negative quantity indicates that this component is present only in the bottoms and is zero in the distillate. A distillate quantity greater than the amount of that component in the feed indicates that this component is present only in the distillate product and is zero in the bottoms. All components whose values in the distillate are between zero and the amount of that component in the feed are distributed to both products. The calculated quantity is the correct amount in distillate for these components.

While preparing results by Underwood's method, it was found that the minimum reflux is distorted if nondistributed components are present. This is caused by the unrealistic values predicted for the nondistributed components. This meaningless quantity may be replaced by a sound value if the θ between the heavy key and next lighter component is used in Equation 7 with the new distillate composition and total. Equation 7 has been rearranged from the form in which it was first presented to avoid the possibility of fixing one too many variables.

The original form is:

$$D \left[\frac{L}{DF} \min + 1 \right] = \sum \frac{\alpha_i d_i}{\alpha_i - \theta_j} \quad (8)$$

Equations 7 and 8 are identical. However, form 8 has often been used erroneously by assuming that the total distillate must be known to find the reflux, when actually the entire left side of the equation is an unknown. The total distillate is known when the composition is determined.

Shiras, Hansen, and Gibson (28) suggested a plate to plate method quite similar to that of Brown and Holcomb. Instead of a trial and error technique to change the tray on which each of the nondistributed components are introduced, they suggest that Lewis and Matheson (20) plate to plate calculations be made from the feed out. The Thiele-Geddes calculations are then made from the pinch zones in again. This method has the same inherent weakness as have those of Jenny, and Brown and Holcomb, that of assuming actual products are equal to those at the minimum reflux.

A number of other investigators (3,6,9,21,23,27) have developed methods of calculating the minimum reflux for multicomponent systems. The majority of these methods involve more assumptions or limitations, are much more difficult to use, and give results no more accurate than the previously described methods. An exception is an unpublished method by Winn (34) which is similar, in many respects, to those of Underwood and Maxwell. This method is quite easy to use but has not been tested extensively against the results of other methods.

The methods of Maxwell, Underwood, and Winn are the simplest to use and, for this reason, the first two have been widely accepted. The results of Underwood's second method are generally comparable to those of Colburn and Jenny; Maxwell's method approximates Gilliland's.

In 1955, Bachelor (1) presented and later published (2) the first method that made none of the classic assumptions mentioned earlier. This method incorporates parts of other distillation calculation methods with some independent derivations. This method was presented as a short cut, but accurate, solution to the problem of multicomponent minimum reflux. It is not much more tedious than many of the methods published earlier, but hardly conducive to hand calculation.

In Bachelor's method, the product compositions and the feed zone compositions can be found as functions of the passing stream ratios in the feed zone and of the equilibrium feed liquid and/or vapor streams. By material balances and equilibrium relationships, the temperatures of the feed streams may be adjusted from the first

assumptions and the product and feed zone compositions adjusted accordingly.

Pseudo-equilibrium plate to plate calculations are made out from the feed, the pinch zone compositions are found using the Souders-Brown equations, and the pinch zone compositions and the products are adjusted again. This sequence is repeated until the desired degree of matching is achieved.

A general outline of the method presented by Bachelor can be found in Appendix A. The derivations pertinent for a bubble point feed are also given in Appendix A. The equations for a dew point or flash feed are presented but not derived as the method is similar to that for the bubble point equations.

The most recent short cut technique is that developed by J. Erbar (14). This method makes use of the generalized distillation equations developed by Edmister (10). From these generalized equations, Erbar derived relationships that pertain to a column operating at the minimum reflux. This method makes no assumptions of constant molal overflow, constant relative volatility and predicts the products at the minimum reflux. Erbar's method is somewhat shorter for hand calculation than that of Bachelor and more readily adaptable to the medium sized or small digital computer. Preliminary results indicate that this method will give results comparable to that of Bachelor.

The pertinent equations and an outline of the method can be found in Appendix B.

CHAPTER IV

DISCUSSION AND EXPLANATION OF NEW METHOD

The minimum reflux method developed in this thesis is similar in many respects to those of Bachelor and of Erbar. The expressions developed by Bachelor are used to determine the feed zone and product compositions.

Using the results of problems solved by the minimum reflux method presented in this thesis, J. Erbar found that the values of L/K_iV for each tray in the rectifying section could be replaced by assuming L/K_iV to be linear over a 5 to 10 tray region. These linear factors produced similar results to those produced by the plate to plate values of L/K_iV . This linear relationship is used to estimate L/K_iV when rigorous calculations would result in a negative material balance. It is also applied when an L/K_iV greater than that in the pinch zone is predicted for a plate.

An example of the linear estimation procedure is given in Figure 4. A plot of the L/KV or V/KL on the trays near the feed is shown for one component. In the stripping section, negative material balances were calculated on the fourth tray. Therefore, the values of VK_i/L were estimated by linear relationships between the VK_i/L on the third tray and in the pinch zone. An examination of the stripping zone curve shows how well the estimations fit the other data.

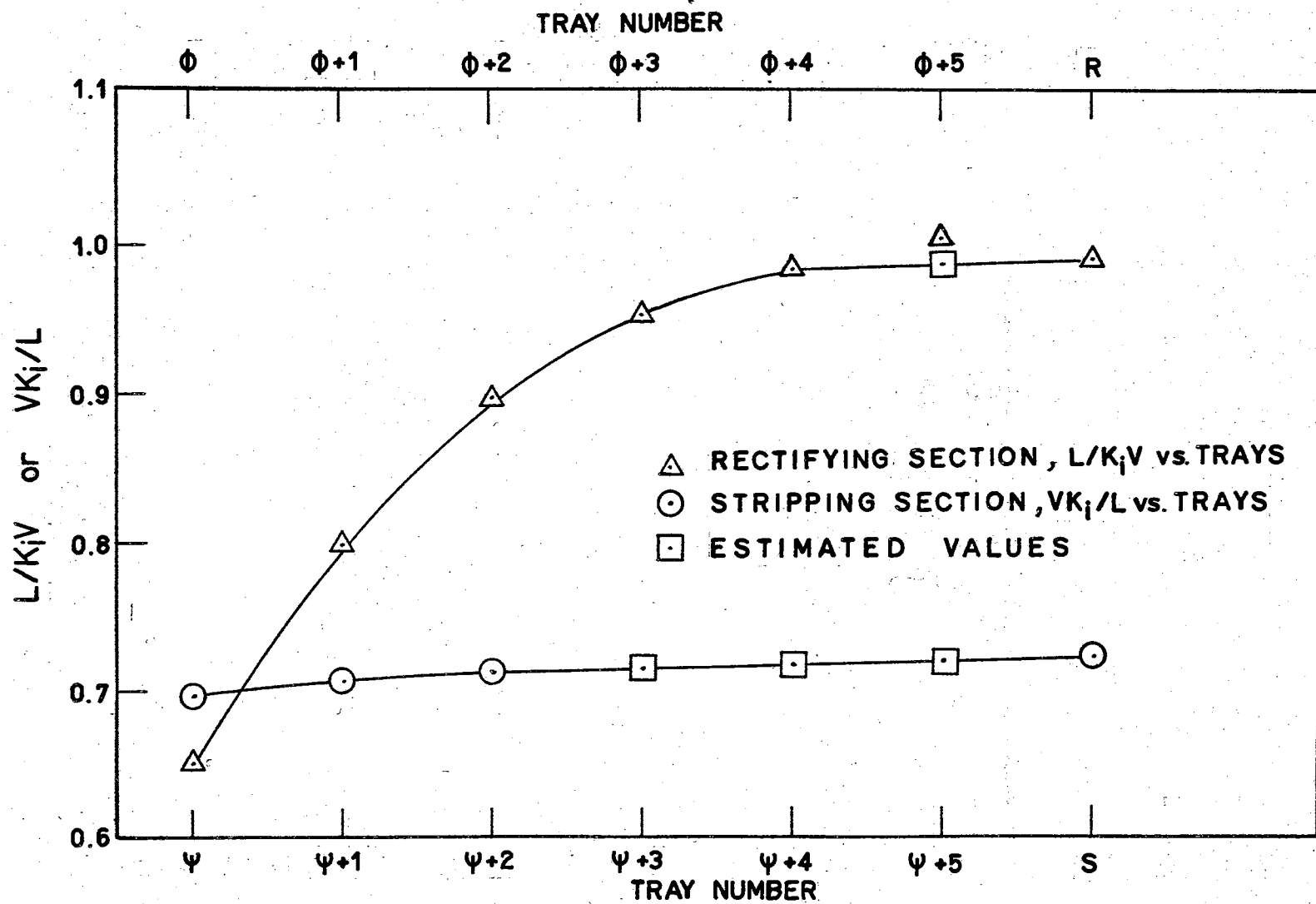


FIGURE 4

L/K_iV , VK_i/L AS FUNCTIONS OF TRAY NUMBER

In the rectifying section, values of L/K_iV greater than those in the pinch zone were calculated for the sixth tray. These values were estimated assuming linearity between the L/K_iV on the fifth tray and the pinch zone. The curve for the rectifying section appears distorted when the incorrect value is considered. This distortion is lessened when the estimated value is used.

Negative material balances and L/K_iV 's that are too large are caused by round out and truncation errors. They are also caused by errors induced by the tolerances applied to the bubble and dew point calculations and heat balances.

When additional trials are carried out, the estimated values of L/K_iV will be gradually replaced by values calculated directly. This procedure applies equally well to the values of VK_i/L in the stripping section.

The major differences between this method and those of Bachelor and J. Erbar are in areas where they use approximation methods and this method uses rigorous plate to plate calculations.

The first area of difference is in the calculation of the pinch zone compositions. Both Erbar and Bachelor approximate these by the use of the Souders-Brown pinch zone equations. It should be remembered that these equations are rigorous only if the pinch zone temperature and total flow quantities are known. These equations are quite sensitive to temperature and total stream quantities. Often a composition will be predicted that is more in error than the one on which the prediction was based. Small errors such as were shown in Figure 4 will produce larger errors in many cases.

This new method predicts the compositions of the pinch zones

by rigorous plate to plate calculations from the extremities of the column to the pinch zones. These plate to plate calculations utilize heat and material balances in conjunction with equilibrium relationships as suggested by Lewis and Matheson. Pinch zone compositions determined in this manner are much more accurate than those determined by other means.

The second and possibly most important difference is the manner in which the plates between the feed zone and pinch zone are handled. J. Erbar uses effective absorption factors which have been determined using the results of this rigorous method as a basis for testing their validity.

Bachelor's method involves "pseudo" plate calculations from the feed zone to the pinch zone. These calculations are rigorous only for distributed products.

For nondistributed products the magnitude of error is dependent upon stream compositions and degree of unbalance in plate heat balances. In some cases, total streams have been overcorrected as much as 70%.

The method presented in this thesis uses rigorous plate to plate calculations from the feed zone out to the pinch zones. These calculations are the same as described for the extremities to the pinch zones. When it becomes necessary to estimate the L/KV or V/KL on a tray that cannot be treated rigorously, the method used has been tested thoroughly and is not subject to the errors developed by a single heat balance correction.

For the first trial the pinch zones are assumed to extend through the feed zone, that is, completely distributed products with

pinch zone compositions equal to the equilibrium feed liquid and vapor compositions are assumed. Corrections are then made using the pinch zone results from plate to plate calculations in from the condenser and reboiler. The next trial is based on the assumption that the pinch zones begin one tray removed from the feed trays. Successive trials move the pinch zones one tray farther away from the feed zone until the change in reflux is considered negligible.

The calculation sequence follows. The theory behind each step will be explained or referenced to an appendix. For consistency, the nomenclature used will be as close as possible to that used by Bachelor.

Data necessary: Liquid and vapor enthalpy data for each component
 Vapor-liquid equilibria data for each component
 Feed composition, quantity and condition
 Light and heavy key component distributions
 (total mols)

1. The temperature, vapor and liquid, and vapor and liquid enthalpy of the feed are calculated.
2. The temperatures of the rectifying and stripping pinch zones are assumed to be equal to the temperature of the feed. (See Appendix C)
3. If, as is first assumed, the pinch zones originate at the feed zone, $g_i = \alpha_{\phi i}$ and $u_i = \alpha_{\psi i}$.

Since, by definition,
$$g_i = \frac{l_{\phi h}/v_{rh}}{l_{\phi i}/v_{ri}}$$

$$\alpha_i = K_i/K_h,$$

and
$$K_i = y_i/x_i = \frac{v_{ri}/V_r}{l_{\phi i}/L_\phi} = \frac{L_\phi v_{ri}}{V_r l_{\phi i}}$$

then,
$$\alpha_{\phi i} = \frac{L_\phi v_{ri}/V_r l_{\phi i}}{L_\phi v_{rh}/V_r l_{\phi h}} = \frac{l_{\phi h}/v_{rh}}{l_{\phi i}/v_{ri}} = g_i$$

Similarly, one can show that $\alpha_{\psi i} = u_i$. In this way g_i and u_i are calculated for the first trial.

4. By definition, $G_i = l_{\phi i}/v_{ri}$, $U_i = v_{\psi i}/l_{\psi i}$,

and
$$g_i = \frac{l_{\phi h}/v_{rh}}{l_{\phi i}/v_{ri}}$$

Therefore,
$$G_i = G_h/g_i$$

In an analogous manner, it can be shown that $U_i = U_h u_i$

Since $U_h = f(u_1, g_1, d_h, d_1, F)$, as is G_h (see Appendix A for equations and derivations), the values of U_i and G_i can be calculated.

5. The distillate composition and the composition of the liquid entering the feed zone from the rectifying section are now calculated. These compositions are functions of U_i , G_i , and F_i . (see Appendix A for equations and derivations)

6. The first trial, as stated in step 3, is based on the assumption that the feed zone is included in the pinch zones. Using material balances and equilibrium relationships, equations to test the validity of the temperature assumptions in the pinch zones can be developed (1,2). For the rectifying pinch zone,

$$K_{hR} = \frac{L_\phi}{(L_\phi + D)G_h}$$

For the stripping pinch zone,

$$K_{hS} = \frac{U_h(L_\phi + L_f)}{L_\phi + D - V_f}$$

The derivation of these equations is given in Appendix A.

If the temperatures for which these K values are valid are the same as those assumed for the pinch zones, the calculation proceeds to step 7. If not, the calculation reverts to step 3, using the calculated temperatures in place of those used before.

7. By material balance, $v_{\psi i}$ and b_i are now calculated.

$$v_{\psi i} = l_{\phi i} - v_{f i} + d_i$$

$$b_i = f_i - d_i$$

8. Since the products, feed liquid and vapor, and the liquid ($l_{\phi i}$) and vapor ($v_{\phi i}$) entering the feed zone are known, the enthalpies for these streams not already known may be calculated. A heat balance is made around the rectifying section of the column to determine the condenser load, Q_c ,

$$Q_c = H_v V_{\psi} + H_v V_f - H_l L_{\phi} - H_d D$$

and the reboiler load, Q_r , is equal to

$$Q_r = H_b B - H_v V_f - H_l L_f + H_d D + Q_c$$

9. Knowing the composition, total quantity and enthalpy of the distillate and knowing the condenser load, one can now proceed plate to plate down the column. The rectifying pinch zone has been reached when no change occurs in the compositions, temperature, and totals of the streams from plate to plate. In a similar manner, calculations are made from the reboiler to the stripping pinch zone.

10. It can be shown (see Appendix C) that

$$\frac{l_{\phi i}}{d_i} = A_{\phi i} + A_{\phi+1 i} A_{\phi i} + A_{\phi+2 i} A_{\phi+1 i} A_{\phi i} + \dots + A_{Ri}^{\infty} \dots A_{\phi+2 i} A_{\phi+1 i} A_{\phi i}$$

for the rectifying section of a column at minimum reflux, where

$$A_i = (L/K_i V).$$

If the pinch zones pass through the feed zone, then

$$A_{\phi i} = A_{\phi+1 i} = A_{\phi+2 i} = \dots = A_{Ri}$$

and $A_{Ri} < 1$ for every component.

Therefore, for completely distributed products,

$$\begin{aligned} \frac{l_{\phi i}}{d_i} &= A_{Ri} + A_{Ri}^2 + A_{Ri}^3 + \dots + A_{Ri}^{\infty} \\ &= A_{Ri} \frac{1}{1 - A_{Ri}} \end{aligned}$$

For the first trial, which assumes distributed products, the series equation is used in the above form. An analogous equation may be derived for the stripping section using $S_i = (VK_i/L)$.

11. The results of calculations using the series equation can be rearranged to find the values of g_i for the next trial.

Remembering that

$$g_i = \frac{l_{\phi h}/v_{rh}}{l_{\phi i}/v_{ri}},$$

then by material balance

$$\frac{l_{\phi i}/d_i + 1}{l_{\phi i}/d_i} = \frac{l_{\phi i} + d_i}{l_{\phi i}} = \frac{v_{ri}}{l_{\phi i}}.$$

Analogous relationships apply in the stripping section of the tower for steps 9, 10, and 11.

12. The calculations now start again at step 4, and step 6 is eliminated. In step 9, a comparison of the new reflux is made with that calculated on the previous trial. Calculations are considered complete when the change in the reflux is small enough.
13. Step 11 is changed somewhat for each trial. For the second trial in which the pinch trays are assumed to be one plate removed from the feed zone, the series equation of step 10 now becomes

$$\begin{aligned} \frac{l_{\phi i}}{d_i} &= A_{\phi i} + A_{\phi i} A_{Ri} + A_{\phi i} A_{Ri}^2 + \dots + A_{\phi i} A_{Ri}^{\infty} \\ &= A_{\phi i} \frac{1}{1 - A_{Ri}} \end{aligned}$$

For all succeeding trials, this equation has the form

$$\frac{l_{\phi i}}{d_i} = \left(\frac{1}{1 - A_{Ri}} \right) A_{\phi+n_i} + 1) A_{\phi+n-1_i} + 1) \dots + 1) A_{\phi i} .$$

14. Step 9 is expanded on trials two through N. On these trials, plate to plate calculations from the feed out to both pinch zones are made. For the second trial, the streams on each side of the feed zone are calculated. This allows the calculation of $A_{\phi i}$ and $S_{\phi i}$ for use in the first series equation in step 13. On each succeeding trial one more tray calculation is made in each direction from the feed zone. The A and S factors from the trays are used in the second equation in step 13 or in the analogous stripping pinch equation.

A comparison of the outlines of Erbar's and of Bachelor's methods with this method will show up the differences very quickly. Inspection of steps 9 through 14 in Bachelor's method show that "equilibrium" streams are not in equilibrium for nondistributed

products. The single liquid rate correction is not followed by a corresponding composition correction, therefore, the streams are not in material or heat balance after the single correction is made. Obviously, if the streams above the first plate do not satisfy these relationships, those on following trays cannot satisfy them either.

In the feed out plate calculations and the pinch zone calculations, the methods of J. Erbar and of Bachelor are good approximations but are rigorous only for distributed products. The pinch zone calculations are made in both methods by the use of the Souders-Brown pinch zone equations.

In summary, the differences between the proposed method and Bachelor's method are:

- I. (a) Bachelor computes pinch zone stream compositions, rates, and temperatures based on feed zone out calculations (Appendix A, p. 54, Step 14).
- (b) The method developed for this thesis computes these quantities by rigorous plate to plate calculations from the column terminals to the pinch zones (Chapter IV, p. 30, Step 9).
- II. (a) Bachelor's "feed out" calculations do not use rigorous equilibrium relationships; heat balance requirements and component material balance requirements are not satisfied (Appendix A, p. 52, Steps 9 - 13).
- (b) The proposed method employs rigorous tray by tray calculations using total stream and component material balances, heat balances, and equilibrium relationships for feed out calculations (Chapter IV, p. 32, Step 14)

- III. (a) Bachelor's initial assumptions of the pinch zone temperatures are $T_R = T_D + 1/3(T_B - T_D)$ and $T_S = T_B + 1/3(T_B - T_D)$. This assumption is not consistent with the initial assumption that the pinch zones coincide with the feed zone (Appendix A, p. 52, Step 3).
- (b) The proposed method initially assumes that the temperatures of the pinch zones are equal to the feed temperature. This assumption is consistent with the assumption that the pinch zones coincide with the feed zone (Chapter IV, p. 28, Step 2; Appendix C, p. 72).
- IV. (a) Bachelor checks U_i and G_i , internal stream ratios, to determine when a satisfactory solution has been reached (Appendix A, p. 54, Step 17).
- (b) The method presented in this thesis checks the calculated reflux rate, an external quantity, to determine if a satisfactory solution has been reached (Chapter IV, p. 28).
- V. (a) For a given cycle number, N , Bachelor uses $N+2$, L/KV or VK/L values to determine new estimates of the internal stream quantities (Appendix A, p. 54, Step 15).
- (b) The rigorous method uses N values of L/KV or VK/L to determine the feed zone and product compositions on trial N (Chapter IV, p. 32, Steps 10 - 13)
- VI. (a) Bachelor's method requires an approximation of the distillate composition (Appendix A, p. 52, data).
- (b) The method presented in this thesis requires only the quantities of the light and heavy keys in the distillate (Chapter IV, p. 28, data).

CHAPTER V

COMPARISON OF NEW METHOD WITH OTHER METHODS

Discussion of Calculation Procedures

A comparison was made of the results of the rigorous method of calculating minimum reflux and the results of several short cut methods. Two of these methods, Underwood's second method and Maxwell's modification of Gilliland's method, have been used extensively. The other, Winn's method, until now has been used only by Winn since it is unpublished.

All four methods were used with the six feed compositions shown in Table I. The light and heavy key quantities in the distillate were taken from J. Erbar-Maddox (11,12,13) plate to plate results.

Tables II through XLVI show the distillate compositions as predicted by the rigorous method. The distillate compositions predicted by Underwood were quite similar in all cases and identical when all components other than the keys were nondistributed. When distributed components other than the keys were present, the quantities predicted by the two methods were only slightly different.

Maxwell's method does not contain a distillate composition prediction feature. Therefore, some means of estimation must be used. A generally accepted method is to use the Fenske minimum plates (15) distribution. While this distribution is obviously in error at minimum reflux, it does provide an estimate of the distillate composition.

Winn's method also lacks a means of predicting the distillate composition. For estimates to be used with this method, Winn's minimum stages (33) distribution was used.

The calculations using Winn's method were carried out at the feed temperature. Maxwell's method was used with the average tower temperature, defined as $1/2(T_{Dist} + T_{Btms})$. The Underwood results are given for both the average and feed temperatures.

All problems were run using a partial reboiler. The condenser type used and tower pressure are noted on each table. Feed condition is noted BP liquid for bubble point liquid feeds, DP vapor for a dew point vapor feed, and as X% liquid for a flash feed.

An "L" after a distillate component denotes light key, and an "H" denotes heavy key.

Both the enthalpy data and the vapor-liquid equilibria data are from the NGSMA Data Book, 1957 (35).

The convergence pressure used with each feed stream is shown in Table I.

Discussion of Results of Calculations

Sufficient problems to warrant comparison were run only with bubble point feeds and adjacent keys. Results for a flash and a dew point feed are included (Tables XLIV, XLV, XLVI) as a point of interest but are not compared. Several problems are included with results for both adjacent and split keys. The effect on composition and reflux is shown by both Underwood's second method and the rigorous method.

The percentage deviation of the results of the short cut methods

from those of the rigorous method was calculated for all bubble point feeds. Maxwell's method showed a maximum error of -71.0% and a minimum error of +1.1%. The average was $\pm 29.9\%$. The largest errors were at extremely low reflux rates with "sloppy" separations. The smallest errors were made with very "sharp" separations between similar components, such as iC_4 and nC_4 .

Winn's method is an improvement over that of Maxwell. The maximum and minimum deviations are of the same general size, -77.5% and -2.1% but the average is -26.3%. The largest errors are again for "sloppy" separations. However, this method is acceptable for any type of very sharp separation.

Underwood's method shows considerable improvement over both Maxwell's and Winn's methods. This should be expected since Underwood's method is rigorous for multicomponent systems with only two limitations. (See Chapter III, page 19)

When the feed temperature is used, the maximum error was found to be 36.2% with a minimum error of -4.9%. The average error was $\pm 17.0\%$. When the average tower temperature was used, the average error was smaller but the range was larger. The average error was $\pm 14.8\%$ with a maximum error of 54.9%, and a minimum error of 1.0%.

When a comparison of the data from the Underwood results at the average temperature was made with those at the feed temperature, it was found that more consistent results were obtained by using the Underwood method at the higher of the two temperatures. In this way, the maximum error becomes -33.4% for the extremely "sloppy" cut and the minimum is +1.0%. Underwood's method, when used in this way, is sensitive only to extremely "sloppy" separations and handles

other separations with little regard to degree of sharpness of the separation. The average error by this method is 11.9%.

It must be remembered that the discussion of results and conclusions drawn apply only to bubble point feeds.

TABLE I
FEED COMPOSITIONS

Component	Feed Composition - Mols		
	1	2	3
C ₂			
C ₃			10
iC ₄		20	20
nC ₄	25	20	20
iC ₅	25	20	20
nC ₅	25	20	20
C ₆	25	20	10
Totals	100	100	100
Convergence Pressure Used	600#	600#	1000#

Component	Feed Composition - Mols		
	4	5	7
C ₁		1	
C ₂	5	5	5
C ₃	20	24	15
iC ₄	15	15	10
nC ₄	15	15	10
iC ₅	15	15	10
nC ₅	15	15	10
C ₆	15	10	10
C ₇			10
C ₁₀			10
Totals	100	100	100
Convergence Pressure Used	1000#	3000#	2000#

TABLE II

Feed Composition 1		Feed Condition		BP Liq.
Total Condenser		Tower Pressure		25 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
nC ₄	24.19614 L	New Method	49.113	
iC ₅	0.91698 H	Underwood @ T _{Ave}	41.771	
Total	25.11312	Underwood @ T _{Feed}	41.876	
		Maxwell	39.840	
		Winn	29.895	

TABLE III

Feed Composition 1		Feed Condition		BP Liq.
Total Condenser		Tower Pressure		25 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
nC ₄	24.32713 L	New Method	47.487	
iC ₅	1.43859 H	Underwood @ T _{Ave}	40.657	
Total	25.76572	Underwood @ T _{Feed}	40.720	
		Maxwell	38.207	
		Winn	28.321	

TABLE IV

Feed Composition 1		Feed Condition		BP Liq.
Total Condenser		Tower Pressure		25 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
nC ₄	23.81698 L	New Method	43.114	
iC ₅	2.14663 H	Underwood @ T _{Ave}	37.757	
Total	25.96361	Underwood @ T _{Feed}	37.889	
		Maxwell	37.350	
		Winn	25.244	

TABLE V

Feed Composition 1		Feed Condition		BP Liq.
Total Condenser		Tower Pressure		25 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
nC ₄	25.00000	New Method	184.870	
iC ₅	23.64628 L	Underwood @ T _{Ave}	169.168	
nC ₅	1.35840 H	Underwood @ T _{Feed}	157.125	
Total	50.00468	Maxwell	152.040	
		Winn	166.543	

TABLE VI

Feed Composition 1		Feed Condition		BP Liq.
Total Condenser		Tower Pressure		25 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
nC ₄	25.00000	New Method	190.474	
iC ₅	23.94206 L	Underwood @ T _{Ave}	174.370	
nC ₅	1.06070 H	Underwood @ T _{Feed}	161.983	
Total	50.00276	Maxwell	156.832	
		Winn	171.338	

TABLE VII

Feed Composition 1		Feed Condition		BP Liq.
Total Condenser		Tower Pressure		25 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
nC ₄	25.00000	New Method	196.095	
iC ₅	24.11807 L	Underwood @ T _{Ave}	177.441	
nC ₅	0.88637 H	Underwood @ T _{Feed}	164.846	
Total	50.00445	Maxwell	159.656	
		Winn	174.166	

TABLE VIII

Feed Composition 1		Feed Condition		BP Liq.
Total Condenser		Tower Pressure		25 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
nC ₄	25.00000	New Method	195.539	
iC ₅	24.24573 L	Underwood @ T _{Ave}	179.727	
nC ₅	0.75336 H	Underwood @ T _{Feed}	166.987	
Total	49.99909	Maxwell	161.766	
		Winn	176.276	

TABLE IX

Feed Composition 2		Feed Condition		BP Liq.
Total Condenser		Tower Pressure		50 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
iC ₄	19.01668 L	New Method	104.048	
nC ₄	0.82294 H	Underwood @ T _{Ave}	101.587	
Total	19.83962	Underwood @ T _{Feed}	111.327	
		Maxwell	105.185	
		Winn	100.148	

TABLE X

Feed Composition 2		Feed Condition	BP Liq.
Total Condenser		Tower Pressure	50 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
iC ₄	19.49084 L	New Method	108.140
nC ₄	0.55977 H	Underwood @ T _{Ave}	106.049
Total	20.05061	Underwood @ T _{Feed}	116.077
		Maxwell	109.810
		Winn	104.800

TABLE XI

Feed Composition 2		Feed Condition	BP Liq.
Total Condenser		Tower Pressure	50 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
iC ₄	19.70647 L	New Method	110.807
nC ₄	0.31303 H	Underwood @ T _{Ave}	108.841
Total	20.01950	Underwood @ T _{Feed}	119.122
		Maxwell	112.806
		Winn	107.878

TABLE XII

Feed Composition 2		Feed Condition	BP Liq.
Total Condenser		Tower Pressure	50 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
iC ₄	20.00000	New Method	54.077
nC ₄	19.47923 L	Underwood @ T _{Ave}	47.750
iC ₅	0.25811 H	Underwood @ T _{Feed}	46.514
Total	39.73735	Maxwell	36.579
		Winn	40.629

TABLE XIII

Feed Composition 2		Feed Condition	BP Liq.
Total Condenser		Tower Pressure	50 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
iC ₄	20.00000	New Method	52.037
nC ₄	19.16387 L	Underwood @ T _{Ave}	46.455
iC ₅	0.44979 H	Underwood @ T _{Feed}	45.300
Total	39.61366	Maxwell	35.213
		Winn	39.400

TABLE XIV

Feed Composition 2		Feed Condition	BP Liq.
Total Condenser		Tower Pressure	50 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
iC ₄	20.00000	New Method	48.632
nC ₄	18.78370 L	Underwood @ T _{Ave}	44.142
iC ₅	0.89316 H	Underwood @ T _{Feed}	43.048
Total	39.67686	Maxwell	32.497
		Winn	37.132

TABLE XV

Feed Composition 2		Feed Condition	BP Liq.
Total Condenser		Tower Pressure	50 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
iC ₄	20.00000	New Method	184.963
nC ₄	20.00000	Underwood @ T _{Ave}	172.315
iC ₅	19.27975 L	Underwood @ T _{Feed}	150.834
nC ₅	1.11443 H	Maxwell	138.928
Total	60.39418	Winn	169.093

TABLE XVI

Feed Composition 2		Feed Condition	BP Liq.
Total Condenser		Tower Pressure	50 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
iC ₄	20.00000	New Method	190.311
nC ₄	20.00000	Underwood @ T _{Ave}	177.223
iC ₅	19.37217 L	Underwood @ T _{Feed}	155.440
nC ₅	0.78802 H	Maxwell	143.323
Total	60.16019	Winn	173.266

TABLE XVII

Feed Composition 2		Feed Condition	BP Liq.
Total Condenser		Tower Pressure	50 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
iC ₄	20.00000	New Method	192.975
nC ₄	20.00000	Underwood @ T _{Ave}	179.731
iC ₅	19.53892 L	Underwood @ T _{Feed}	157.589
nC ₅	0.71201 H	Maxwell	145.366
Total	60.25093	Winn	175.458

TABLE XVIII

Feed Composition 3		Feed Condition	BP Liq.
Total Condenser		Tower Pressure 100 psia	
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₃	10.00000	New Method	123.487
iC ₄	18.36573 L	Underwood @ T _{Ave}	115.742
nC ₄	1.61941 H	Underwood @ T _{Feed}	117.746
Total	29.98514	Maxwell	99.928
		Winn	113.043

TABLE XIX

Feed Composition 3		Feed Condition	BP Liq.
Total Condenser		Tower Pressure 100 psia	
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₃	10.00000	New Method	118.061
iC ₄	17.90530 L	Underwood @ T _{Ave}	109.892
nC ₄	1.94810 H	Underwood @ T _{Feed}	111.894
Total	29.85340	Maxwell	94.675
		Winn	107.199

TABLE XX

Feed Composition 3		Feed Condition	BP Liq.
Total Condenser		Tower Pressure 75 psia	
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₃	10.00000	New Method	46.075
iC ₄	20.00000	Underwood @ T _{Ave}	41.628
nC ₄	19.27919 L	Underwood @ T _{Feed}	37.301
iC ₅	1.10445 H	Maxwell	29.375
Total	50.38364	Winn	35.046

TABLE XXI

Feed Composition 3		Feed Condition	BP Liq.
Total Condenser		Tower Pressure 75 psia	
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₃	10.00000	New Method	46.850
iC ₄	20.00000	Underwood @ T _{Ave}	42.392
nC ₄	19.40874 L	Underwood @ T _{Feed}	38.008
iC ₅	0.96838 H	Maxwell	30.261
Total	50.37712	Winn	35.713

TABLE XXII

Feed Composition 4		Feed Condition	BP Liq.
Partial Condenser		Tower Pressure 150 psia	
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₂	5.00000	New Method	48.596
C ₃	18.66793 L	Underwood @ T _{Ave}	40.498
iC ₄	0.66297 H	Underwood @ T _{Feed}	40.234
Total	24.33090	Maxwell	35.276
		Winn	31.090

TABLE XXIII

Feed Composition 4		Feed Condition	BP Liq.
Partial Condenser		Tower Pressure 150 psia	
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₂	5.00000	New Method	47.682
C ₃	18.56424 L	Underwood @ T _{Ave}	39.866
iC ₄	0.77572 H	Underwood @ T _{Feed}	39.585
Total	24.33996	Maxwell	34.521
		Winn	30.377

TABLE XXIV

Feed Composition 4		Feed Condition	BP Liq.
Partial Condenser		Tower Pressure 100 psia	
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₂	5.00000	New Method	86.434
C ₃	20.00000	Underwood @ T _{Ave}	92.703
iC ₄	14.17280 L	Underwood @ T _{Feed}	77.526
nC ₄	0.75932 H	Maxwell	69.259
Total	39.93212	Winn	83.313

TABLE XXV

Feed Composition 4		Feed Condition	BP Liq.
Partial Condenser		Tower Pressure 100 psia	
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₂	5.00000	New Method	88.615
C ₃	20.00000	Underwood @ T _{Ave}	96.688
iC ₄	14.47215 L	Underwood @ T _{Feed}	80.987
nC ₄	0.52592 H	Maxwell	72.570
Total	39.99807	Winn	86.725

TABLE XXVI

Feed Composition 4		Feed Condition	BP Liq.
Partial Condenser		Tower Pressure	75 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₂	5.00000	New Method	33.506
C ₃	20.00000	Underwood @ T _{Ave}	34.352
iC ₄	15.00000	Underwood @ T _{Feed}	27.073
nC ₄	14.91426 L	Maxwell	20.695
iC ₅	0.36575 H	Winn	29.237
Total	55.28001		

TABLE XXVII

Feed Composition 4		Feed Condition	BP Liq.
Partial Condenser		Tower Pressure	75 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₂	5.00000	New Method	32.089
C ₃	20.00000	Underwood @ T _{Ave}	33.923
iC ₄	15.00000	Underwood @ T _{Feed}	26.546
nC ₄	14.98883 L	Maxwell	20.079
iC ₅	0.48801 H	Winn	28.927
Total	55.47684		

TABLE XXVIII

Feed Composition 5		Feed Condition	BP Liq.
Partial Condenser		Tower Pressure	300 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₁	1.00000	New Method	60.576
C ₂	5.00000	Underwood @ T _{Ave}	54.577
C ₃	22.88938 L	Underwood @ T _{Feed}	52.073
iC ₄	0.95873 H	Maxwell	40.405
Total	29.84811	Winn	39.614

TABLE XXIX

Feed Composition 5		Feed Condition	BP Liq.
Partial Condenser		Tower Pressure	300 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₁	1.00000	New Method	59.467
C ₂	5.00000	Underwood @ T _{Ave}	53.902
C ₃	22.84916 L	Underwood @ T _{Feed}	51.243
iC ₄	1.10660 H	Maxwell	39.559
Total	29.95577	Winn	38.705

TABLE XXX

Feed Composition 5		Feed Condition	BP Liq.
Partial Condenser		Tower Pressure	150 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₁	1.00000	New Method	47.745
C ₂	5.00000	Underwood @ T _{Ave}	50.472
C ₃	24.00000	Underwood @ T _{Feed}	31.641
iC ₄	15.00000	Maxwell	24.309
nC ₄	14.80045 L	Winn	33.863
iC ₅	0.22947 H		
Total	60.02992		

TABLE XXXI

Feed Composition 5		Feed Condition	BP Liq.
Partial Condenser		Tower Pressure	150 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₁	1.00000	New Method	51.093
C ₂	5.00000	Underwood @ T _{Ave}	51.622
C ₃	24.00000	Underwood @ T _{Feed}	32.612
iC ₄	15.00000	Maxwell	25.346
nC ₄	14.95079 L	Winn	34.603
iC ₅	0.08176 H		
Total	60.03255		

TABLE XXXII

Feed Composition 7		Feed Condition	BP Liq.
Partial Condenser		Tower Pressure	300 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₂	5.00000	New Method	46.743
C ₃	13.76581 L	Underwood @ T _{Ave}	34.516
iC ₄	1.84454 H	Underwood @ T _{Feed}	36.356
Total	20.61035	Maxwell	19.254
		Winn	23.164

TABLE XXXIII

Feed Composition 7		Feed Condition	BP Liq.
Partial Condenser		Tower Pressure	300 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₂	5.00000	New Method	34.644
C ₃	12.62757 L	Underwood @ T _{Ave}	23.427
iC ₄	2.89561 H	Underwood @ T _{Feed}	24.051
nC ₄	0.84097	Maxwell	10.906
Total	21.36415	Winn	14.170

TABLE XXXIV

Feed Composition 7		Feed Condition	BP Liq.
Partial Condenser		Tower Pressure 100 psia	
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₂	5.00000	New Method	28.447
C ₃	15.00000	Underwood @ T _{Ave}	32.498
iC ₄	10.00000	Underwood @ T _{Feed}	20.475
nC ₄	9.84604 L	Maxwell	13.005
iC ₅	0.32002 H	Winn	21.384
Total	40.16606		

TABLE XXXV

Feed Composition 7		Feed Condition	BP Liq.
Partial Condenser		Tower Pressure 100 psia	
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols	
C ₂	5.00000	New Method	29.188
C ₃	15.00000	Underwood @ T _{Ave}	33.299
iC ₄	10.00000	Underwood @ T _{Feed}	21.141
nC ₄	9.97511 L	Maxwell	13.769
iC ₅	0.21595 H	Winn	21.951
Total	40.19107		

TABLE XXXVI

Feed Composition 3		Feed Condition		BP Liq.
Total Condenser		Tower Pressure 150 psia		
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
C ₃	8.21174 L	New Method	35.915	
iC ₄	5.23096 H	Underwood @ T _{Ave}	24.419	
nC ₄	1.46132	Underwood @ T _{Feed}	28.018	
Total	14.90402	Maxwell	20.075	
		Winn	11.618	

TABLE XXXVII

Feed Composition 3		Feed Condition		BP Liq.
Total Condenser		Tower Pressure 150 psia		
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
C ₃	8.21174 L	New Method	32.526	
iC ₄	5.70542	Underwood @ T _{Ave}	25.113	
nC ₄	2.25254 H	Underwood @ T _{Feed}	28.491	
Total	16.16970	Maxwell		
		Winn		

TABLE XXXVIII

Feed Composition 3		Feed Condition		BP Liq.
Total Condenser		Tower Pressure 150 psia		
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
C ₃	7.89727 L	New Method	32.534	
iC ₄	5.26751 H	Underwood @ T _{Ave}	22.339	
nC ₄	1.88156	Underwood @ T _{Feed}	25.718	
Total	15.04634	Maxwell	18.034	
		Winn	10.407	

TABLE XXXIX

Feed Composition 3		Feed Condition		BP Liq.
Total Condenser		Tower Pressure 150 psia		
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
C ₃	7.89727 L	New Method	30.684	
iC ₄	5.57643	Underwood @ T _{Ave}	23.542	
nC ₄	2.31478 H	Underwood @ T _{Feed}	26.788	
Total	15.78648	Maxwell		
		Winn		

TABLE XL

Feed Composition 4		Feed Condition		BP Liq.
Partial Condenser		Tower Pressure 300 psia		
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
C ₂	3.19791 L	New Method	19.42188	
C ₃	4.38610 H	Underwood @ T _{Ave}	8.7608	
iC ₄	0.08184	Underwood @ T _{Feed}	12.939	
Total	7.66585	Maxwell	5.620	
		Winn	4.377	

TABLE XLI

Feed Composition 4		Feed Condition		BP Liq.
Partial Condenser		Tower Pressure 300 psia		
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
C ₂	3.19791 L	New Method	17.113	
C ₃	4.67504	Underwood @ T _{Ave}	11.151	
iC ₄	0.53009 H	Underwood @ T _{Feed}	14.605	
Total	8.40304	Maxwell		
		Winn		

TABLE XLII

Feed Composition 4		Feed Condition		BP Liq.
Partial Condenser		Tower Pressure 300 psia		
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
C ₂	3.62115 L	New Method	23.356	
C ₃	4.10628 H	Underwood @ T _{Ave}	12.471	
Total	7.72743	Underwood @ T _{Feed}	18.201	
		Maxwell	7.616	
		Winn	7.035	

TABLE XLIII

Feed Composition 4		Feed Condition		BP Liq.
Partial Condenser		Tower Pressure 300 psia		
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
C ₂	3.62115 L	New Method	20.575	
C ₃	5.16585	Underwood @ T _{Ave}	13.314	
iC ₄	0.37154 H	Underwood @ T _{Feed}	17.366	
Total	9.15854	Maxwell		
		Winn		

TABLE XLIV

Feed Composition 1		Feed Condition		BP Liq.
Total Condenser		Tower Pressure		25 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
nC ₄	23.89377 L	New Method	45.340	
iC ₅	1.65478 H	Underwood @ T _{Ave}	37.360	
Total	25.54855	Underwood @ T _{Feed}	39.349	
		Maxwell	36.584	
		Winn	27.003	

TABLE XLV

Feed Composition 1		Feed Condition		50% Liq.
Total Condenser		Tower Pressure		25 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
nC ₄	23.89377 L	New Method	85.785	
iC ₅	1.65478 H	Underwood @ T _{Ave}	66.758	
Total	25.54855	Underwood @ T _{Feed}	72.651	
		Maxwell	62.132	
		Winn	68.502	

TABLE XLVI

Feed Composition 1		Feed Condition		DP Vap.
Total Condenser		Tower Pressure		25 psia
Distillate Composition Total Mols		Minimum Reflux Rate Total Mols		
nC ₄	23.89377 L	New Method	139.687	
iC ₅	1.65478 H	Underwood @ T _{Ave}	107.856	
Total	25.54855	Underwood @ T _{Feed}	117.217	
		Maxwell	87.680	
		Winn	92.170	

CHAPTER VI

CONCLUSIONS

At the time of publication, Bachelor's method was probably the best general method of minimum reflux calculation that had been proposed. It was the only method available that included a product correction feature that was free of the assumptions of constant molal overflow and constant relative volatility. While requiring a large amount of hand calculation, the results are more accurate than any of the plate to plate calculations proposed earlier, since the products are correct for the feed condition and amounts of key components in each product.

J. Erbar's trial and error short cut method is somewhat easier to use by hand. Erbar's calculation procedure is also free of the classical assumptions usually made in minimum reflux calculations and predicts the distillate composition.

If the problem can tolerate the assumptions of constant molal overflow and constant relative volatility, or if the products are distributed, Underwood's second method of calculation is much shorter than either of the above mentioned methods. Underwood's method does contain a product prediction feature.

For feeds wherein the rigorous method predicted that all components except the keys were nondistributed, Underwood's method also predicted the same distribution. If one or more components other

other than the keys were distributed according to the rigorous method, Underwood's method made the same type of prediction. However, the amounts of the distributed non-key components were somewhat different.

The assumption of constant relative volatility is no longer present if the products are distributed and relative volatilities at the feed temperature are used. The liquid thus calculated is the liquid entering the feed zone. Heat balances can be made around the rectifying section and the condenser to determine the minimum reflux. Hence, constant molal overflow need no longer to be assumed.

The method presented in this thesis is rigorous and the minimum reflux may be found to any degree of accuracy desired. This method is not feasible for hand calculation, but is easily adaptable to medium size digital computers. This method could be used to great advantage in checking the reliability of short cut methods. This is suggested as a means of discovering just which short cut methods can be used for a fairly good estimate of the minimum reflux, under what conditions the short cut methods are most reliable, and what the degree of reliability might be for the various methods.

This use has been made in this thesis for bubble point feeds. It has shown that Underwood's second method is fairly reliable considering the assumptions inherent in it.

LIST OF NOMENCLATURE

- A - component ratio in equilibrium streams, $L/K_i V = l_i/v_i$
- B - bottoms, total mols
- D - distillate, total mols
- F - feed, total mols
- G - component ratio in passing streams above feed entry, $l_{\phi i}/v_{ri}$
- K - vapor-liquid equilibrium ratio, y_i/x_i
- L - liquid, total mols
- N - trial number
- Q - heat load, Btu
- S - component ratio in equilibrium streams, $VK_i/L = v_i/l_i$
- U - component ratio in passing streams below feed entry, $v_{\psi i}/l_{si}$
- V - vapor, total mols
- b - individual bottoms component, mols
- d - individual distillate component, mols
- f - individual feed component, mols
- g - relative passing stream ratio above feed entry
- l - individual liquid component, mols
- m - plates in stripping section of distillation column
- n - plates in rectifying section of distillation column
- q - feed condition specification
- r, s, t - terms in equations pertaining to Bachelor's method for flashed feeds
- u - relative passing stream ratio below feed entry

v - individual vapor component, moles
x - mol fraction of a component in the liquid phase
y - mol fraction of a component in the vapor phase
 ϕ_A - fraction of component not absorbed
 ϕ_S - fraction of component not stripped
 ϕ - tray above feed entry
 ψ - tray below feed entry
 θ - root in Underwood method
 α - relative volatility

Subscripts

b - bottoms
d - distillate
F - feed zone
f - feed
h - heavy key
i - individual component
l - light key
L - liquid
R - rectifying pinch zone
RZ - rectifying zone
r - stream entering rectifying section
S - stripping pinch zone
SZ - stripping zone
s - stream entering stripping section
V - vapor
 ϕ - tray above feed entry
 ψ - tray below feed entry

A SELECTED BIBLIOGRAPHY

1. Bachelor, J. B., "Multicomponent Distillation Calculation of Minimum Reflux," presented at the 48th Annual Meeting of the American Institute of Chemical Engineers, Detroit, Michigan (November, 1955).
2. Bachelor, J. B., Pet. Ref., 36, No. 6, 161 (1957).
3. Bailey, R. V. and J. Coates, Pet. Ref., 27, 141 (1948).
4. Brown, G. G. and D. E. Holcomb, Pet. Engr., 11, No. 8, 23 (1940).
5. Brown, G. G. and D. E. Holcomb, Pet. Engr., 11, No. 9, 27 (1940).
6. Brown, G. G. and H. F. Martin, Trans. Am. Inst. Chem. Engrs. 35, 679 (1939).
7. Brown, G. G. and Mott Souders, Jr., Trans. Am. Inst. Chem. Engrs. 30, 438 (1934).
8. Colburn, A. P., Trans. Am. Inst. Chem. Engrs., 37, 805 (1941).
9. Edmister, W. C., Notes distributed in Distillation Class, Oklahoma State University, 1959.
- ✓ 10. Edmister, W. C., A.I.Ch.E. Journal, 2, No. 2, 165 (1957).
- ✓ 11. Erbar, J. H. and R. N. Maddox, "Distillation Calculations on the IBM 650," presented at the 38th Annual Convention of the Natural Gasoline Association of America, Dallas, Texas (April, 1959).
12. Erbar, J. H. and R. N. Maddox, Oil and Gas Jour., 57, No. 18, 116 (1959).
13. Erbar, J. H. and R. N. Maddox, Ref. Engr., 31, No. 10, C-35 (1959).
14. Erbar, J. H., "Minimum Reflux Ratio Calculations," Unpublished paper (1960).
15. Fenske, M. R., Ind. Eng. Chem., 24, 482 (1932).
16. Gilliland, E. R., Ind. Eng. Chem., 32, 1101 (1940).
- ✓ 17. Gilliland, E. R. and C. E. Reed, Ind. Eng. Chem., 34, 551 (1942).
18. Jenny, F. J., Trans. Am. Inst. Chem. Engrs., 35, 635 (1939).

- ✓ 19. Kwauk, Mooson, A.I.Ch.E. Jour., 2, No. 2, 240 (1956).
20. Lewis, W. K. and G. L. Matheson, Ind. Eng. Chem., 24, 494 (1932).
21. Mayfield, F. D. and J. A. May, Pet. Ref., 25, No. 4, 141 (1946).
22. Maxwell, J. B., Data Book on Hydrocarbons. New York: D. Van Nostrand Company, Inc. (1955), pp. 231.
23. Murdock, P. G. and C. D. Holland, Chem. Eng. Prog., 48, No. 6, 287 (1952).
24. McCabe, W. L. and E. W. Thiele, Ind. Eng. Chem., 17, 605 (1925).
25. Ponchon, M., Tech. Moderne, 13, No. 20, 55 (1921).
26. Savarit, P., Arts et Metiers 75, 65, 142, 178, et al (1922).
27. Scheibel, E. G. and C. F. Montross, Ind. Eng. Chem., 38, 268 (1946).
- ✓ 28. Shiras, R. N., D. N. Hanser, and C. W. Gibson, Ind. Eng. Chem., 42, 871 (1950).
29. Thiele, E. W. and R. L. Geddes, Ind. Eng. Chem., 25, 289 (1933).
30. Underwood, A. J. V., Chem. Eng. Prog., 44, No. 8, 603 (1948).
31. Underwood, A. J. V., Trans. Inst. Chem. Engr. (London), 32, No. 274, 614 (1946).
32. Underwood, A. J. V., Trans. Inst. Chem. Engr. (London), 10, 112 (1932).
- ✓ 33. Winn, F. W., Pet. Ref., 37, No. 5, 216 (1958).
34. Winn, F. W., Private communication with Dr. R. N. Maddox, Oklahoma State University, (April, 1959).
35. _____ Natural Gasoline Supply Men's Association Engineering Data Book, 7th Edition, Tulsa, Oklahoma (1957).

APPENDIX A

OUTLINE OF BACHELOR'S METHOD OF CALCULATING MINIMUM REFLUX

Data necessary: Liquid and vapor enthalpy data

Vapor-liquid equilibria data

Feed composition, quantity and condition

Light and heavy key component distributions (mols)

An approximation of the distillate composition

1. Choose totals of key components in the distillate.
2. Determine feed condition, temperature and enthalpy.
3. Assume T_ϕ and $T_\psi = \pm 1/6(T_b + T_d) + 1/2(T_d + T_b)$.
4. Calculate g_i and $u_i = \alpha_i$ at assumed temperatures.
5. Calculate G_i and U_i .
6. Calculate d_i and $l_{\phi i}$.
7. Check assumed temperatures against calculated temperatures. If the two do not agree, recalculate, starting at 3 with the new temperatures. If the calculated and assumed temperatures agree within the limits set, proceed to 8.
8. Calculate $v_{\psi i}$ and b_i by material balance.
9. Calculate trays out from the feed in both directions. There are the trial number plus two trays in each section. These calculations are made as shown below for the rectifying zones, assuming trial number six for purposes of illustration.

Tray No.	Components Appearing in the Distillate	Components Not Appearing in the Distillate
φ	$v_{\varphi i} = (l_{\varphi+1 i} / d_i + 1) d_i$	$= l_{\varphi i} / (L/K_i V)_{\varphi}$
$\varphi+1$	$v_{\varphi+1 i} = (l_{\varphi+2 i} / d_i + 1) d_i$	$= v_{\varphi i} / (L/K_i V)_{\varphi+1}$
$\varphi+2$	$v_{\varphi+2 i} = (l_{\varphi+3 i} / d_i + 1) d_i$	$= v_{\varphi+1 i} / (L/K_i V)_{\varphi+2}$
$\varphi+3$	$v_{\varphi+3 i} = (l_{\varphi+4 i} / d_i + 1) d_i$	$= v_{\varphi+2 i} / (L/K_i V)_{\varphi+3}$
$\varphi+4$	$v_{\varphi+4 i} = (l_{\varphi+5 i} / d_i + 1) d_i$	$= v_{\varphi+3 i} / (L/K_i V)_{\varphi+4}$
$\varphi+5$	$v_{\varphi+5 i} = v_{\varphi+4 i}$	$= v_{\varphi+4 i} / (L/K_i V)_{\varphi+5}$
$\varphi+6$	$v_{\varphi+6 i} = v_{\varphi+5 i} = v_{\varphi+4 i}$	$= v_{\varphi+5 i} / (L/K_i V)_{\varphi+5}$
$\varphi+7$	$v_{\varphi+7 i} = v_{\varphi+6 i} = v_{\varphi+5 i} = v_{\varphi+4 i} = v_{Ri} = 0$	

10. The compositions of the liquid streams above the feed tray are not necessary since Bachelor recommends that the over-all rates and average molecular weights of the vapor streams and the distillate be used to determine the average molecular weights and rates of the liquid streams.

11. Dew points are calculated on all vapor streams to determine the plate temperatures.

12. Make a single liquid rate correction based on a heat balance around the tray. For example, for the first tray:

$$L'_{\varphi+1} = \frac{H_V V_{\varphi} + H_V V_f - H_L L_{\varphi} - H_V D}{H_V - H_{L_{\varphi+1}}}$$

This new value of the liquid entering tray φ plus the distillate is equal to the total vapor leaving tray φ . Since the

compositions are assumed to remain the same, no further correction of the total quantities of the passing streams above tray ϕ can be made. Similar calculations are made on the other trays above the feed.

13. Calculate the enthalpies of the vapor and liquid streams above the first tray using enthalpies based on average molecular weights.
14. The results of the last tray are assumed to be the conditions in the pinch zone, and the Souders-Brown rectifying pinch zone equation is used to correct the total stream quantities and temperature.
15. A series equation is used to correct the feed zone to product ratios. Bachelor recommends that this equation be initiated at the third correction from a distributed feed. This will allow it to be correct if the feed is distributed and gives a better second guess if there are nondistributed components. The ratios of $l_{\phi i}/d_i$ are now used to calculate the new values of g_i .
16. Steps 9 through 15 apply specifically to the rectifying section of the column. Similar calculations are made for the stripping section of the column and new values of u_i are found.
17. Calculations are now resumed at step 5. Of course, step 7 is no longer included. Bachelor suggests that the calculations be considered complete when there is no longer a significant change in G_i and U_i .
18. Heat and material balances are now made around the rectifying section and around the condenser to determine the minimum reflux rate.

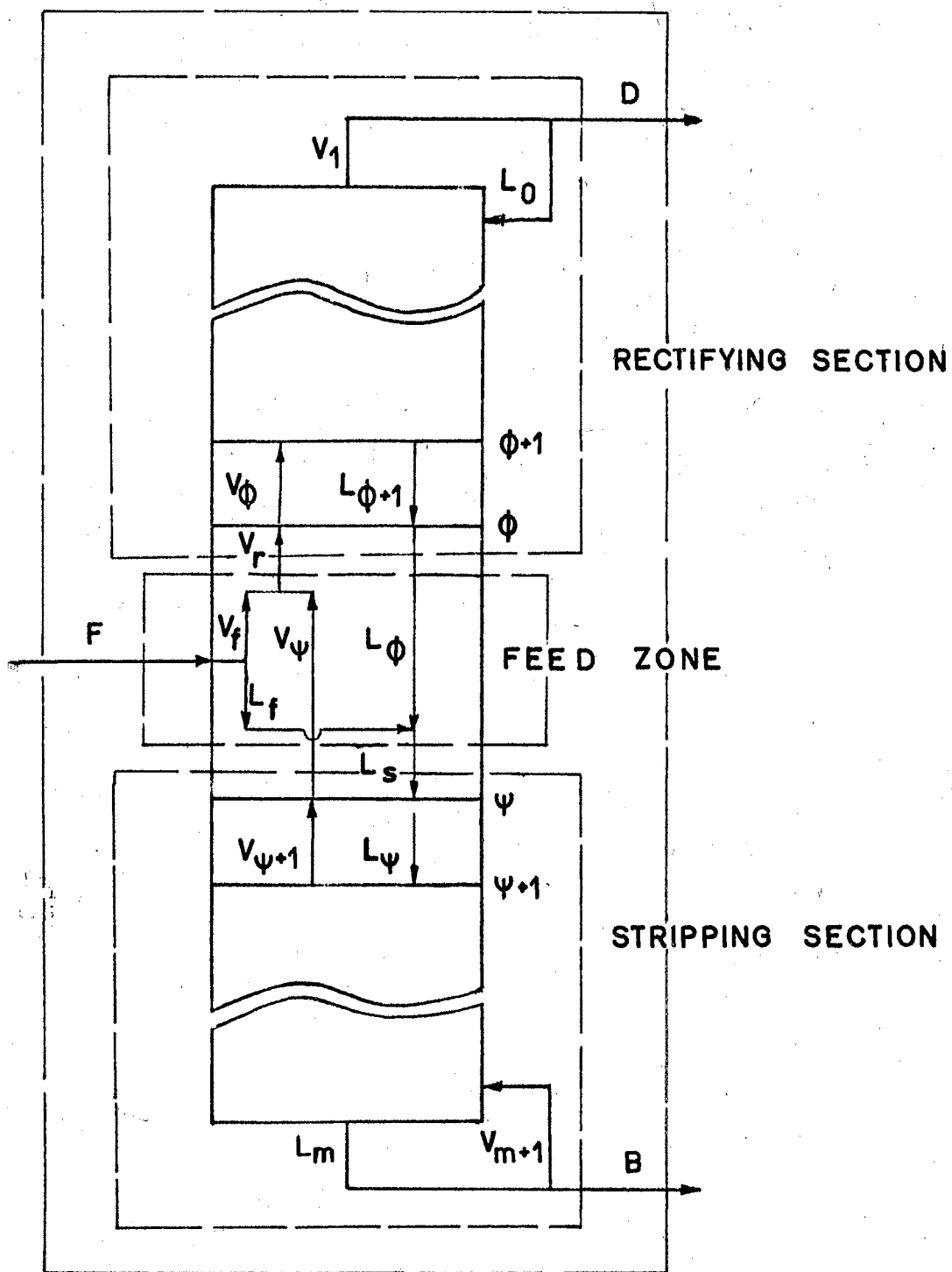


FIGURE 5

COLUMN AT MINIMUM REFLUX
BACHELOR'S METHOD

Derivation of Equations for Bachelor's Method
Pertaining to Bubble Point Feeds

All equations refer to Figure 5.

Basic equations for a bubble point feed:

$$V_f = 0$$

$$\therefore V_r = V_\psi$$

Material balance 'A' around feed

$$f_i + v_{\psi i} + l_{\phi i} = l_{si} + v_{ri}$$

$$(A) \quad f_i = l_{si} - l_{\phi i}$$

By definition

$$(1) \quad G_i = \frac{l_{\phi i}}{v_{ri}} \quad \text{and} \quad (2) \quad U_i = \frac{v_{\psi i}}{l_{si}}$$

rearranging,

$$(3) \quad l_{\phi i} = G_i v_{ri} \quad (4) \quad l_{si} = \frac{v_{\psi i}}{U_i}$$

$$(5) \quad v_{ri} = \frac{l_{\phi i}}{G_i} = v_{\psi i} = l_{si} U_i$$

$$(6) \quad l_{\phi i} = l_{si} U_i G_i \quad (7) \quad l_{si} = \frac{l_{\phi i}}{G_i U_i}$$

Derivation of:

$$l_{\phi i} = \frac{f_i U_i G_i}{1 - U_i G_i}$$

$$(A) \quad f_i = l_{si} - l_{\phi i}$$

Substituting Equation (7):

$$f_i = \frac{l_{\phi i}}{G_i U_i} - l_{\phi i}$$

$$f_i U_i G_i = l_{\phi i} - l_{\phi i} U_i G_i$$

$$f_i U_i G_i = (1 - U_i G_i) l_{\phi i}$$

therefore,
$$l_{\phi i} = \frac{f_i U_i G_i}{(1 - U_i G_i)} \quad (1a)$$

Derivation of:

$$l_{si} = \frac{f_i}{1 - U_i G_i}$$

(A)
$$f_i = l_{si} - l_{\phi i}$$

Substituting Equation (6):

$$f_i = l_{si} - l_{si} U_i G_i$$

$$f_i = (1 - U_i G_i) l_{si}$$

therefore,
$$l_{si} = \frac{f_i}{1 - U_i G_i} \quad (1b)$$

Derivation of:

$$v_{\psi i} = v_{ri} = \frac{f_i U_i}{1 - U_i G_i}$$

From (1b)
$$l_{si} = \frac{f_i}{1 - U_i G_i}$$

$$(4) \quad l_{si} = \frac{v_{\psi i}}{U_i} = \frac{v_{ri}}{U_i}$$

$$\frac{v_{\psi i}}{U_i} = \frac{v_{ri}}{U_i} = \frac{f_i}{1 - U_i G_i}$$

therefore,

$$v_{\psi i} = v_{ri} = \frac{f_i U_i}{1 - U_i G_i} \quad (1c)$$

Derivation of:

$$d_i = \frac{f_i U_i}{1 - U_i G_i} (1 - G_i)$$

Material balance 'B'

$$d_i + l_{\phi i} = v_{ri}$$

$$d_i = v_{ri} - l_{\phi i}$$

Substituting Equation (3):

$$d_i = v_{ri} - G_i v_{ri}$$

$$d_i = (1 - G_i) v_{ri}$$

from (1c)

$$v_{ri} = \frac{f_i U_i}{1 - U_i G_i}$$

therefore,

$$d_i = \frac{f_i U_i}{1 - U_i G_i} (1 - G_i) \quad (1d)$$

Derivation of:

$$b_i = \frac{f_i}{1 - U_i G_i} (1 - U_i)$$

Material balance 'C'

$$b_i + v_{\psi_i} = l_{si}$$

$$b_i = l_{si} - v_{\psi_i}$$

Substituting Equation (5):

$$b_i = l_{si} - l_{si} U_i$$

$$b_i = (1 - U_i) l_{si}$$

From Equation (1b)

$$l_{si} = \frac{f_i}{(1 - U_i G_i)}$$

therefore,

$$b_i = \frac{f_i}{1 - U_i G_i} (1 - U_i) \quad (1e)$$

Derivation of:

$$G_i = \frac{f_i U_i - d_i}{U_i b_i}$$

(1d)

$$d_i = \frac{f_i U_i (1 - G_i)}{1 - U_i b_i}$$

$$d_i - d_i U_i G_i = f_i U_i - f_i U_i G_i$$

$$f_i U_i G_i - d_i U_i G_i = f_i U_i - d_i$$

$$(f_i - d_i) U_i G_i = f_i U_i - d_i$$

Substituting material balance 'D',

$$f_i = b_i + d_i$$

$$b_i U_i G_i = f_i U_i - d_i$$

$$G_i = \frac{f_i U_i - d_i}{U_i b_i} \quad (1f)$$

Definitions of other basic relationships:

$$(8) \quad \varepsilon_i = \frac{l_{\phi i}}{v_{ri}} / \frac{l_{\phi i}}{v_{ri}} = \frac{G_h}{G_i}$$

$$(9) \quad u_i = \frac{v_i}{l_{si}} / \frac{v_{\psi h}}{l_{sh}} = \frac{U_i}{U_h}$$

$$(10) \quad G_1 = \frac{G_h}{\varepsilon_1}$$

$$(11) \quad U_1 = U_h u_1$$

Derivation of:

$$U_h = \frac{d_1 b_h (\varepsilon_1 / u_1) - d_h b_1}{f_1 b_h \varepsilon_1 - f_h b_1}$$

$$d_1 = \frac{f_1 U_1 (1 - G_1)}{1 - U_1 G_1}$$

rearranging,

$$d_1 - d_1 U_1 G_1 = f_1 U_1 - f_1 U_1 G_1$$

Substituting Equations (10) and (11),

$$d_1 - d_1 U_h u_1 \frac{G_h}{\varepsilon_1} = f_1 U_h u_1 - f_1 U_h u_1 \frac{G_h}{\varepsilon_1}$$

Substituting Equation (1f)

$$d_1 - \frac{d_1 U_h u_1 (f_h U_h - d_h)}{\varepsilon_1 b_h U_h} = f_1 U_h u_1 - \frac{f_1 U_h u_1 (f_h U_h - d_h)}{\varepsilon_1 b_h U_h}$$

rearranging,

$$d_1 + \frac{d_1 u_1 f_h U_h}{g_1 b_h} + \frac{d_1 u_1 d_h}{g_1 b_h} = f_1 U_h u_1 - \frac{f_1 u_1 f_h U_h}{g_1 b_h} + \frac{f_1 u_1 d_h}{g_1 b_h}$$

$$d_1 + \frac{d_1 u_1 d_h}{g_1 b_h} - \frac{f_1 u_1 d_h}{g_1 b_h} = f_1 U_h u_1 - \frac{f_1 u_1 f_h U_h}{g_1 b_h} + \frac{d_1 U_h u_1 f_h}{g_1 b_h}$$

$$d_1 - (f_1 - d_1) \frac{u_1 d_h}{g_1 b_h} = f_1 U_h u_1 - (f_1 - d_1) \frac{u_1 f_h U_h}{g_1 b_h}$$

$$g_1 b_h d_1 - (f_1 - d_1) u_1 d_h = f_1 U_h u_1 g_1 b_h - (f_1 - d_1) u_1 f_h U_h$$

Substituting material balance 'D'

$$f_i = b_i + d_i$$

$$\frac{g_1 b_h d_1 - b_1 u_1 d_h}{f_1 u_1 g_1 b_h - b_1 u_1 f_h} = U_h$$

Dividing through by u_1

$$U_h = \frac{d_1 b_h (g_1 / u_1) - d_h b_1}{f_1 b_h g_1 - f_h b_1} \quad (1g)$$

It should be noted that when solving problems using these equations, only Equations (1a), (1d), (1f), and (1g) need be used. Also, Equations (2a) and (2b) for a flash feed may be used in place of Equations (1a) and (1d) for a bubble point feed and (3a) and (3b) for a dew point feed since terms not applicable automatically drop out.

Bachelor's Method - Equations for Flash Feeds

$$(2a) \quad d_i = \frac{(v_{fi} + l_{fi} U_i)}{1 - U_i G_i} (1 - G_i)$$

$$(2b) \quad l_{\phi i} = \frac{v_{fi} G_i + l_{fi} G_i U_i}{1 - U_i U_i}$$

$$(2c) \quad G_h = \frac{(d_h - v_{fh}) - l_{fh} U_h}{(d_h - l_{fh}) U_h - v_{fh}}$$

$$(2d) \quad U_h = \frac{-s \pm \sqrt{s^2 - 4rt}}{2r}$$

$$\text{where: } r = l_{fh} \frac{U_1}{g_1} (d_1 - l_{fh}) - l_{fl} U_1 (d_h - l_{fh})$$

$$s = (d_1 - v_{fl})(d_h - l_{fh}) - (d_h - v_{fh})(d_1 - l_{fl}) \frac{U_1}{g_1} \\ + l_{fl} v_{fh} U_1 - \frac{l_{fh} v_{fl}}{g_1}$$

$$t = (d_h - v_{fh}) \frac{v_{fl}}{g_1} - (d_1 - v_{fl}) v_{fh}$$

Bachelor's Method - Equations for Dew Point Feeds

$$(3a) \quad d_i = \frac{f_i (1 - G_i)}{1 - U_i G_i}$$

$$(3b) \quad l_{\phi i} = \frac{f_i G_i}{1 - U_i G_i}$$

$$(3c) \quad G_h = \frac{b_h}{f_h - d_h U_h}$$

$$(3d) \quad U_h = \frac{f_h b_l - (f_l b_h / g_l)}{b_l d_h - b_h d_l (U_l / g_l)}$$

APPENDIX B

OUTLINE OF J. ERBAR'S MINIMUM REFLUX CALCULATION PROCEDURE

Data necessary: Vapor and liquid enthalpy data

Vapor-liquid equilibria data

Feed composition, rate and condition

Light and heavy key component quantities

An approximation of the distillate composition

1. If distributed products are suspected, assume T_R and T_S equal to the feed temperature. If nondistributed products are expected, one can assume $T_R = T_f - 1/6(T_d + T_b)$ and $T_S = T_f + 1/6(T_d + T_b)$.
2. Assume values for $(L/V)_R$ and $(V/L)_S$, using the criteria that $(L/K_h V)_R < 1$ and $(VK_l/L)_S < 1$. A good first approximation is that $(L/K_h V)_R$ and $(VK_h/L)_R = 0.95$. Calculate values for both the light and heavy keys in each pinch zone.
3. For the first trial, the pinch zones can be assumed to extend through the feed zone, therefore,

$$(L/K_i V)_R = (L/K_i V)_\phi \quad \text{and} \quad (VK_i/L)_S = (VK_i/L)$$
4. Since A_{R_h} , A_{R_l} , A_{ϕ_h} , and A_{ϕ_l} are known, A_{eRZ_l} and A_{eRZ_h} can be found using Figure 7. The same is true for the stripping section so S_{eSZ_l} and S_{eSZ_h} may also be found.
5. The values of ϕ_{ARZ} and ϕ_{SRZ} are now calculated for the light and heavy key components.

$$\phi_{ARZ_i} = 1 - A_{eRZ_i}$$

$$\phi_{SSZ_i} = 1 - S_{eSZ_i}$$

For the second through n^{th} trials, these values are compared with those of the preceding trial if the feed zone was in heat balance in step 16. If the values from successive trials agree within 1 to 2% and the feed zone heat balance is within tolerance, 1 to 5%, calculations may be completed in step 22.

6. The values of A_F for the light and heavy keys can be calculated from

$$(b/d)_i = A_{F_i} \frac{\phi_{SSZ_i}}{\phi_{ARZ_i}}$$

7. Since $A_{F_l} \neq \alpha_l A_{F_h}$, the feed zone temperature can be checked. If this temperature, T_F , is smaller than T_R , both $(L/V)_R$ and $(V/L)_S$ should be decreased. If T_F is greater than T_S , both ratios should be increased. The changes in these ratios must be made, remembering the limiting criteria mentioned in step 2. Calculations now revert to step 3.

If the feed zone temperature calculated is within range between T_R and T_S , calculations proceed to step 8.

8. Since T_F is known and A_{F_l} and A_{F_h} have been calculated, $(L/V)_F$ can be computed from the definition,

$$A_{F_i} = (L/K_i V)_F$$

9. Values of A_{F_i} , ϕ_{ARZ_i} and ϕ_{SSZ_i} are calculated for the remaining components.
10. Using the data calculated in step 9, the product distributions are calculated using Equation 7. Nondistributed components are indicated by ratios of 0 or ∞ .

11. Using material balances, the compositions of the products are computed.

$$f_i = d_i + b_i \qquad \frac{f_i}{d_i} = 1 + \frac{b_i}{d_i}$$

$$d_i = \frac{f_i}{1 + (b/d)_i}$$

12. The composition of the liquid, l_F , leaving the feed zone is calculated by

$$l_{Fi} = \frac{b_i}{\phi_{SSZ_i}}$$

The vapor, v_F , is found using

$$v_{Fi} = \frac{d_i}{\phi_{ARZ_i}}$$

These equations are valid for all distributed components and for those nondistributed components appearing in the product from each section. For example, a feed stream contains five components; the lightest component appears only in the distillate; the next three heavier components are present in both products; and the heaviest component appears only in the bottoms. Then l_F can be calculated for the heaviest component and the three distributed components. The v_F equation above, applies also to the three distributed components and to the lightest component.

13. The nondistributed component quantities leaving the feed zone may be computed, applying the definition

$$A_{Fi} = (L/K_i V)_F = l_{Fi}/v_{Fi}.$$

A_F was calculated in step 9 and one of the feed zone quantities is known from step 12.

14. By material balance, calculate $v_{\psi i}$ and $l_{\phi i}$
15. The temperature and enthalpy of each stream entering and leaving the feed zone are calculated.
16. A heat balance is made around the feed zone. If the feed zone is in heat balance, calculations are continued but the values calculated in step 5 should be checked.

If the heat leaving the feed zone is greater than the heat entering, the total stream quantities in the rectifying section are adjusted. If the heat entering the feed zone is greater than the heat leaving leaving the feed zone, the total stream quantities are adjusted in the stripping section. In either case, component material balances are adjusted by holding the composition of the smaller stream constant in the affected section. This procedure eliminates the possibility of negative material balance quantities.

17. Plate calculations are made around plates ϕ and ψ to find new values for $(L/K)_{\phi}$ and $(V/L)_{\psi}$. T_{ϕ} and T_{ψ} were calculated in step 15.

If a negative material balance is encountered, constant molal overflow is assumed for this trial. The temperatures T_{ϕ} and T_{ψ} are modified to reduced cycling.

$$T_{\phi 2} = \frac{T_{\phi \text{ CALC}} + T_{\phi \text{ ASSM}}}{2}, \quad T_{\psi 2} = \frac{T_{\psi \text{ CALC}} + T_{\psi \text{ ASSM}}}{2}$$

For the next trial, $T_{\phi 3} = \frac{T_{\phi 3 \text{ CALC}} + T_{\phi 2}}{2}$

18. From the results of step 17, the values of $A_{\phi i}$ and $S_{\psi i}$ are calculated.

19. The pinch zone compositions are found by the Brown-Souders pinch zone equations.

$$vR_i = \frac{d_i}{1 - AR_i} \qquad lS_i = \frac{b_i}{1 - SS_i}$$

Carry out pinch zone tray calculations based on adjusted heat quantities. Here again, use smaller stream quantities and compositions and adjust larger.

20. The temperature of each pinch zone should be found by bubble or dew point calculation. The temperature thus found for each zone is averaged with that from the preceding trial to reduce oscillation in convergence.
21. New values of AR_i and SS_i can be calculated. Calculations are resumed at step 4. Step 7 is used simply to find the feed zone temperature, not for checking purposes.
22. Heat and material balances are made around the upper section of the column and condenser in the conventional manner to determine the heat load on the condenser and the minimum reflux.

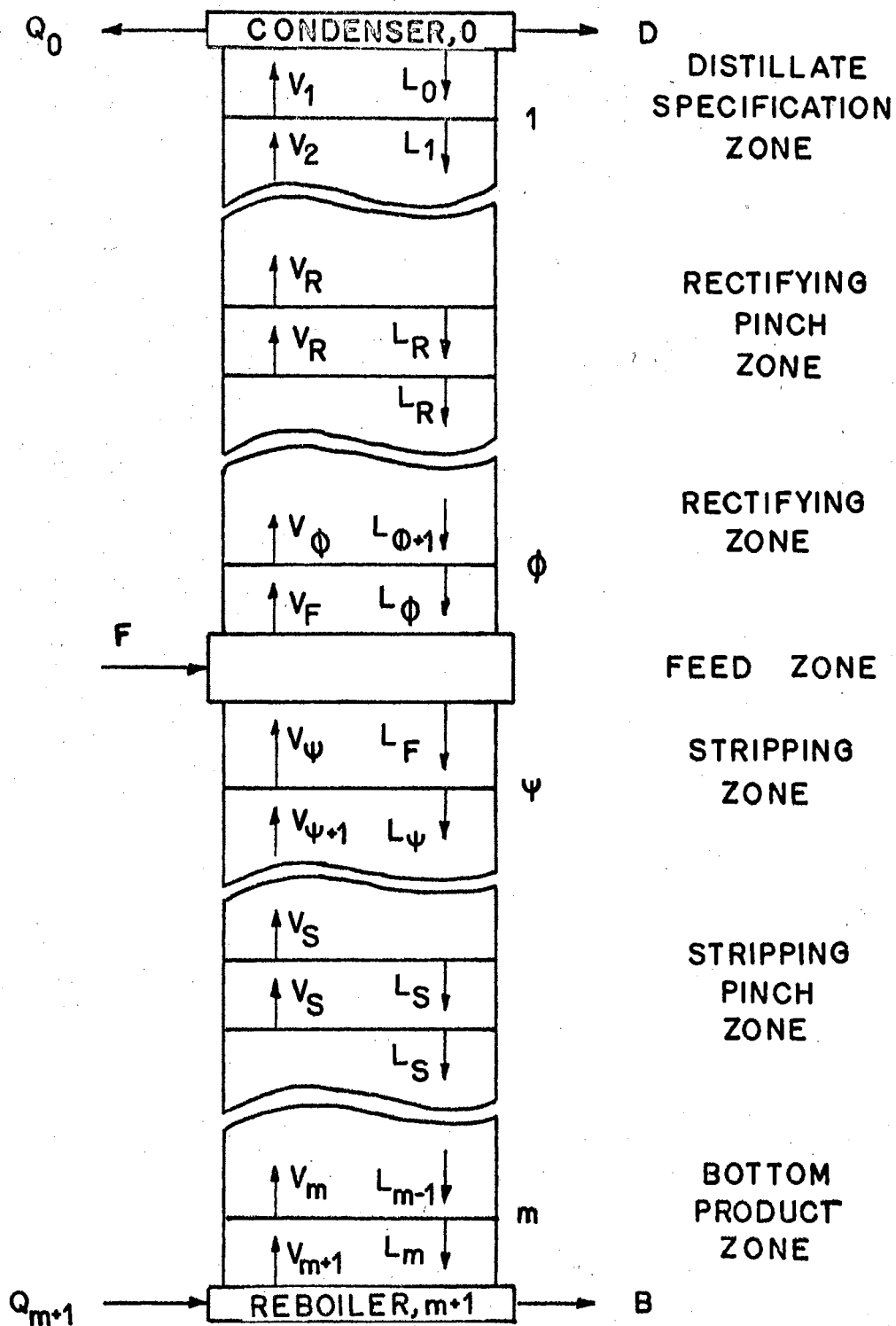


FIGURE 6

COLUMN AT MINIMUM REFLUX

J. ERBAR METHOD

J. Erbar's Method - Equations for Minimum Reflux Calculation

All equations in Erbar's method refer to Figure 6.

$$\phi_{ARZ_i} = 1 - A_{eRZ_i} \quad (1)$$

$$\phi_{SSZ_i} = 1 - S_{eSZ_i} \quad (2)$$

By definition,

$$A_{F_i} = (L/K_i V)_F = l_{F_i}/v_{F_i} \quad (3)$$

dividing through by b_i/d_i , and rearranging

$$\frac{b_i}{d_i} = A_{F_i} \frac{v_{F_i}/d_i}{l_{F_i}/b_i} \quad (4)$$

Since

$$v_{F_i}/d_i = \frac{1}{\phi_{ARZ_i}} \quad (5)$$

$$l_{F_i}/b_i = \frac{1}{\phi_{SSZ_i}} \quad (6)$$

then, substituting Equations (5) and (6) in Equation (4),

$$\frac{b_i}{d_i} = A_{F_i} \frac{\phi_{SSZ_i}}{\phi_{ARZ_i}} \quad (7)$$

For the derivation of these equations for general application, refer to Edmister (10). For the derivation of the equations and applications to the minimum reflux, refer to Erbar (14).

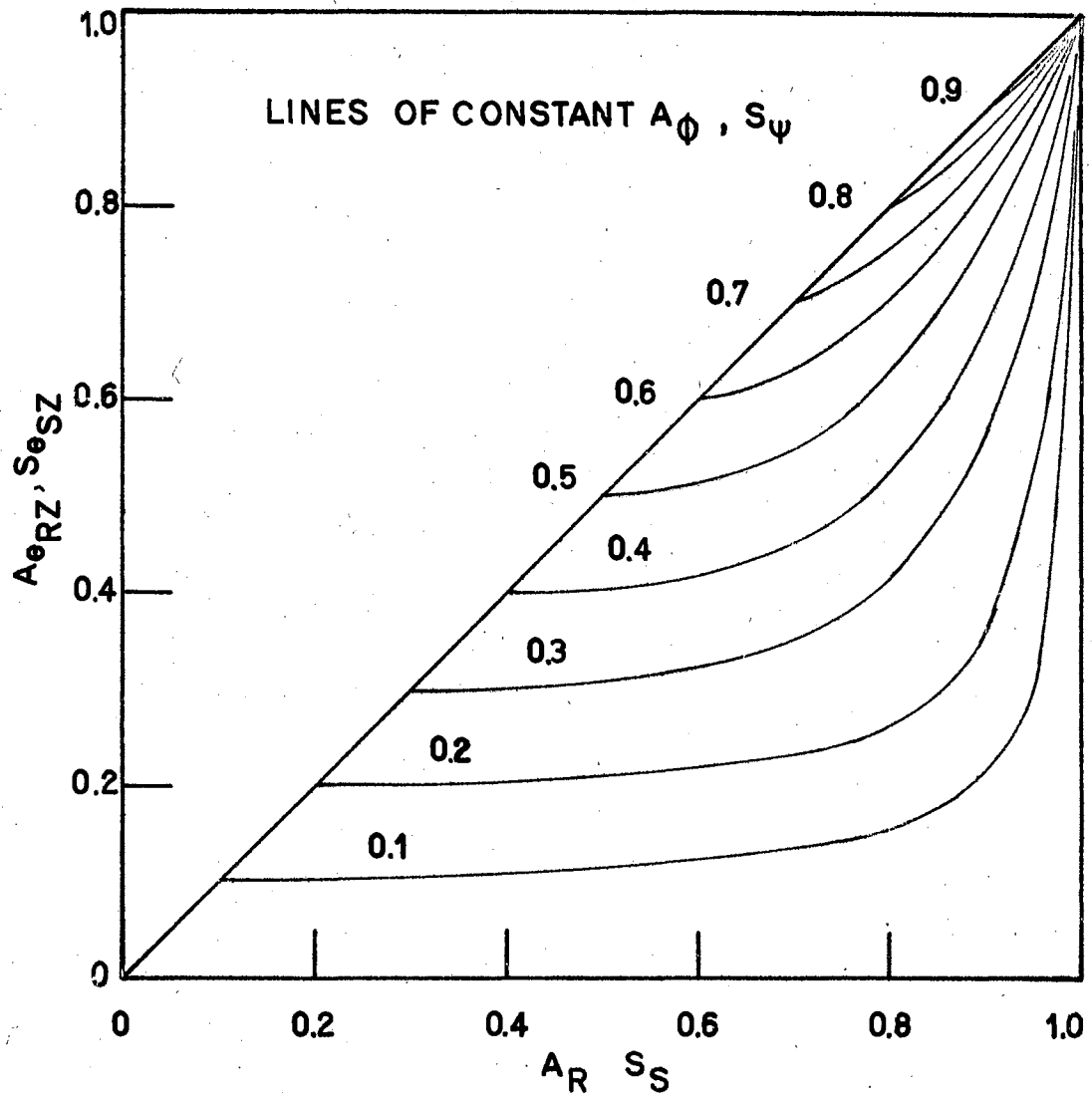


FIGURE 7

EFFECTIVE ABSORPTION, STRIPPING FACTORS

APPENDIX C

Reference to step 2, p. 29: In Bachelor's method, the recommendation is made that the temperature of the rectifying pinch zone be first assumed equal to the approximate distillate temperature plus $1/3$ of the "average" tower temperature. The temperature of the stripping pinch is assumed to be the bottoms temperature minus $1/3$ of the average tower temperature. This requires an approximation of the distillate and bottoms compositions in addition to unnecessary calculations on these approximate compositions. In addition, and of most importance, quite often this first approximation of T_R and T_S will result in temperatures both of which are above the actual temperature of the stripping pinch zone or below the temperature of the rectifying pinch zone. If this occurs, it becomes impossible to calculate realistic values of U_i or G_i (see Appendix A) and forces negative compositions in the distillate and/or feed zone. This is immediately obvious to an experienced engineer who is making hand calculations. It would not be obvious to those unfamiliar with the intricacies of distillation calculation. In addition, such conditions would require complex testing on the computer. For this reason, the method reported in this thesis makes the initial assumption that the pinch zone temperatures are equal to the feed temperatures.

Derivation of the General Series Equation
For Internal Stream — Product Ratios

For simplicity, "i" will be left off as a subscript. However, all "l"s, "v"s, "A"s, and "K"s indicate single components.

A material balance around some plate, $\phi + n$, in the rectifying section gives

$$l_{\phi+n} + v_{\phi+n} = l_{\phi+n+1} + v_{\phi+n-1} \quad (1)$$

Since, by definition, $K = y/x$, $y = v/V$ and $x = l/L$, then

$$K = \frac{v/V}{l/L}, \quad \frac{l}{v} = \frac{L}{KV}, \quad \text{and} \quad v = \frac{l}{(L/KV)}$$

By definition, $A = (L/KV)$

then $v = l/A$ (2)

Substituting Equation (2) into (1)

$$l_{\phi+n} + v_{\phi+n} = l_{\phi+n+1} + \frac{l_{\phi+n-1}}{A_{\phi+n-1}}$$

rearranging,

$$l_{\phi+n-1} = (l_{\phi+n} + v_{\phi+n} - l_{\phi+n+1})A_{\phi+n-1} \quad (3)$$

By combining a number of relationships similar to those of Equation (3) for the plates in the rectifying section of a column, the following general equation is obtained.

$$l_{\phi} = v_1 (A_{\phi} + A_{\phi+1}A_{\phi} + A_{\phi+2}A_{\phi+1}A_{\phi} + \dots + A_1A_2 \dots A_{\phi+n} \dots A_{\phi+1}A_{\phi}) \\ - l_0 (A_{\phi} + A_{\phi+1}A_{\phi} + A_{\phi+2}A_{\phi+1}A_{\phi} + \dots + A_2 \dots A_{\phi+n} \dots A_{\phi+1}A_{\phi}) \quad (4)$$

The above equation was first derived by Brown and Souders and has

been used in many distillation calculations (1,2,7,10,14).

Rearranging Equation (4)

$$l_{\varphi} = d(A_{\varphi} + A_{\varphi} A_{\varphi+1} + \dots + A_{\varphi} A_{\varphi+1} \dots A_{\varphi+n} \dots A_2) + v_1 (A_{\varphi} A_{\varphi+1} \dots A_{\varphi+2} \dots A_1) \quad (5)$$

Since, at the minimum reflux, there is a zone of infinite plates over which the compositions and total quantities of the stream remain constant, the "A"s will also remain constant. If the A for some component is less than 1.0 in this infinite zone, all terms above this zone become zero. Therefore, Equation (5) becomes at minimum reflux

$$l_{\varphi} = d(A_{\varphi} + A_{\varphi} A_{\varphi+1} + \dots + A_{\varphi} A_{\varphi+1} \dots A_{RP} + A_{\varphi} A_{\varphi+1} \dots A_R^2 + \dots + A_{\varphi} A_{\varphi+1} \dots A_R^{\infty})$$

where the term containing $A_R^{\infty} = 0$, and all preceding terms are in order of decreasing magnitude.

APPENDIX D

PERCENT DEVIATION OF APPROXIMATE METHODS
FROM RIGOROUS CALCULATION RESULTS

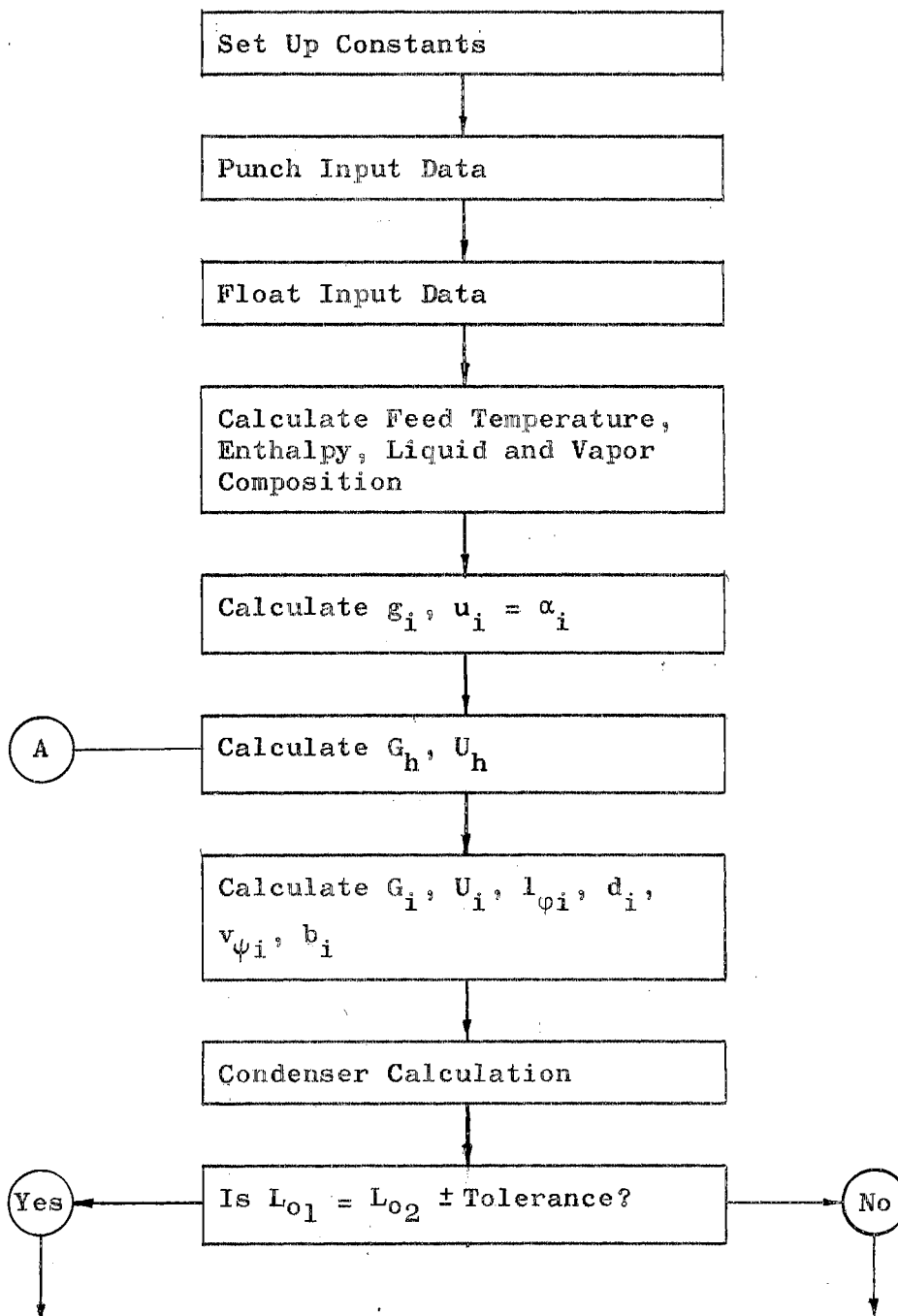
Table No.	Underwood T _{Ave}	Underwood T _{Feed}	Maxwell	Winn
II	-14.950	-14.736*	-18.882	-39.131
III	-14.742	-14.252*	-19.544	-40.362
IV	-17.599	-13.212*	-19.310	-40.442
V	- 8.494*	-15.008	-17.759	- 9.914
VI	- 8.454*	-14.957	-17.662	-10.046
VII	- 9.512*	-15.935	-18.582	-11.182
VIII	- 8.086*	-14.601	-17.271	- 9.851
IX	- 2.366	+ 6.995*	+ 1.092	- 3.749
X	- 2.933	+ 7.340*	+ 1.545	- 3.088
XI	- 1.774	+ 7.504*	- 1.804	- 2.642
XII	-11.701*	-13.986	-32.358	-24.869
XIII	-10.727*	-12.947	-32.331	-20.285
XIV	- 9.231*	-11.480	-33.176	-23.645
XV	- 6.838*	-18.452	-24.889	- 8.580
XVI	- 6.876*	-18.322	-24.680	- 8.956
XVII	- 6.863*	-18.337	-24.671	- 9.078
XVIII	- 5.402	- 4.875*	-19.154	- 8.491
XIX	- 6.919	- 5.224*	-19.808	- 9.200
XX	- 9.652*	-19.143	-36.245	-23.937
XXI	- 9.515*	-18.873	-35.409	-23.772
XXII	-16.664*	-17.207	-27.410	-36.024
XXIII	-16.392*	-16.981	-27.601	-36.292
XXIV	- 7.253	-10.307	-19.871	- 3.611
XXV	- 9.110	- 8.608	-18.107	- 2.133

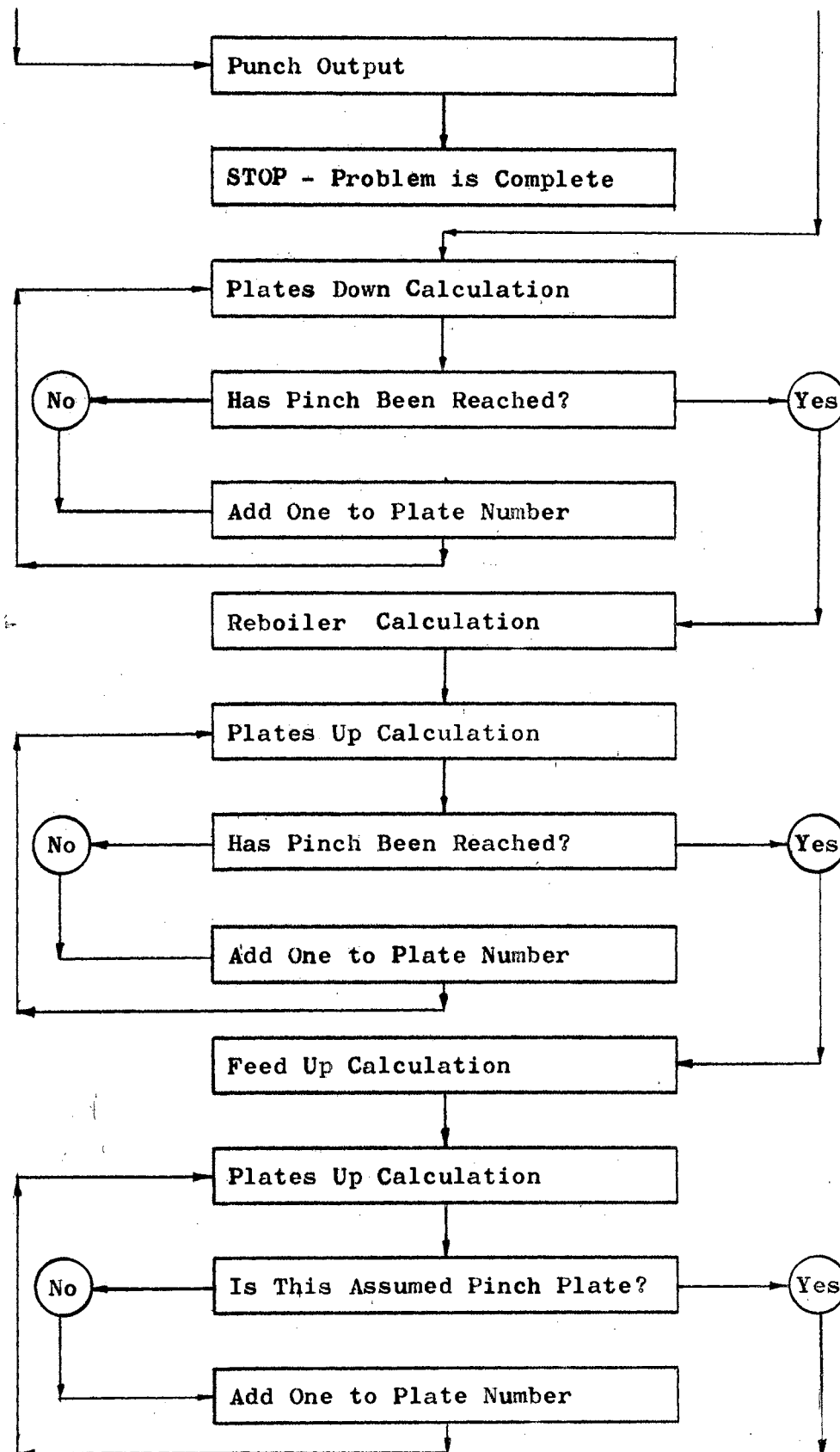
XXVI	+ 2.525*	-19.199	-38.234	-12.741
XXVII	+ 5.715*	-20.390	-37.027	- 9.854
XXVIII	- 9.903*	-14.037	-33.298	-34.604
XXIX	- 9.358*	-13.661	-33.492	-34.913
XXX	+ 5.712*	-33.730	-49.087	-29.076
XXXI	+ 1.035*	-36.171	-50.392	-32.247
XXXII	-26.158	-22.203*	-58.810	-50.445
XXXIII	-32.378	-30.577*	-68.520	-59.098
XXXIV	+14.240	-28.024	-54.283	-24.829
XXXV	+14.085	-27.570	-52.827	-24.795
XXXVI	-32.009	-21.988*	-44.104	-67.651
XXXVII	-22.791	-12.405*		
XXXVIII	-31.336	-20.950*	-44.569	-68.012
XXXIX	-23.276	-12.697*		
XL	-54.927	-33.380*	-71.012	-77.463
XLI	-34.843	-14.661*		
XLII	-46.605	-22.072*	-67.392	-69.880
XLIII	-35.291	-15.597*		
XLIV	-12.427	-12.120*	-13.370	-41.449
Max.Error	-54.927	-36.171	-71.012	-77.463
Min.Error	+ 1.035	- 4.875	+ 1.092	- 2.133
Ave.Error	±14.806	±16.993	±29.869	-26.258

* Indicates the deviation for the higher temperature of the Under-wood calculations. For the U* Max.Error = -33.380, Min.Error = +1.035, Ave.Error = ±11.900.

APPENDIX E

BLOCK DIAGRAM FOR RIGOROUS METHOD





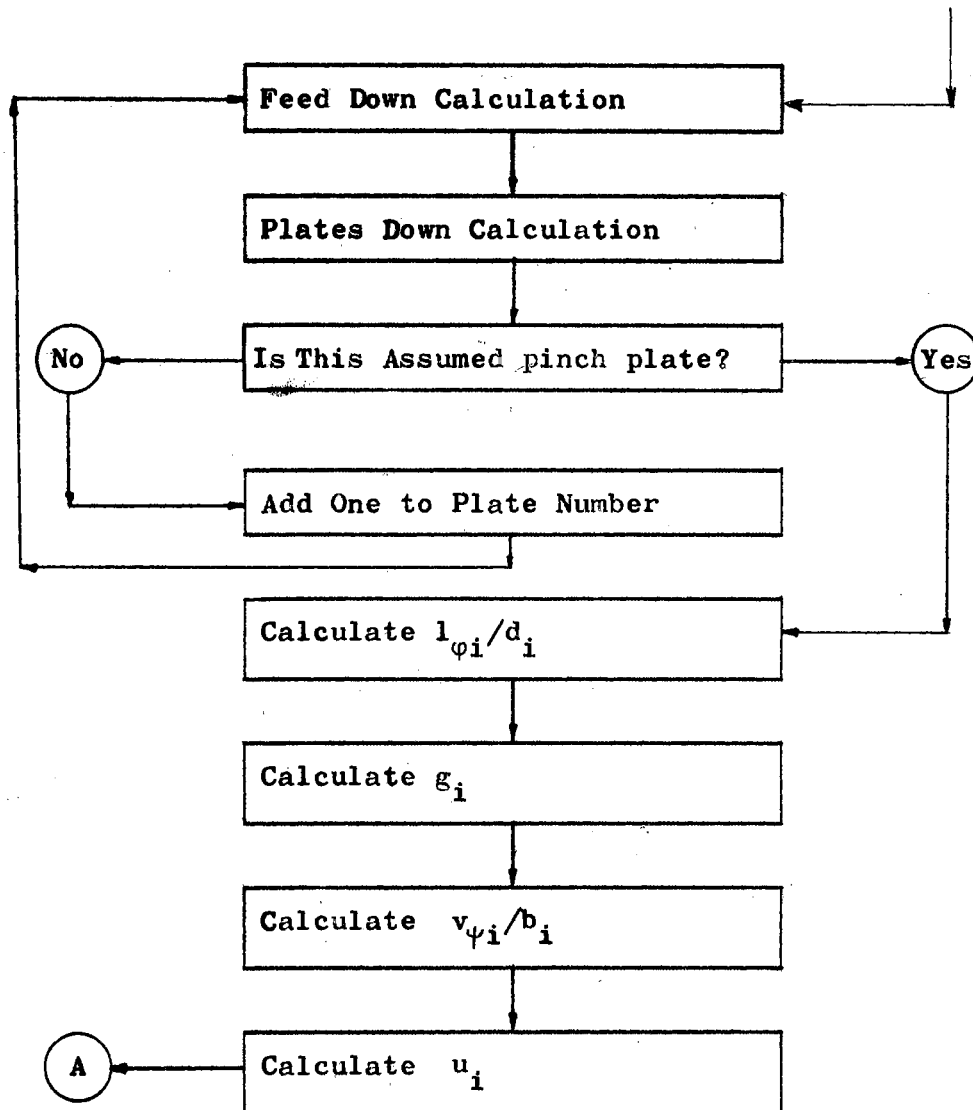
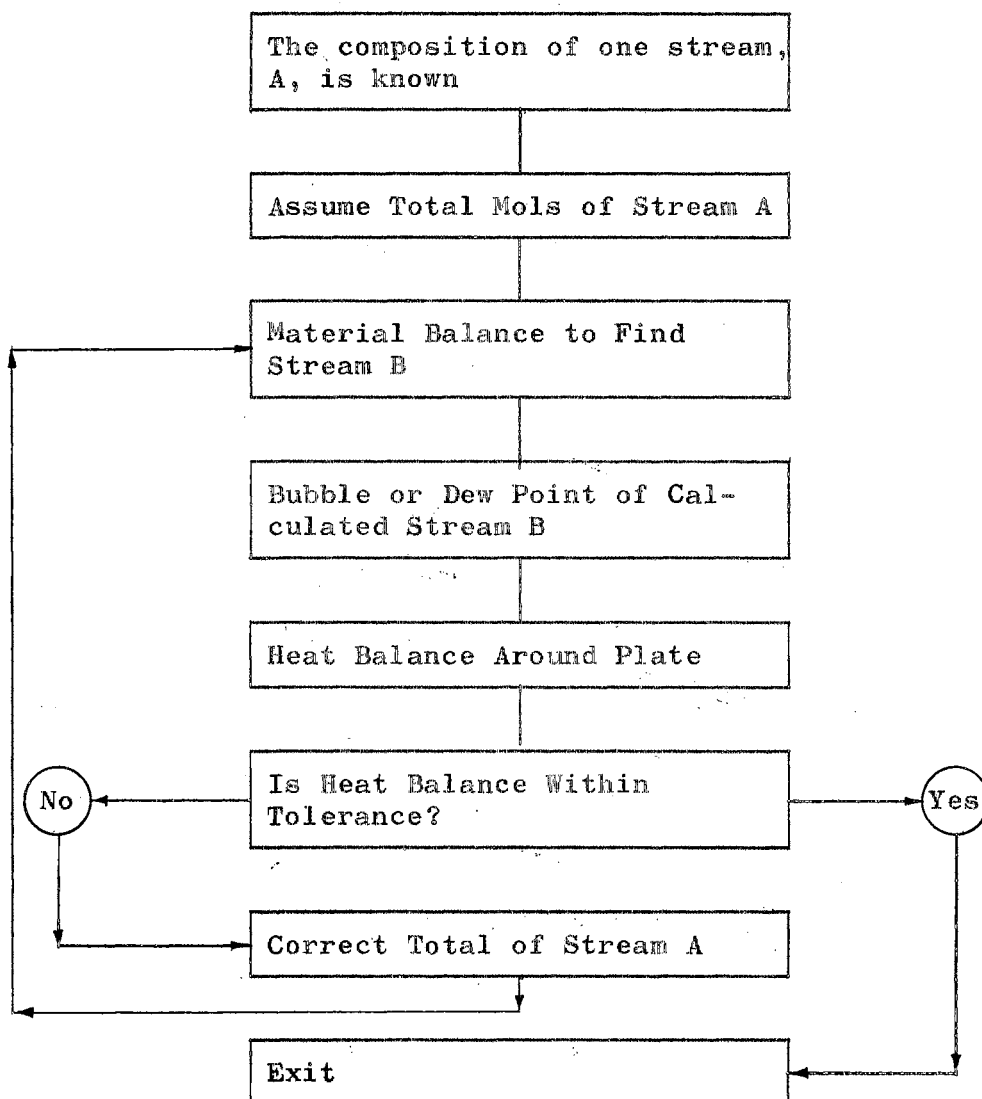


Plate Calculation Loop



VITA

Ruth Campbell Erbar

Candidate for the Degree of
Master of Science

Thesis: MINIMUM REFLUX IN MULTICOMPONENT DISTILLATION SYSTEMS

Major Field: Chemical Engineering

Biographical:

Personal Data: Born in Claremore, Oklahoma, January 19, 1936, the daughter of William David and Beatrice Johnson Campbell.

Education: Attended elementary and secondary school in Stillwater, Oklahoma, graduating from Eugene Field grade school, Stillwater Junior High School, and Stillwater High School; received the Bachelor of Science degree from Oklahoma State University in May, 1958; completed requirements for Master of Science degree in May, 1960. Membership in scholarly or professional societies includes Sigma Tau and the American Institute of Chemical Engineers.

Professional experience: Summer employment in the Planning Engineering Division of Esso Research and Engineering Company, Linden, New Jersey from June to September, 1957.