National Library of Canada
Bibliothèque nationale du Canada

Canadian Theses Service
Service des thèses canadiennes

Ottawa, Canada
K1A 0N4

NOTICE

The quality of this microform is heavily dependent upon the quality of the original thesis submitted for microfilming. Every effort has been made to ensure the highest quality of reproduction possible.

If pages are missing, contact the university which granted the degree.

Some pages may have indistinct print especially if the original pages were typed with a poor typewriter ribbon or if the university sent us an inferior photocopy.

Reproduction in full or in part of this microform is governed by the Canadian Copyright Act, R.S.C. 1970, c. C-30, and subsequent amendments.

AVIS

La qualité de cette microforme dépend grandement de la qualité de la thèse soumise au microfilmage. Nous avons tout fait pour assurer une qualité supérieure de reproduction.

S'il manque des pages, veuillez communiquer avec l'université qui a conféré le grade.

La qualité d'impression de certaines pages peut laisser à désirer, surtout si les pages originales ont été dactylographiées à l'aide d'un ruban usé ou si l'université nous a fait parvenir une photocopie de qualité inférieure.

La reproduction, même partielle, de cette microforme est soumise à la Loi canadienne sur le droit d'auteur, SRC 1970, c. C-30, et ses amendements subséquents.

[illegible]

Canada

UNIVERSITY OF ALBERTA

MINIMUM REFLUX FOR MULTIFEED DISTILLATION COLUMNS
WITH GENERALIZED UNDERWOOD METHOD

BY

FRANÇOIS BATAILLE ©

A THESIS
SUBMITTED TO THE FACULTY OF GRADUATE STUDIES AND RESEARCH
IN PARTIAL FULFILMENT OF THE REQUIREMENTS FOR THE DEGREE
OF MASTER OF SCIENCE

DEPARTMENT OF CHEMICAL ENGINEERING

EDMONTON, ALBERTA
FALL 1990

National Library of Canada
Bibliothèque nationale du Canada

Canadian Theses Service
Service des thèses canadiennes

Ottawa, Canada
K1A 0N4

ISBN 0-315-64967-4

UNIVERSITY OF ALBERTA

RELEASE FORM

NAME OF AUTHOR :	FRANÇOIS BATAILLE
TITLE OF THESIS :	MINIMUM REFLUX FOR MULTIFEED DISTILLATION COLUMNS WITH GENERALIZED UNDERWOOD METHOD
DEGREE :	MASTER OF SCIENCE
YEAR THIS DEGREE GRANTED :	1990

Permission is hereby granted to the UNIVERSITY OF ALBERTA LIBRARY to reproduce single copies of this thesis and to lend or sell such copies for private, scholarly or scientific research purposes only.

The author reserves other publication rights, and neither the thesis nor extensive extracts from it may be printed or otherwise reproduced without the author's written permission.

François Bataille

Permanent address :
3455 Dudemaine Street
Montréal, Québec
H3M 1R4
Canada

Date : Oct 5, 1990

UNIVERSITY OF ALBERTA

FACULTY OF GRADUATE STUDIES AND RESEARCH

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research for acceptance, a thesis entitled MINIMUM REFLUX FOR MULTIFEED DISTILLATION COLUMNS WITH GENERALIZED UNDERWOOD METHOD submitted by FRANÇOIS BATAILLE in partial fulfillment of the requirements for the degree of Master of Science.

K. Nandakumar, supervisor

P.J. Crickmore

P. J. Crickmore

A. Ambastha

Date : Oct 4, 90

ABSTRACT

A shortcut method for the calculation of the minimum reflux in multicomponent distillation is presented. This method extends the "Generalized Underwood Model" proposed by Nandakumar and Andres (1981a) to multiple feed columns. The basic assumptions of this model are constant relative volatilities and constant liquid and vapor enthalpies of the components. The "Generalized Underwood Model" differs from the original Underwood model by replacing the assumption of constant molal overflow with the assumption of constant enthalpies.

It is shown that this algorithm is correct within the limits of the assumptions by its comparison with a plate-by-plate simulation using the same equilibrium and enthalpy data. The accuracy of this algorithm is also verified by comparing it with a rigorous plate-by-plate simulation using the Peng-Robinson correlations. This analysis is completed by a comparison with Underwood's model.

In the case studies examined here, the comparisons made with the Peng-Robinson simulation indicate that Underwood's model tends to underestimate the minimum reflux ratio, whereas the Generalized Underwood model tends to overestimate it. They also indicate that Underwood model tends to predict more accurate values of the minimum reflux ratio for narrow-boiling mixtures, with a maximum error of 5.9%, compared with the Generalized Underwood model with a maximum error of 10%. In opposition, Generalized Underwood model tends to predict more accurate values for wide-boiling mixtures, with a maximum error of 8.3%, compared with Underwood model with a 22% error. It is also shown that, for the prediction of the top product, the two shortcut methods are in close agreement with the Peng-Robinson simulation.

RÉSUMÉ

Une méthode approximative servant au calcul du reflux minimum pour la distillation à plusieurs constituants est présentée. Cette méthode applique le « Modèle Underwood généralisé » proposé par Nandakumar et Andres (1981a) aux colonnes à alimentations multiples. Dans ce modèle, les volatilités relatives et les enthalpies en phases liquide et vapeur des constituants sont considérées comme constantes. Le « Modèle Underwood généralisé » se distingue du modèle développé à l'origine par Underwood en remplaçant l'approximation du trafic liquide-vapeur constant d'Underwood par l'approximation des enthalpies constantes.

Il est démontré que cette méthode est exacte à l'intérieur des limites des approximations utilisées. Ceci est établi en comparant cette méthode à une simulation plateau-par-plateau utilisant les mêmes propriétés thermodynamiques. La précision de la méthode est évaluée en la comparant à une simulation plateau-par-plateau utilisant les corrélations développées par Peng-Robinson. Cette méthode est aussi comparée à celle élaborée par Underwood.

Dans les exemples présentés, les comparaisons faites avec la simulation Peng-Robinson montrent que le modèle d'Underwood tend à sous-évaluer le rapport du reflux minimum, alors que le modèle Underwood généralisé tend à le sur-évaluer. Ces comparaisons indiquent aussi que le modèle d'Underwood tend à obtenir des valeurs plus précises du rapport du reflux minimum pour les mélanges à coupe étroite, avec une erreur maximale de 5,9%, en comparaison avec le modèle Underwood généralisé dont l'erreur maximale est de 10%. En contrepartie, le modèle Underwood généralisé tend à obtenir des valeurs plus précises pour les mélanges à coupe large, avec une erreur

maximale de 8,3%, en comparaison avec le modèle Underwood dont l'erreur maximale est de 22%. Les résultats montrent aussi que les valeurs obtenues par les deux modèles pour le produit de tête sont essentiellement équivalentes à celles obtenues avec la simulation Peng-Robinson.

ACKNOWLEDGMENTS

I wish to express my gratitude to my research supervisor Dr Krishnaswamy Nandakumar for his direction and encouragement.

I would like to thank the Department of Chemical Engineering of the University of Alberta for giving me the opportunity to pursue postgraduate studies.

I would like to thank Y. Ishii and F.D. Otto, as well as D.B. Robinson & Associates Ltd for the usage of their computer programs.

I also would like to thank the Natural Sciences and Engineering Research Council of Canada (NSERC) and the University of Alberta for their financial support.

Finally, I keep good memories of the friends I met in Alberta and will be happy to see them again in the future.

TABLE OF CONTENTS

APPENDICES

LIST OF TABLES

TABLE PAGE

LIST OF TABLES (continued)

LIST OF TABLES (continued)

LIST OF FIGURES

LIST OF FIGURES (continued)

LIST OF SYMBOLS

b : partial flowrate of a component in the bottom product (moles)

d : partial flowrate of a component in the distillate (moles)

D : distillate flowrate (moles)

f : partial flowrate of a component in the feed (moles)

F : feed flowrate (moles)

h : liquid enthalpy of a component (energy / mole)

H : vapor enthalpy of a component (energy / mole)

H_F : enthalpy of the feed per mole (energy / mole)

HF : total enthalpy of the feed (energy)

ΔHF : total enthalpy of the feed with reference to the saturated liquid state (Equation C.14) (energy)

HK : heavy key component

HDC : heaviest component that distributes

LDC : lightest component that distributes

l : partial liquid flowrate of a component (moles)

L : liquid flowrate (moles)

L_F : liquid portion of the feed (moles)

LK : light key component

m : number of plates

n : number of components

N : number of feeds

p : partial net upward flowrate of a component (Equation 3.2) (moles)

P : net upward flowrate (Equation 3.1) (moles)

R_m : minimum reflux ratio

LIST OF SYMBOLS (continued)

SK : split-key component
v : partial vapor flowrate of a component (moles)
V : vapor flowrate (moles)
V_F : vaporized portion of the feed (moles)
ΔV : change of vapor flowrate on the feed plate (moles)
x : liquid mole fraction of a component
y : vapor mole fraction of a component
z : mole fraction of a component (vapor and liquid mixed)

GREEK LETTERS :

α : relative volatility
Γ : quantity defined in Equation 4.4 (energy)
$\Delta\Gamma$: difference between values of Γ for two adjacent sections of a column (Equation 6.14)
λ : latent heat of vaporization of a component (Equation 4.1)
Λ_i : quantity defined in Equation 4.6 for section 'i' of a column (energy / mole of mixture)
ϕ : root for a section of a column
Φ : common root at the feed level or on the feed plate

SUBSCRIPTS :

f : related to the feed plate
F : related to the feed or the feed level
HK : related to the heavy key component
LK : related to the light key component
V_F : related to the vaporized portion of the feed

SUPERSCRIPTS :

∞ : indicates the pinch region

Introduction

There are two limiting cases in the operation of a multicomponent distillation column. These are the *minimum reflux* and *total reflux* limits. There is a relationship between the required number of trays and the reflux. For a specified separation, the required number of trays increases as the reflux is reduced. The first limiting case of this dependence is the total reflux condition. Since there is no product withdrawal the reflux is at its maximum. Under this condition we then determine the minimum number of plates necessary for the given fractionation.

The other limiting case is the minimum reflux condition. The basic hypothesis of this condition is the requirement of infinite number of trays. This is an important limit as in practice, the effective reflux ratio is 1.1 to 1.5 times the minimum reflux ratio. In the present work, we concentrate on this second limiting case.

Several authors have developed a number of methods to predict the minimum reflux. These methods may be divided into two categories : plate-by-plate algorithms and analytical solutions. The advantage of plate-by-plate algorithms is the possibility to use rigorous correlations for K-values and enthalpies. However, such a simulation may require a lot of computer time, especially for multiple feed columns. One must assume a large number of trays to reproduce the condition of the infinite number of trays.

On the other hand, analytical solutions may be shortcut methods requiring little computer time and not dependent upon the number of trays as the infinite plate limit is built into the development of the algorithms. These methods, however, are limited by the assumptions made for the equilibrium and enthalpy data.

The shortcut method developed in the present work is the adaptation of the "Generalized Underwood Model" presented by Nandakumar and Andres (1981a) to the treatment of Underwood's (1948) model for multiple feed columns by Barnés, Hanson and King (1972). The basic assumptions of Underwood's model are constant relative volatilities and constant molal overflow. The basic assumptions of the Generalized Underwood model are constant relative volatilities and constant liquid and vapor enthalpies of the components. The Generalized Underwood model has the same form but permits the relaxation of the assumption of constant molal overflow of the previous model.

We first analyse Underwood's model for single feed columns and derive the pertinent equations related to minimum reflux calculation. We then show how they are applied to multiple feed columns. The Generalized Underwood model is derived in the same fashion as Underwood's. Finally we describe the steps of the computer program developed in this work. This description is completed by a block diagram. This program computes the minimum reflux ratio for the fractionation of multicomponent mixtures with multiple feed columns using the Generalized Underwood model.

The analysis comprises two sections. We first verify the exactness of the Generalized Underwood model algorithm by comparing it with a plate-by-plate simulation using the same equilibrium and enthalpy data. Secondly, we evaluate the accuracy of the model by comparing it with a rigorous plate-by-plate simulation using the Peng-Robinson correlations. The Generalized Underwood model is also compared with the Underwood model to assess the effect of the constant latent heats of vaporization in the Generalized Underwood model.

Chapter 1
Literature Review

Through the years, minimum reflux calculation for multicomponent distillation has been the subject of numerous investigations. Different considerations, assumptions, and calculation procedures have been presented. Authors developed shortcut and rigorous methods. The evolution of computers allowed more rigorous calculations to be performed. However, shortcut methods are still useful depending on the precision required, as long as we realize that they have limitations.

The class of separation is very important for minimum reflux calculation since several methods use the properties of the pinch zones which are necessarily present because the number of plates is infinite. The distinction between class 1 and class 2 separations was discussed indirectly by Brown and Holcomb (1940a) (1940b) and Gilliland (1940) and made very precise by Shiras, Hanson and Gibson (1950). In summary, class 1 separation occurs when all components present in the feed appear in both the top and the bottom products. For the rectifying and the stripping sections, the pinch zones are located at the feed. Class 2 separation occurs when one or more components are present in only one product. In this case, the pinches occur away from the feed because additional plates are needed to exhaust the non-distributing components. These considerations are discussed further in Chapter 2. Classes of separation were introduced to facilitate the comprehension of the different approaches for the calculation of the minimum reflux presented in this chapter.

Fenske (1932) presented equations for the calculation of minimum reflux for multicomponent fractionation. The author simplified the problem by treating the separation of a multicomponent mixture like the separation of a binary mixture after identifying two components as key components. This method does not take into account the contribution of the other non-key components. Plate-by-plate calculation is based on a material balance and uses equations built with ratios of two components. In this application, the two components selected are the key components. Constant liquid and vapor flows are assumed. Raoult's law is assumed to apply with constant α. Since the equations are basically built for binary mixtures, it implies that the feed enters the column at the feed tray conditions. It also means that the pinch region is located around the feed. This is correct for binary mixtures, but for multicomponent mixtures it does not apply unless all components distribute. The author reduces any separation to class 1.

Lewis and Matheson (1932) presented a general plate-by-plate algorithm that can be used for minimum reflux calculation by assuming a very large number of plates ($m \to \infty$). The equations are written for one component from one plate to the next one and are based on equations for binary mixtures. We have to assume the top product and proceed with the calculations towards the feed. Equilibria follow Raoult's law and constant L and V are assumed. As for the previous method, this one really applies to class 1 separations only.

Underwood (1932) derived an analytical equation for minimum reflux calculation. The equation is written for two components and is applied to multicomponent mixtures by assuming the same minimum reflux as for the binary mixture of the key components. The method is based on a pinch being located around the feed plate. Only the two adjacent keys distribute meaning that the top product composition is known. Constant L, V, and α are assumed. This shortcut method has the advantage not to require the number of trays since the condition of an infinite number of trays ($m \to \infty$) is built into the analytical solution. This method really applies to class 1 separations.

Thiele and Geddes (1933) developed a general plate-by-plate method. In this iterative procedure, one must fix the number of plates, the reflux ratio, and the amount of top product. Also, the temperature profile must be guessed. While it is assumed that Raoult's law applies, the method has the advantage to allow variable L and V and to accept class 1 or class 2 separations. It was developed for columns with multiple feeds and side-stream strippers. Having to fix a number of plates large enough and to perform several runs to identify the minimum reflux are the major drawbacks of this method. It requires experience from the user.

Jenny (1939) presented a plate-by-plate method for minimum reflux. Basically, the top product must be known and the minimum reflux be guessed. This is a trial and error method. The reflux ratio is corrected, if necessary, and the calculation performed again. This method requires no assumption on L, V, nor α.

Brown and Holcomb (1940a) (1940b) presented an approximate method and a rigorous method for the calculation of minimum reflux. For the approximate method, they consider that the pinch region is always around the feed. Since the concentrations of the keys at the pinch correspond to those in the feed, a material balance is made around the top and the feed plate. Basically, they find the minimum reflux that reduces the ratio between the keys to the ratio existing in the liquid part of the feed. This is correct for class 1 separation, but for class 2, it predicts a higher minimum reflux ratio.

In the rigorous method, the pinch may be located away from the feed if we have a class 2 separation. This method is a plate-by-plate calculation and the minimum reflux is found by trial and error. The top composition and the number of plates are specified. The calculation starts at the top and moves towards the feed plate. However, since the pinch is away from the feed, concentrations of components not present in the top product have to be assumed so that the calculation can be carried to the feed. The same type of calculation is done from the bottom and the two results have to match. For someone who does not have much experience, this process may be lengthy.

Gilliland (1940) established two limiting cases for the minimum reflux. He pointed out the error made in previous work where equations for binary systems are applied to multicomponent systems.

The higher limit is found through the following reasoning. A mixture contains four components, A-B-C-D, and only A-B-C are present in the top product. Components A-B-C-D are said to be present in the pinch located around the feed meaning that the section of the column between the pinch and the top fractionates completely component D. This procedure predicts a higher minimum reflux because the separation is made harder than it is in reality. In fact, the plates between the feed and the pinch should fractionate D. This corresponds to previous works like the Underwood's (1932) and Brown and Holcomb's (1940a) approximate methods.

The lower limit follows these considerations. The feed contains components A-B-C-D, and the top product, A-B-C. Components A-B-C are said to be present in the pinch located around the feed. The pinch region should be away from the feed and it is as if the plates between the feed and the pinch were not required. These considerations make the fractionation of D look easier, therefore a lower minimum reflux is predicted.

Underwood (1945) presented a general analytical method for the fractionation of ternary mixtures. This method is based on material balance and the basic assumptions are constant L, V and α. Equations are of the n^{th} degree (here $n = 3$) and are satisfied by the roots ϕ. The equations are developed so that we can find the composition on any plate without plate-by-plate calculation.

Underwood (1948a) then applied the same equations to minimum reflux. It is assumed that only the key components distribute. The minimum reflux is specified and the corresponding roots ϕ are found for each section of the column. From this, the composition of the pinch regions can be determined.

Following the same idea, Underwood (1946b) extended his method to multicomponent mixtures. However, the roots Φ are found to be common to the rectifying and the stripping section at the feed level. The roots Φ can then be found first and the minimum reflux can be determined without guesses. Still, only the adjacent keys distribute.

Finally, Underwood (1946) (1948) presented his method for the fractional distillation of multicomponent mixtures as we know it. It is based on material balance only and the basic assumptions are constant L, V, and α. The feed condition and the amount of keys in the top product must be specified. Unlike the previous work, split-key components are permitted and any component may distribute. Roots Φ are found at the feed and L, V, the product composition as well as the reflux are then determined. The general method is applied to minimum reflux when $m \to \infty$ for the rectifying and the stripping sections. The simplified equations form a linear system of equations easily solved. Contrary to his first method (1932), this one is exact for class 2 separation (within the assumptions) and, since class 1 is a special case of class 2 separation, it is also valid for class 1.

Shiras, Hanson and Gibson (1950) presented three methods for calculating the minimum reflux. The first one is based on the early work of Underwood (1932) and the second one is an extension of the latest work of Underwood (1948). The third one is an adaptation of Thiele and Geddes' (1933) plate-by-plate method for minimum reflux. The latter is not a shortcut method and applies to both types of separations. Aside the equations, the important aspect brought to the reader's attention is the clear distinction made between class 1 and class 2 separations.

Acrivos and Amundson (1955) made use of eigen values for the calculation of minimum reflux with the assumptions of constant L, V, and α. Equations are derived for discrete or continuous mixtures. We notice that the equation obtained for discrete mixtures is the same as the one derived by Underwood (1948).

Bachelor (1957) presented a semi-rigorous method for the calculation of minimum reflux that utilizes approximations for the material and the heat balances. There are no restrictions on L, V, nor α. This scheme differs from others by the relaxation technique of convergence using successive mathematical models. The calculation is initiated at the feed. For class 1 separation, the pinch is located around the feed and the procedure is fairly straightforward. For class 2 separation, the pinch starts around the feed, but slowly it is moved away from it by the addition of plates until the minimum reflux is reached. Basically, class 1 is the first guess for class 2 separation. This method requires minimum dependance on the operator's experience.

Erbar and Maddox (1962) published a rigorous method to calculate the minimum reflux for multicomponent distillation. It is based on Lewis and Matheson's (1932) work and borrows equations from other authors. In this iterative procedure, it is first assumed that all components distribute and, then, the feed tray and the pinch regions compositions are computed. Plates are added until satisfactory results are obtained. For every iteration, each plate is in complete material and heat balance. The iterations stop when the reflux does not change as plates are added. This method does not apply to subcooled nor overheated feeds.

McDonough and Holland (1962a) presented a plate-by-plate method which is a combination of Thiele and Geddes' (1933) scheme and the θ-method of convergence developed by Holland. The top product and the reflux ratio are specified. The temperature profile and the ratios L/V on the plates are assumed to start the iterations. Material and equilibrium relationships are applied between the two pinch regions. The convergence method is then used to obtain the composition and the temperature on each plate. Following this, L and V are calculated from enthalpy balance. Iterations stop when the temperature profile is stable. As with Bachelor's (1957) method, plates may be added to satisfy the minimum reflux conditions. In a companion paper, McDonough and Holland (1962b) extend the method to columns with any number of feeds and side-streams.

Petlyuk, Avet'yan and Platonov (1966) based their work on Underwood's (1948) equations. The idea is to find the limiting cases. The reflux is specified and graphics are built. Minimum reflux condition is one of the limiting cases of a distillation process.

Sugie and Lu (1970) extended Acrivos and Amundson's (1955) work to columns with one feed and any number of side-cut streams. They find that the side-cuts do not influence the number of pinch regions because they have no effect on the characteristic roots. The calculation is done on the basis that only the key components distribute. A balance is completed between the pinch regions and the iterative process stops when the concentrations match. They find that the pinch is located around the feed for class 1 separation and between the feed and the first side-cut stream for class 2 separation.

Barnés, Hanson and King (1972) extended the application of Underwood's (1948) equations to multiple feed columns.

Ramkrishna and Amundson (1973) derived Underwood's (1948) equations by using self-adjoint operators.

Lee (1974) developed a new approach for the calculation of minimum reflux. Unlike several plate-by-plate methods, the minimum reflux does not have to be assumed. It is obtained simultaneously with the composition of the top product by using quasilinearization. However, the number of trays between the pinch regions has to be specified. The system is built as a multipoint boundary value problem of a difference equation.

Chien (1978) designed a totally rigorous method for minimum reflux calculation. This plate-by-plate scheme is formulated for high speed computers and may use damping, if required. Again, the number of plates between the feed and the pinches must be known. Like other methods, class 1 calculation is performed to provide an initial guess for class 2 separations.

Cerda and Westerberg (1981) presented another shortcut method for the minimum reflux. Like Underwood's (1948) model, the assumptions are constant L, V, and α, but it applies to sharp separation of the key components only. Sharp separation means that $(d/f)_{LK} = 1$ and $(b/f)_{HK} = 1$. The minimum reflux and the recovery of the split-key components are guessed and verified after each iteration. This procedure tends to predict lower values of minimum reflux than Underwood's (1948) method.

Nandakumar and Andres (1981a) (1981b) extended Underwood's (1948) method by replacing the assumption of constant molal overflow by the assumption of constant liquid and vapor enthalpies of the components. This method is called the "Generalized Underwood Model". In the second part, they propose a new approach for minimum reflux calculation which is called "Shock Model". This rigorous method is based on a continuum model.

Glinos and Malone (1984) developed a method for minimum reflux which applies to saturated liquid feeds only. Basically the calculation is made for sharp split of the key components. Minimum reflux for a sloppy separation of the keys is then presented as a function of the minimum reflux for the sharp separation of the keys.

Tsuo, Yaws and Chang (1986) found an analytical method for minimum reflux calculation. It is valid for binary mixtures fractionated in columns with any number of side-streams. The effect of each side-stream is added one at a time and it is found that only the side-streams above the feed have an effect on the minimum reflux.

It is interesting to see in detail what previous authors have accomplished. Reviewing their work enables us to appreciate the different approaches. At the beginning, computers were not available and the authors had to make assumptions to simplify the calculations. The most common ones were constant L, V, and α as well as reducing class 2 separations to class 1 separations. The different methods can be grouped in two types, plate-by-plate calculations and analytical solutions, each one having its own merit.

Plate-by-plate calculation allows more sophisticated equilibrium relationships and no restrictions on flowrates. However, the user must assume a number of plates large enough to simulate the minimum reflux condition of infinite number of plates $(m \rightarrow \infty)$ and not too large to render the calculation too laborious. Besides the fact that the process can be lengthy, if the number of plates is not adequate, the calculation has to be done again.

Analytical methods require more assumptions to keep the equations simple, however, the condition of infinite number of plates $(m \rightarrow \infty)$ is built-in. It is interesting to note that Nandakumar and Andres' (1981a) method is rigorous while including the infinite number of plates condition.

Nowadays, plate-by-plate calculations are made easier but shortcut methods remain a useful tool to lead us in the right direction prior to carrying more rigorous computation.

Chapter 2
Review of Basic Concepts

2.1 Pinch Region and Minimum Reflux

In any exchange process, such as heat transfer and fractionation, sections of the process where driving forces are small or simply non-existent may appear. In a co-current heat exchanger, two fluids enter at different temperatures and heat is transfered from the warmer to the colder fluid. The temperature gap reduces as the process takes place. If the heat exchanger is long enough, the two fluids reach the same temperature. At the inlet, the temperature gap, which is the driving force, is high. At the outlet, there is no driving force left. There is heat exchange as long as the temperatures are not the same. But since the transfer is very slow at the outlet, it is said to be negligible. At this point, the pinch region starts. It means that an infinite length of tubing is required to exchange heat. Every length added is less efficient than the previous one. Finally no interaction is observed.

In fractionation, the driving forces are the concentrations of the components in the liquid and vapor phases with respect to the thermodynamic equilibria. If a fractionation column is longer than required to perform a certain separation, some stages have the same or almost the same composition. No net material exchange is performed and the efficiency of the process in the region including these stages tends to zero. For a given stage, the liquid and vapor phases are in equilibrium, even before being in contact.

This portion of the fractionation process may be called under different names : pinch point, pinch region, point of infinitude, or region of infinitude. While all these terms describe the same phenomenon, they point out different aspects of it. Pinch point is well illustrated by the intersection of the equilibrium curve and the operating lines for a binary mixture. The point of intersection is the pinch point. Pinch region refers to the surroundings of the pinch point where the driving forces tend to zero. Point of infinitude and region of infinitude highlight the fact that, near the pinch point, an infinite number of plates is required to perform infinitesimal fractionation. The notion of region is probably better because the pinch is recognized when the concentrations do not change from one plate to the next.

In real life operation, pinch regions must be avoided because the efficiency is reduced. This situation generates unnecessary losses and shows overdesigned equipment, which can be costly.

Since minimum reflux condition implies an infinite number of plates, it is directly linked to the pinch region phenomenon. Many methods discussed in Chapter 1 use the properties of the pinch region to calculate the minimum reflux ratio. However, to use these properties properly, the location of the pinch region must be determined. This is discussed in the next section.

2.2 Class 1 and Class 2 Separations for Single Feed Columns

2.2.1 Distinction Between Class 1 and Class 2 Separations

Multicomponent distillation can be grouped into two classes. For class 1 separation, all components present in the feed are found in non negligible amounts in both the top and the bottom products. For class 2 separation one or more components are not found in either products. The class of separation indicates where the pinch regions are located : immediately around the feed or away from the feed. Let us illustrate the principle with a single feed column without side-cuts.

Figures 1, 2, and 3 show the fractionation of six component mixtures. The liquid mole fraction of each component is plotted as a function of the location in the column (plate number) where plate number 1 is at the top. The three graphs in Figures 1, 2, and 3 are built from plate-by-plate simulations. The precision of the liquid mole fractions is 0.001. The boundaries of the pinch regions are determined when the liquid mole fraction of no more than one component changes by a value of 0.001. For all three cases, the feed enters on plate 45. In Figure 1, all components distribute. This is class 1 separation. In Figure 2, components A and F do not appear in the bottom product and the top product, respectively. In Figure 3, components A and B are not present in the bottom product, and components E and F are not present in the top product. These two cases are class 2 separations. In all three figures, we notice regions where concentrations are constant for all components.

In Figure 2, we can identify the following six regions :

- Region 1 : between the top and the top pinch (plates 1 to 15), where some fractionation occurs.
- Region 2 : the top pinch itself (plates 15 to 25), where no fractionation occurs.
- Region 3 : between the top pinch and the feed (plates 25 to 45), where some fractionation occurs.
- Region 4 : between the feed and the bottom pinch (plates 45 to 55), where some fractionation occurs.
- Region 5 : the bottom pinch itself (plates 55 to 70), where no fractionation occurs.
- Region 6 : between the bottom pinch and the bottom (plates 70 to 90), where some fractionation occurs.

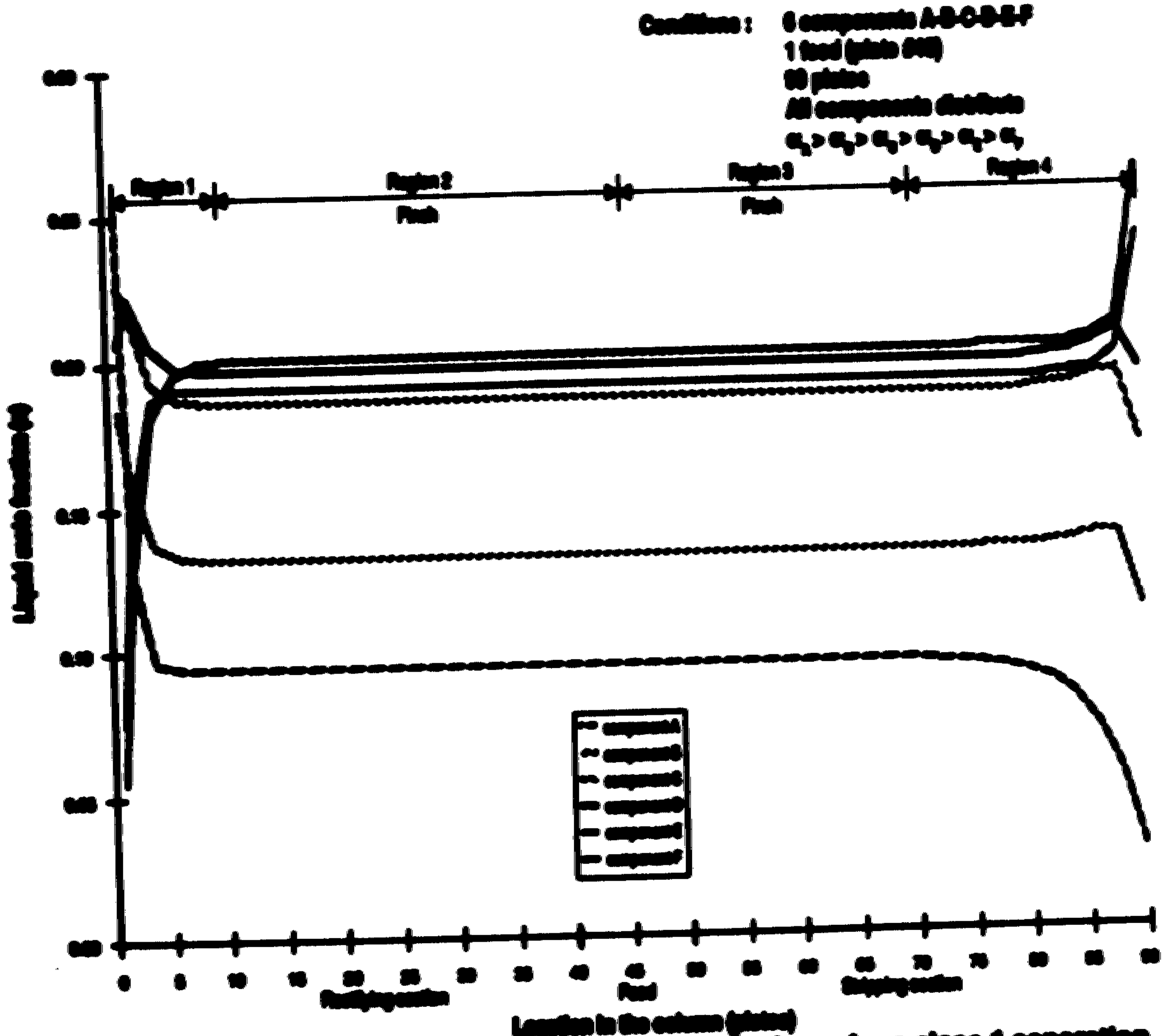

FIGURE 1. Concentration profiles of components through a column for a class 1 separation. (All 6 components distribute.)

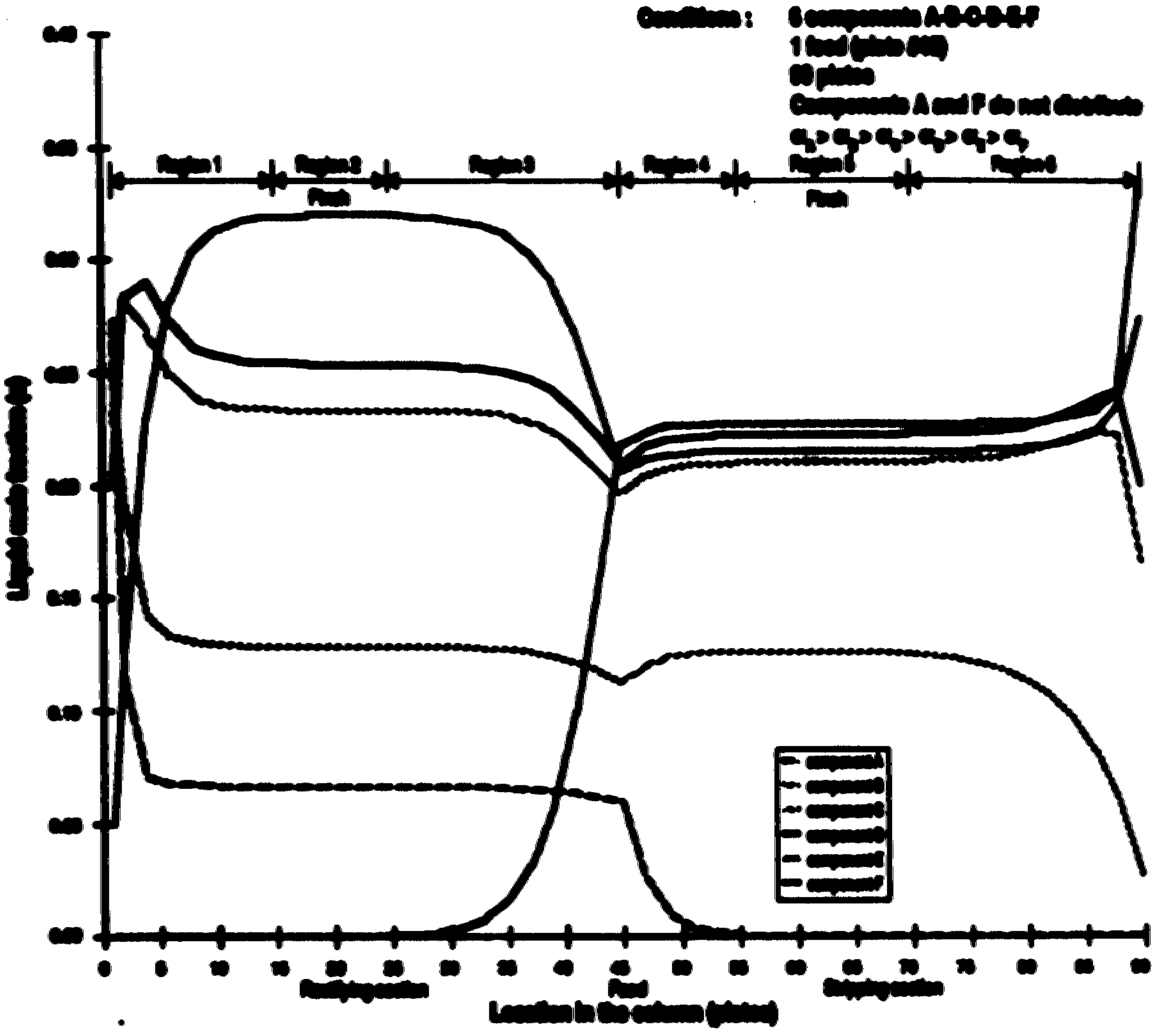

FIGURE 2. Concentration profiles of components through a column for a class 2 separation. (Components A and F do not distribute.)

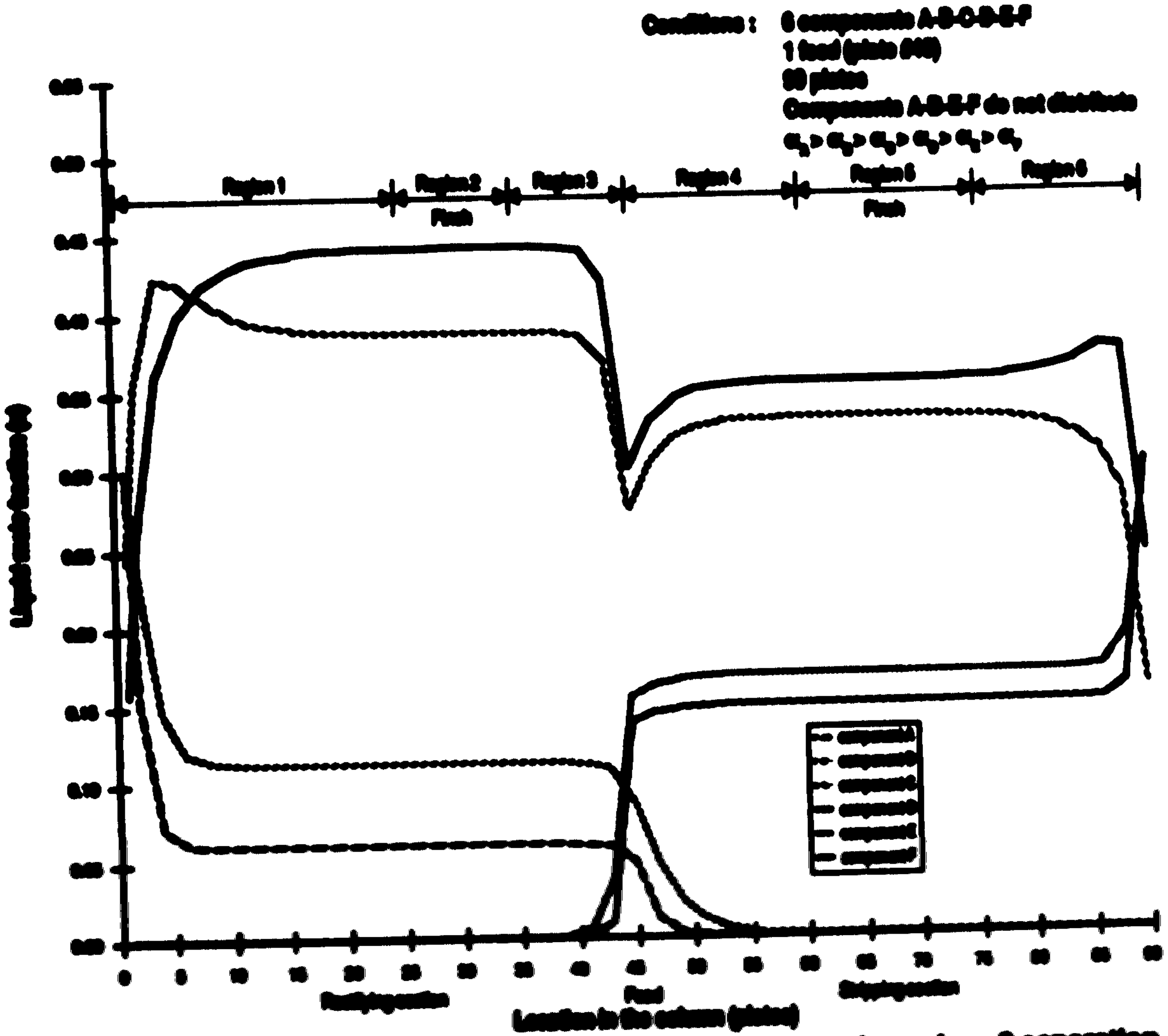

FIGURE 3. Concentration profiles of components through a column for a class 2 separation. (Components A-B-E-F do not distribute.)

In this case (Figure 2), starting from the feed, component A (most volatile) is exhausted in region 4 and its concentration reaches zero where the bottom pinch starts (plate 55). Component F (least volatile) is exhausted in region 3 and its concentration reaches zero where the top pinch starts (plate 25).

In Figure 3, we identify the same six regions but located at different plates :

- Region 1 : between the top and the top pinch (plates 1 to 25), where some fractionation occurs.
- Region 2 : the top pinch itself (plates 25 to 35), where no fractionation occurs.
- Region 3 : between the top pinch and the feed (plates 35 to 45), where some fractionation occurs.
- Region 4 : between the feed and the bottom pinch (plates 45 to 60), where some fractionation occurs.
- Region 5 : the bottom pinch itself (plates 60 to 75), where no fractionation occurs.
- Region 6 : between the bottom pinch and the bottom (plates 75 to 90), where some fractionation occurs.

In this case (Figure 3), components A and B are exhausted in region 4. Even though component A is removed between plates 50 and 55, the bottom pinch can only occur once component B is removed, at plate 60. Components E and F are exhausted in region 3. Component F is removed between plates 45 and 40 and component E is removed higher in the column between plates 40 and 35. The top pinch starts near plate 35. By definition a pinch is a region where no fractionation occurs, so it can only appear when all components present in only one product are exhausted in the regions mentioned previously.

In Figure 1, we identify only four regions :

- Region 1 : between the top and the top pinch (plates 1 to 10), where some fractionation occurs.
- Region 2 : the top pinch itself (plates 10 to 45) bounded by the feed at its lower end, where no fractionation occurs.
- Region 3 : the bottom pinch itself (plates 45 to 70) bounded by the feed at its upper end, where no fractionation occurs.
- Region 4 : between bottom pinch and the bottom (plates 70 to 90), where some fractionation occurs.

In this case (Figure 1), all components are present in both products. Since no component needs to be exhausted, the fractionating regions located between the feed and the pinches, unlike the two other cases, are not required. This is why the two pinches are adjacent to the feed and make one large pinch around the feed.

Cases 2 and 3 belong to class 2 separation and case 1 belongs to class 1 separation. Class 2 separation collapses to class 1 when all components distribute.

The class of separation indicates the location of the pinch regions. Failure to make the distinction between the two classes can lead to wrong calculations of the minimum reflux. For example, in class 1 separation, the feed enters the column at the feed tray condition and the pinch concentrations are readily known by a flash calculation of the feed. For class 2 separation, this is not true. When class 1 considerations are applied to class 2 separation, the result cannot be correct. On the other hand, using class 2 considerations for class 1 separation is correct, but renders the calculations much more complicated than necessary.

2.2.2 Schematics of Pinch Region Location

In relation with Figure 1, Figure 4 shows the different regions in the column with the shaded areas being the pinch regions. Since the feed enters the column at the feed plate conditions, the concentrations, the temperature and the pressure are the same. Only changes of liquid and vapor flowrates occur on the feed plates. By definition, binary fractionation belongs to class 1, see Figure 5. For multicomponent mixtures, it is less obvious. Class 1 separation may apply to multicomponent systems, but most likely class 2 will apply since the components have a broader range of volatilities.

Different cases of class 2 separation are presented in Figures 6 through 11. The schematic diagrams in Figures 6 and 7 correspond respectively to the concentration profiles shown in Figures 2 and 3. The pinch regions are shown away from the feed, leaving the exhausting regions between the feed and the pinches.

In Figure 8, all components appear in the top product and no exhausting region is required in the top section, this is why the top pinch is located right above the feed plate. Component A is not present in the bottom product and is exhausted in the region between the feed and the bottom pinch. Figure 9 shows a similar case, but components A and B do not distribute. This is represented by a bottom pinch region located further away from the feed. The latter two are hybrid cases between class 1 and class 2 separations. However, they are considered as class 2 cases. The same considerations apply to Figures 10 and 11 with the exception that components E and F do not distribute instead of A and B.

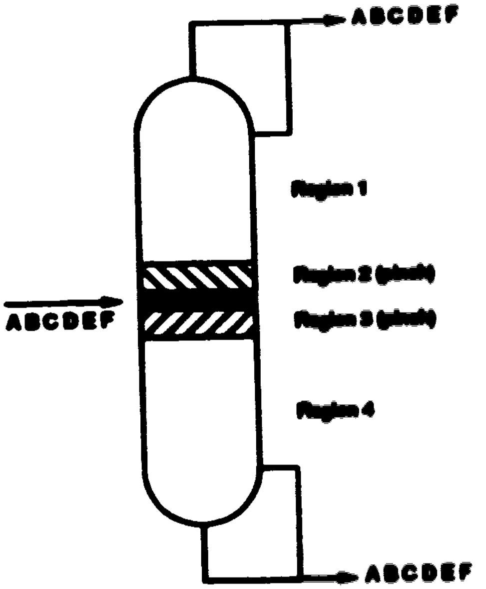

FIGURE 4. Pinch regions for class 1 separation of multicomponent mixture.

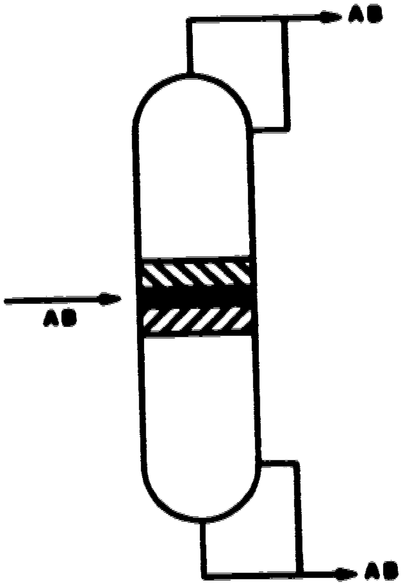

FIGURE 5. Pinch regions for binary separation.

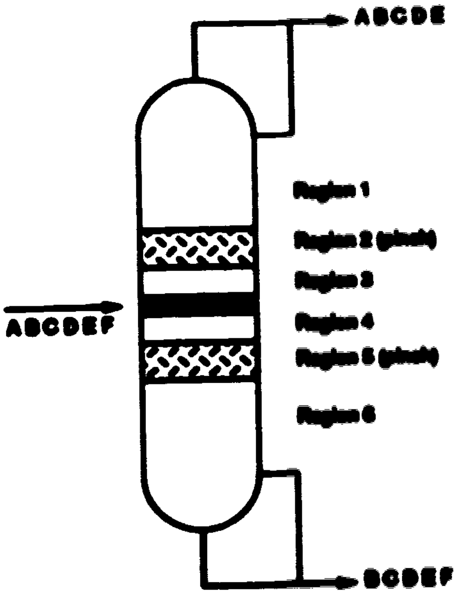

FIGURE 6. Pinch regions for class 2 separation. (Components A and F do not distribute.)

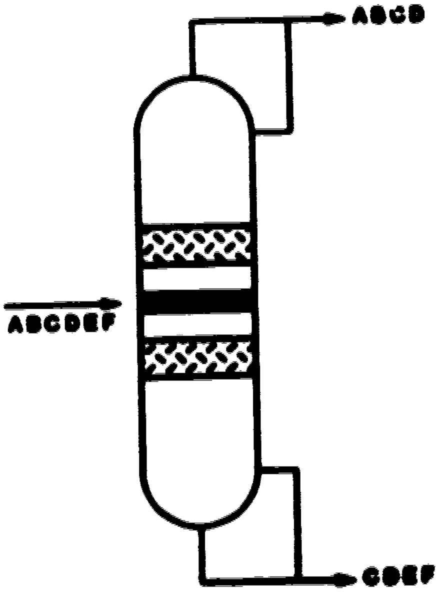

FIGURE 7. Pinch regions for class 2 separation. (Components A, B, E, F do not distribute.)

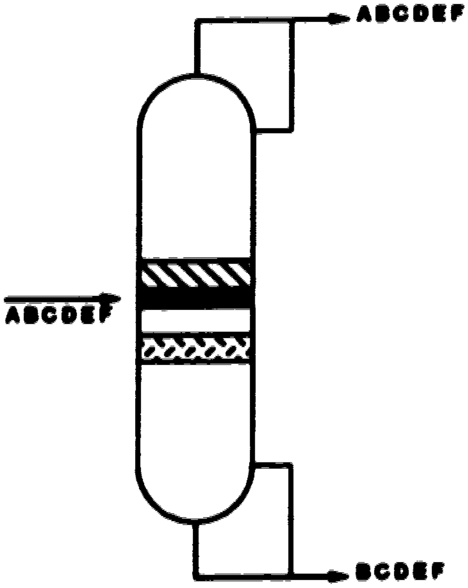

FIGURE 8. Pinch regions for class 2 separation. (Component A does not distribute.)

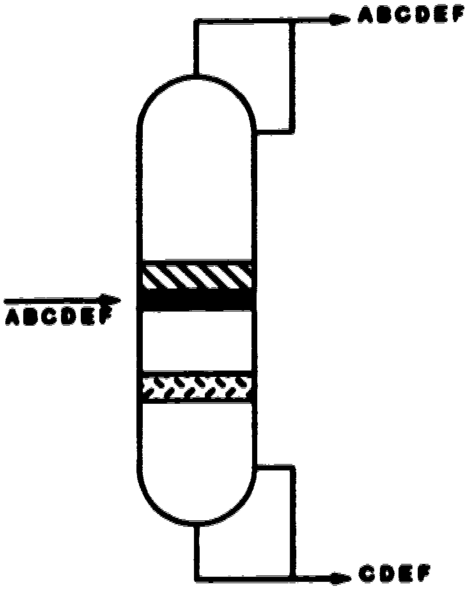

FIGURE 9. Pinch regions for class 2 separation. (Components A and B do not distribute.)

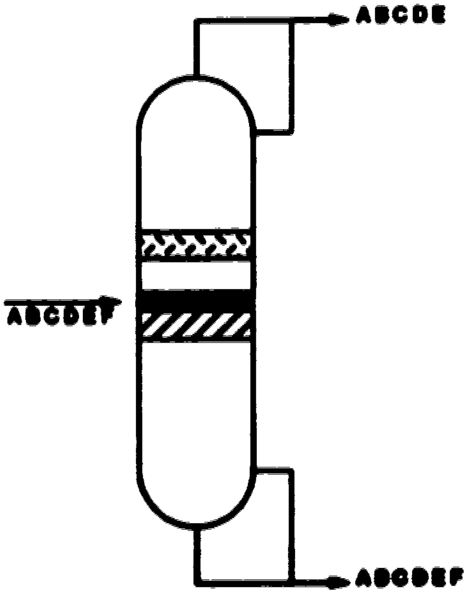

FIGURE 10. Pinch regions for class 2 separation. (Component F does not distribute.)

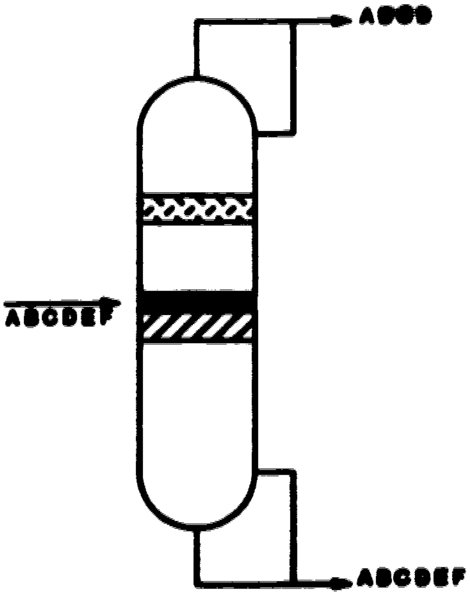

FIGURE 11. Pinch regions for class 2 separation. (Components E and F do not distribute.)

2.3 Pinch Regions for Multiple Feed Columns

The location of a pinch is the consequence of the type of separation. For single feed columns, a pinch around the feed indicates class 1 separation. With a two feed column, the upper pinch is right above the first feed and the lower pinch right below the second feed. The intermediate pinch may be anywhere between the two feeds. This is shown in Figure 12. The same thing is shown in Figure 13 for class 2 separations and for hybrid class 2 in Figure 14. It may also occur that no fractionation is performed on either side of the pinch in the intermediate section. This is shown in Figure 15 with the intermediate pinch located right above the feed plate.

In most cases, the intermediate pinch is located away from the feeds. Unlike pinches for rectifying and stripping sections, it does not necessarily indicate that a component is exhausted. It remains a region where no fractionation is performed.

2.4 Columns with One Pinch Region Only

Basically, to assure that a distillation process operates under minimum reflux condition, one pinch region must appear in each section of the column. The requirement of infinite number of plates is then respected.

It may happen that one section does not exhibit pinch condition. For example, in Figure 16, the feed should be moved upward to increase the efficiency of the column by transfering the unused plates from the upper pinch region to the stripping section. After this operation, the upper pinch may disappear before a lower pinch appears. This means that, in reality, minimum reflux conditions were not prevailing. On the other hand, a pinch region may appear in the stripping section, showing that minimum reflux operation is reached.

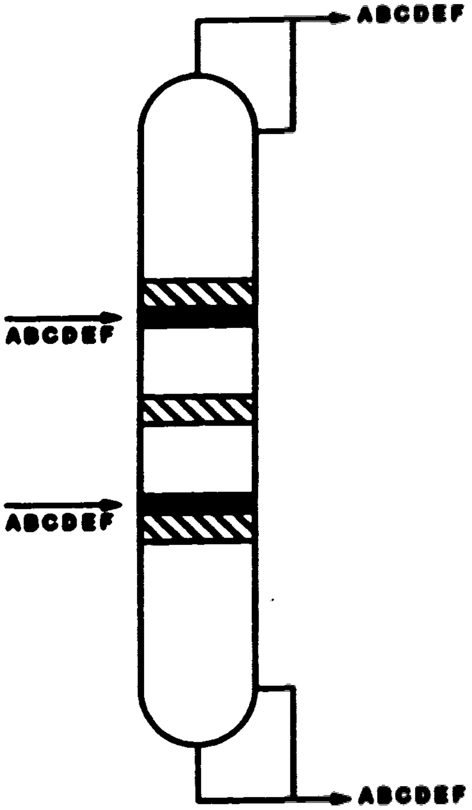

FIGURE 12. Pinch regions for class 1 separation, multiple feed column.

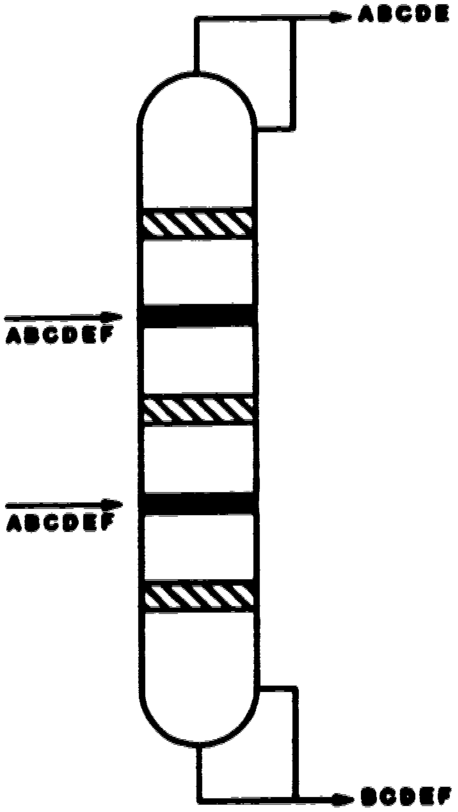

FIGURE 13. Pinch regions for class 2 separation, multiple feed column. (Components A and F do not distribute.)

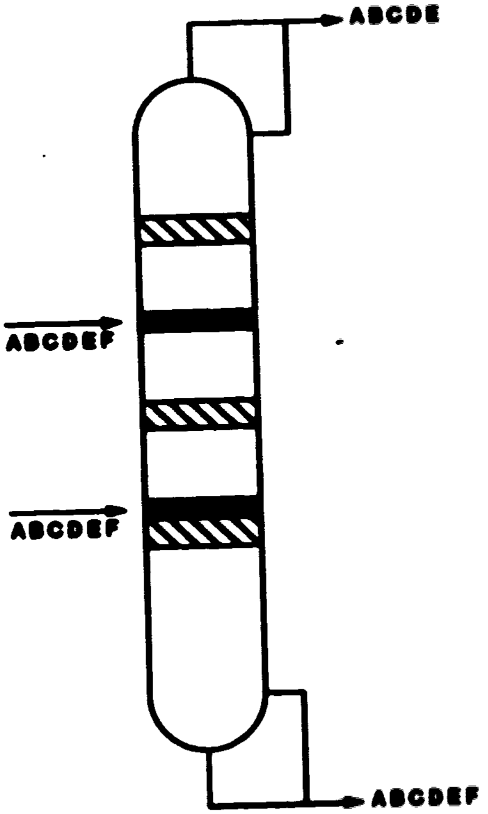

FIGURE 14. Pinch regions for class 2 separation, multiple feed column. (Component F does not distribute.)

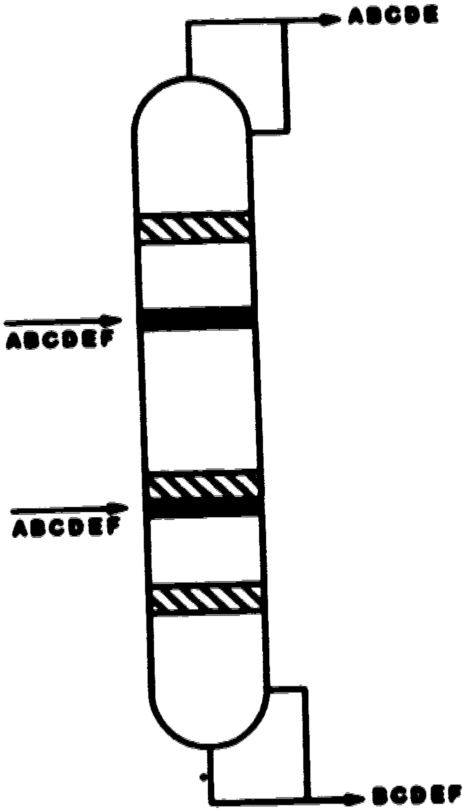

FIGURE 15. Pinch regions for class 2 separation, multiple feed column. (Intermediate pinch adjacent to feed.)

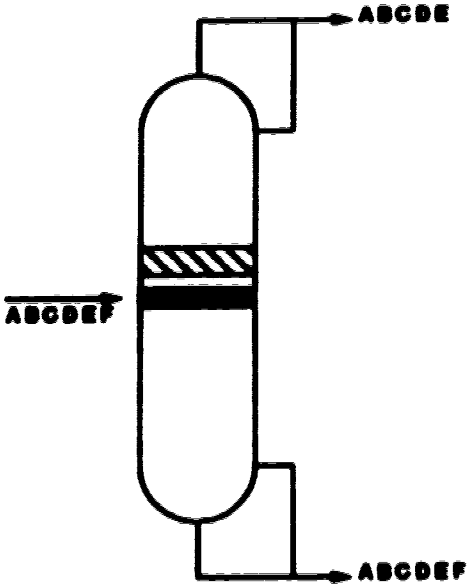

FIGURE 16. Column with one pinch region.

To complete these considerations, one must point out that the exact location of the feed is not an issue, as long as each section exhibits a pinch region. Additional plates do not increase the separation. Only the length of the pinch would increase.

Chapter 3
Underwood's Theory

This work is based on Barnés, Hanson and King (1972) treatment of Underwood's (1948) equations. The derivation of Underwood's equations will be reviewed to show that they can be easily modified to include energy balance considerations. This chapter will also show the application of Underwood's work to multiple feed columns by Barnés, Hanson and King. The method based on energy balance is called "Generalized Underwood Model" and will be shown in Chapter 4.

3.1 Underwood's Equations Applied to Single Feed Columns

3.1.1 Introduction

Underwood developed an analytical method for class 2 separation, assuming constant L, V, and α. The specifications required are the composition of the feed (f_i), the feed condition (V_F), and the amount of LK and HK recovered in the top product. This method applies to columns with one feed. It takes into account the contribution of the other components which are the "light components" (lighter than LK) and the "heavy components" (heavier than HK). It even allows for "split-key components" (between LK and HK).

Section 3.1.2 will show the starting equations utilized to derive the four basic equations that we use from Underwood's work. These equations are derived in Sections 3.1.3, 3.1.4, 3.1.5, and 3.1.6. The equations are summarized in Section 3.1.7 and their application is briefly explained in Section 3.1.8.

3.1.2 Basis for Underwood's Equations

The net upward molal flow (P) is a very useful quantity because it is, by definition, constant throughout a given section. It is defined as follows on plate "i", with plate "i+1" being below plate "i" :

$$P = V_{i+1} - L_i \tag{3.1}$$

and for a given component "j", it is written :

$$p_j = (v_j)_{i+1} - (l_j)_i \tag{3.2}$$

or

$$P(z_j)_P = V_{i+1}\,(y_j)_{i+1} - L_i(x_j)_i \tag{3.3}$$

As for the equilibrium relationship, the following equation applies (where α_j is constant) :

$$y_j = \frac{\alpha_j x_j}{\sum_{j=1}^{n} \alpha_j x_j} \tag{3.4}$$

Substituting Equation 3.4 in Equation 3.3 and having the assumptions that V_{i+1} and L_i are constant for a section of the column, we can write for component "j" on plate "i" :

$$\frac{L}{V}(x_j)_i + \frac{P}{V}(z_j)_P = \frac{\alpha_j (x_j)_{i+1}}{\sum_{j=1}^{n} \alpha_j (x_j)_{i+1}} \tag{3.5}$$

Now, Equation 3.5 can be multiplied by $\dfrac{\alpha_j}{\alpha_j - \phi}$ to yield :

$$\frac{L}{V}\frac{(x_j)_i\,\alpha_j}{\alpha_j-\phi}+\frac{P}{V}\frac{(z_j)_P\,\alpha_j}{\alpha_j-\phi}=\frac{\alpha_j(x_j)_{i+1}\,\frac{\alpha_j}{\alpha_j-\phi}}{\sum\limits_{j=1}^{n}\alpha_j(x_j)_{i+1}} \tag{3.6}$$

Adding Equation 3.6 applied to each n components :

$$\frac{L}{V}\sum_{j=1}^{n}\frac{\alpha_j(x_j)_i}{\alpha_j-\phi}+\frac{P}{V}\sum_{j=1}^{n}\frac{\alpha_j(z_j)_P}{\alpha_j-\phi}=\frac{\sum\limits_{j=1}^{n}\alpha_j(x_j)_{i+1}\,\frac{\alpha_j}{\alpha_j-\phi}}{\sum\limits_{j=1}^{n}\alpha_j(x_j)_{i+1}} \tag{3.7}$$

and ϕ is chosen so that :

$$\frac{P}{V}\sum_{j=1}^{n}\frac{\alpha_j(z_j)_P}{\alpha_j-\phi}=1 \tag{3.8}$$

3.1.3 Derivation of the First Equation

The first equation links the liquids compositions of any tray to any other tray. The case of interest is to link the upper and the lower ends of a given section.

Substituting Equation 3.8 in 3.7 :

$$\frac{L}{V}\left(\sum_{j=1}^{n}\frac{\alpha_j(x_j)_i}{\alpha_j-\phi}\right)=\frac{\sum\limits_{j=1}^{n}\alpha_j(x_j)_{i+1}\left[\frac{\alpha_j}{\alpha_j-\phi}-1\right]}{\sum\limits_{j=1}^{n}\alpha_j(x_j)_{i+1}} \tag{3.9}$$

and grouping the terms :

$$\sum_{j=1}^{n} \frac{\alpha_j \beta_j x_{j,i}}{\alpha_j - \phi} = \frac{\phi \displaystyle\sum_{j=1}^{n} \frac{\alpha_j \beta_j x_{j,i+1}}{\alpha_j - \phi}}{\frac{L}{V} \displaystyle\sum_{j=1}^{n} \alpha_j \beta_j x_{j,i+1}} \qquad (3.10)$$

Equation 3.10 is of the n^{th} degree and n different real roots ϕ satisfy the equation. Ramkrishna and Amundson (1973) showed that Underwood's equations could be derived by using self-adjoint operators for nonsymmetric real matrices. Let us denote them as follows :

$$\phi_1, \phi_2, \ldots, \phi_k, \ldots, \phi_n \quad \text{where } \phi_1 > \phi_2 > \phi_k > \phi_n$$

Applying Equation 3.10 to any two roots ϕ_k and ϕ_l and dividing one equation generated by the other enables us to eliminate the factor L/V in the denominator :

$$\frac{\displaystyle\sum_{j=1}^{n} \frac{\alpha_j \beta_j x_{j,i}}{\alpha_j - \phi_l}}{\displaystyle\sum_{j=1}^{n} \frac{\alpha_j \beta_j x_{j,i}}{\alpha_j - \phi_k}} = \frac{\phi_l}{\phi_k} \cdot \frac{\displaystyle\sum_{j=1}^{n} \frac{\alpha_j \beta_j x_{j,i+1}}{\alpha_j - \phi_l}}{\displaystyle\sum_{j=1}^{n} \frac{\alpha_j \beta_j x_{j,i+1}}{\alpha_j - \phi_k}} \qquad (3.11)$$

Equation 3.11 can be written with any combination of ϕ_k and ϕ_l where k = 1, 2, ..., n and l = 1, 2, ..., n with the restriction $k \neq l$. The number of combinations is equal to $(n^2-n)/2$. Equation 3.11 is written for two adjacent plates "i" and "i + 1". Writing it for plates "i + 1" and "i + 2" yields :

$$\frac{\displaystyle\sum_{j=1}^{n}\frac{\alpha_j (x_j)_{i+1}}{\alpha_j-\phi_l}}{\displaystyle\sum_{j=1}^{n}\frac{\alpha_j (x_j)_{i+1}}{\alpha_j-\phi_k}}=\frac{\phi_l}{\phi_k}\cdot\frac{\displaystyle\sum_{j=1}^{n}\frac{\alpha_j (x_j)_{i+2}}{\alpha_j-\phi_l}}{\displaystyle\sum_{j=1}^{n}\frac{\alpha_j (x_j)_{i+2}}{\alpha_j-\phi_k}} \qquad (3.12)$$

Combining Equations 3.11 and 3.12 gives a relationship between the compositions of plates "i" and "i + 2" :

$$\frac{\displaystyle\sum_{j=1}^{n}\frac{\alpha_j (x_j)_i}{\alpha_j-\phi_l}}{\displaystyle\sum_{j=1}^{n}\frac{\alpha_j (x_j)_i}{\alpha_j-\phi_k}}=\left(\frac{\phi_l}{\phi_k}\right)^2\cdot\frac{\displaystyle\sum_{j=1}^{n}\frac{\alpha_j (x_j)_{i+2}}{\alpha_j-\phi_l}}{\displaystyle\sum_{j=1}^{n}\frac{\alpha_j (x_j)_{i+2}}{\alpha_j-\phi_k}} \qquad (3.13)$$

Equation 3.13 can be generalized for plates "i" and "i + m" :

$$\frac{\displaystyle\sum_{j=1}^{n}\frac{\alpha_j (x_j)_i}{\alpha_j-\phi_l}}{\displaystyle\sum_{j=1}^{n}\frac{\alpha_j (x_j)_i}{\alpha_j-\phi_k}}=\left(\frac{\phi_l}{\phi_k}\right)^m\cdot\frac{\displaystyle\sum_{j=1}^{n}\frac{\alpha_j (x_j)_{i+m}}{\alpha_j-\phi_l}}{\displaystyle\sum_{j=1}^{n}\frac{\alpha_j (x_j)_{i+m}}{\alpha_j-\phi_k}} \qquad (3.14)$$

Equation 3.14 is general for any reflux ratio. For minimum reflux calculation, it is written in a more convenient form with the restriction $\phi_k > \phi_l$:

$$\frac{\sum_{j=1}^{n} \frac{\alpha_j p_j x_{j,i}}{\alpha_j - \phi_l}}{\sum_{j=1}^{n} \frac{\alpha_j p_j x_{j,i}}{\alpha_j - \phi_k}} \cdot \frac{\sum_{j=1}^{n} \frac{\alpha_j p_j x_{j,i+m}}{\alpha_j - \phi_k}}{\sum_{j=1}^{n} \frac{\alpha_j p_j x_{j,i+m}}{\alpha_j - \phi_l}} = \left(\frac{\phi_l}{\phi_k}\right)^{m} \tag{3.15}$$

where : ϕ_k and ϕ_l are any root ϕ
$k = 1, 2, \ldots, n$
$l = 1, 2, \ldots, n$
$k < l$ or $\phi_k > \phi_l$

Minimum reflux ratio implies that $m \to \infty$ and, since $\phi_k > \phi_l$, $\left(\frac{\phi_l}{\phi_k}\right)^{m \to \infty} \to 0$. Equation 3.15 reduces to :

$$\sum_{j=1}^{n} \frac{\alpha_j p_j x_{j,i}}{\alpha_j - \phi_l} \cdot \sum_{j=1}^{n} \frac{\alpha_j p_j x_{j,i+m}}{\alpha_j - \phi_k} = 0 \tag{3.16}$$

Equation 3.16 applies to any plates "i" and "i + m" of the same section. Finally, the case of interest is when Equation 3.16 links the upper tray and the lower tray of a given section of the column. This is noted by the "u" and "l" subscripts :

$$\sum_{j=1}^{n} \frac{\alpha_j p_j x_{j,u}}{\alpha_j - \phi_l} \cdot \sum_{j=1}^{n} \frac{\alpha_j p_j x_{j,l}}{\alpha_j - \phi_k} = 0 \tag{3.17}$$

3.1.4 Derivation of the Second Equation

The second equation describes the relationship between the composition of the net upward flowrates of the components "j" (p_j) and the total vapor flowrate (V) for a given section of a column. Note that, by definition, p_j is constant throughout the section. Also, V is assumed to be constant. Rewriting Equation 3.8 gives :

$$\sum_{j=1}^{n} \frac{\alpha_j F(z_j)_F}{\alpha_j - \phi} = V \tag{3.18}$$

or

$$\sum_{j=1}^{n} \frac{\alpha_j \beta_j}{\alpha_j - \phi} = V \tag{3.19}$$

The two cases, viz., when all components distribute and when some components are non-distributed, are treated separately next.

3.1.4.1 All components distribute — case 1

Figures 17a and 17b show an example of the solution for a six component mixture (components A, B, C, D, E, F). Figure 17a is for the rectifying section where all $\beta_j > 0$ ($j = 1, 2, \ldots, n$) and Figure 17b is for the stripping section where all $\beta_j < 0$ ($j = 1, 2, \ldots, n$).

Roots ϕ are on the x-axis and the vapor flow in the section on the y-axis. Relative volatilities α_j of the components constitute the asymptotes crossing the x-axis. The locations of the intersections between the graph and the horizontal line V are the different roots satisfying Equation 3.19. V_1 stands for vapor flowrate in section 1 which is the rectifying section. V_2 stands for vapor flowrate in section 2 which is the stripping section.

Until now, subscripts for the roots ϕ were numbers : ϕ_1, ϕ_2, ...ϕ_n. Since they are located between the different α_j, they can also be noted by ϕ_{AB} if it is located between α_A and α_B. Also, we observe that one root for each section is not located between two α_j. For the rectifying section, since it is smaller than α_F the notation is ϕ_{F-}. For the

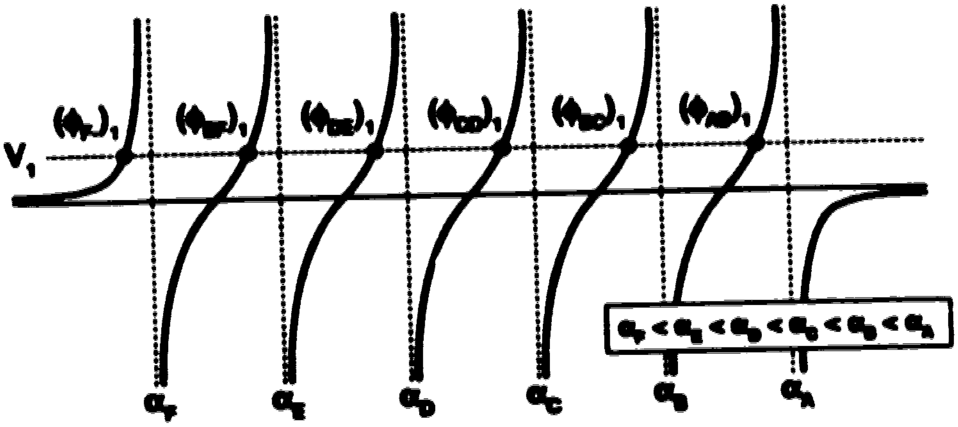

FIGURE 17a. Representation of the roots ϕ for the rectifying section. 6 components, all components distribute.

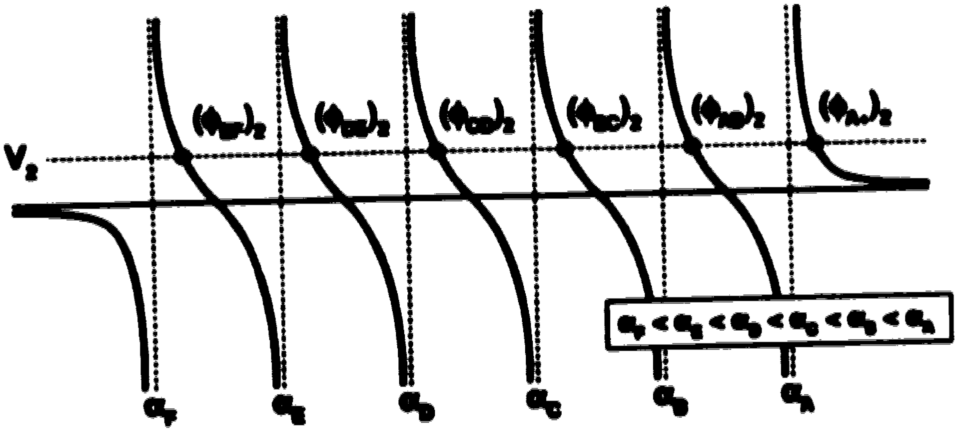

FIGURE 17b. Representation of the roots ϕ for the stripping section. 6 components, all components distribute.

stripping section, it is larger than α_A and the notation is ϕ_{A+} . Also, $(\phi_{AB})_1$ stands for ϕ_{AB} in section 1 (rectifying section) and $(\phi_{AB})_2$ for ϕ_{AB} in section 2 (stripping section).

The roots for each section are :

section 1 : $(\phi_{AB})_1$ $(\phi_{BC})_1$ $(\phi_{CD})_1$ $(\phi_{DE})_1$ $(\phi_{EF})_1$ $(\phi_{F-})_1$
section 2 : $(\phi_{A+})_2$ $(\phi_{AB})_2$ $(\phi_{BC})_2$ $(\phi_{CD})_2$ $(\phi_{DE})_2$ $(\phi_{EF})_2$

For each section, there are as many roots as there are components for which $p_j \neq 0$. This will be shown in the next case.

3.1.4.2 Some components do not distribute — case 2

Figures 18a and 18b show also the solution for a six component mixture with the exception that components A and F do not distribute. Component A is only found in the top product and component F, in the bottom product. This means that $(p_A)_2 = 0$ and $(p_F)_1 = 0$. As for the construction of the graphics, α_A is no longer an assymptote for the stripping section solution nor is α_F an assymptote for the rectifying section solution.

The roots for each section are :

section 1 : $(\phi_{AB})_1$ $(\phi_{BC})_1$ $(\phi_{CD})_1$ $(\phi_{DE})_1$ (ϕ_{E-})
section 2 : $(\phi_{B+})_2$ $(\phi_{BC})_2$ $(\phi_{CD})_2$ $(\phi_{DE})_2$ $(\phi_{EF})_2$

This shows that the number of roots is equal to the number of components for which $(p_j)_i \neq 0$, "j" being the component and "i", the section.

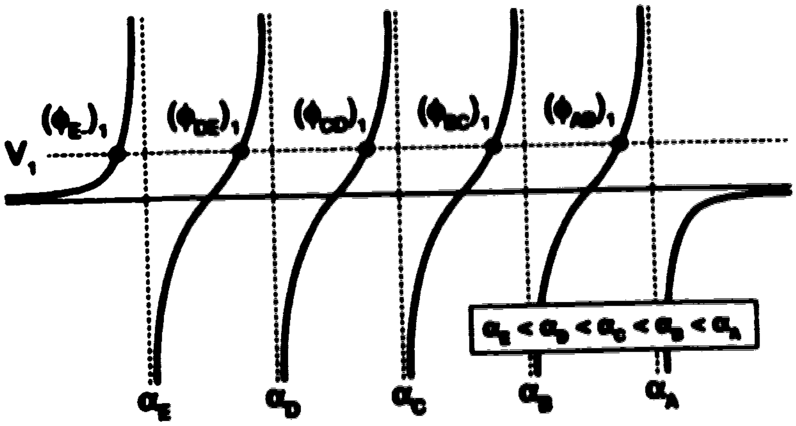

FIGURE 18a. Representation of the roots φ for the rectifying section. 6 components, components A and F do not distribute.

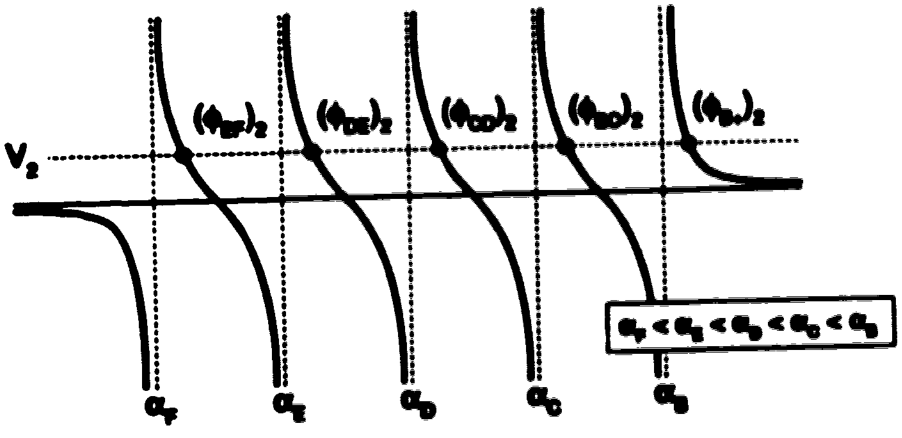

FIGURE 18b. Representation of the roots φ for the stripping section. 6 components, components A and F do not distribute.

3.1.5 Derivation of the Third Equation

It was already shown that each section has its own roots when applying Equation 3.19. It is also found that some of these roots can be common to two adjacent sections. Roots for section "i" are noted $(\phi_k)_i$ and the roots that are common on the feed plate are noted $(\Phi_k)_f$.

The derivation of the third equation is based on Equation 3.17. For this application, we find that the lower plate of the top section is the feed plate, and that the upper plate of the bottom section is also the feed plate. Writing Equation 3.17 for both sections :

section 1 : $$\sum_{j=1}^{n}\frac{\alpha_j (x_j)_t}{\alpha_j-(\phi_k)_1} - \sum_{j=1}^{n}\frac{\alpha_j (x_j)_f}{\alpha_j-(\phi_k)_1} = 0 \qquad (3.20)$$

section 2 : $$\sum_{j=1}^{n}\frac{\alpha_j (x_j)_f}{\alpha_j-(\phi_k)_2} - \sum_{j=1}^{n}\frac{\alpha_j (x_j)_l}{\alpha_j-(\phi_k)_2} = 0 \qquad (3.21)$$

The second term of Equation 3.20 and the first term of Equation 3.21 describe the same point in the column. Therefore $(\phi_k)_1$ and $(\phi_k)_2$ should be the same. Since only one term for each equation must be equal to zero, both equations are satisfied when the term related to the feed is equal to zero. From Equations 3.20 and 3.21 these considerations are summarized in one equation :

$$\sum_{j=1}^{n}\frac{\alpha_j (x_j)_f}{\alpha_j-(\Phi_k)_f} = 0 \qquad (3.22)$$

where : $(x_j)_f$: liquid mole fraction of component "j" on the feed plate
$(\Phi_k)_f$: common roots on the feed plate

3.1.6 Derivation of the Fourth Equation

The fourth and final equation is derived using the fact that the roots corresponding to the distributed components are common for two adjacent sections. The way to use these roots is dictated by Equations 3.20, 3.21, and 3.22, but let us first derive the equation. Writing Equation 3.19 for the rectifying section and the stripping section :

section 1 : $$\sum_{j=1}^{n} \frac{\alpha_j (D_j)_1}{\alpha_j - (\theta_k)_1} = V_1 \tag{3.23}$$

section 2 : $$\sum_{j=1}^{n} \frac{\alpha_j (D_j)_2}{\alpha_j - (\theta_k)_2} = V_2 \tag{3.24}$$

where V_1 and V_2 are the vapor flows in the rectifying and the stripping sections, respectively. Since roots can be common where two sections meet, we can subtract Equation 3.24 from 3.23 knowing that $(D_j)_1 - (D_j)_2 = f_j$:

$$\sum_{j=1}^{n} \frac{\alpha_j f_j}{\alpha_j - (\theta_k)_F} = \Delta V = V_1 - V_2 = V_F \tag{3.25}$$

$$\text{if } (\theta_k)_1 = (\theta_k)_2 = (\theta_k)_F$$

Now we have to determine which roots $(\theta_k)_F$ can satisfy Equation 3.25. This will be illustrated with two cases.

3.1.6.1 All components distribute — case 1

Application of Equation 3.20 for the rectifying section to a six component mixture enables us to determine which roots $(\Phi_{l,k})_F$ may be common. Let us recall that roots $(\Phi_{l,k})_F$ are not the same as roots $(\Phi_{l,k})_f$. Roots $(\Phi_{l,k})_f$ are valid on the feed tray and $(\Phi_{l,k})_F$ satisfy Equation 3.25 at the feed level.

As seen in Section 3.1.4.1, roots for the rectifying section are : $(\phi_{AB})_1$, $(\phi_{BC})_1$, $(\phi_{CD})_1$, $(\phi_{DE})_1$, $(\phi_{EF})_1$, $(\phi_{F-})_1$. The roots combine to satisfy Equation 3.20 as shown below. On top, we have Equation 3.20 and, underneath it, we show the roots that apply to each term. Since either term has to be equal to zero and recalling that $\phi_k > \phi_l$, we have :

$\sum_{j=1}^{n} \frac{\alpha_j d_j}{\alpha_j - (\phi_k)_1} = 0$	or	$\sum_{j=1}^{n} \frac{\alpha_j d_j}{\alpha_j - (\phi_l)_1} = 0$
$(\phi_{BC})_1$	or	$(\phi_{AB})_1$
$(\phi_{CD})_1$	or	$(\phi_{BC})_1$
$(\phi_{DE})_1$	or	$(\phi_{CD})_1$
$(\phi_{EF})_1$	or	$(\phi_{DE})_1$
$(\phi_{F-})_1$	or	$(\phi_{EF})_1$

Application of Equation 3.21 for the stripping section in the same manner will complete the picture. As seen in Section 3.1.4.1, roots for the stripping section are : $(\phi_{A-})_2$, $(\phi_{AB})_2$, $(\phi_{BC})_2$, $(\phi_{CD})_2$, $(\phi_{DE})_2$, $(\phi_{EF})_2$. We have :

$\sum_{j=1}^{n} \frac{\alpha_j b_j}{\alpha_j - (\phi_k)_2} = 0$	or	$\sum_{j=1}^{n} \frac{\alpha_j b_j}{\alpha_j - (\phi_l)_2} = 0$
$(\phi_{AB})_2$	or	$(\phi_{A-})_2$
$(\phi_{BC})_2$	or	$(\phi_{AB})_2$
$(\phi_{CD})_2$	or	$(\phi_{BC})_2$
$(\phi_{DE})_2$	or	$(\phi_{CD})_2$
$(\phi_{EF})_2$	or	$(\phi_{DE})_2$

As said previously, common roots are found at the feed level. Common roots $(\Phi_k)_F$ are then $(\Phi_{AB})_F$, $(\Phi_{BC})_F$, $(\Phi_{CD})_F$, $(\Phi_{DE})_F$, $(\Phi_{EF})_F$. Roots $(\theta_{F-})_1$ and $(\theta_{A-})_2$ cannot be common.

3.1.6.2 Some components do not distribute — case 2

Again, we apply Equation 3.20 with the exception that component F does not distribute, meaning that it does not appear in the top product. As seen in Section 3.1.4.2, roots for the rectifying section are : $(\theta_{AB})_1$, $(\theta_{BC})_1$, $(\theta_{CD})_1$, $(\theta_{DE})_1$, $(\theta_{E-})_1$.

$$\sum_{j=1}^{n} \frac{\alpha_j x_{jD}}{\alpha_j - (\theta_i)_1} = 0 \qquad \text{or} \qquad \sum_{j=1}^{n} \frac{\alpha_j x_{jD}}{\alpha_j - (\theta_k)_1} = 0$$

$(\theta_{BC})_1$ or $(\theta_{AB})_1$
$(\theta_{CD})_1$ or $(\theta_{BC})_1$
$(\theta_{DE})_1$ or $(\theta_{CD})_1$
$(\theta_{E-})_1$ or $(\theta_{DE})_1$

Now, we apply Equation 3.21 with the exception that component A does not distribute, meaning that it does not appear in the bottom product. As seen in Section 3.1.4.2, roots for the stripping section are : $(\theta_{B-})_2$, $(\theta_{BC})_2$, $(\theta_{CD})_2$, $(\theta_{DE})_2$, $(\theta_{EF})_2$.

$$\sum_{j=1}^{n} \frac{\alpha_j x_{jB}}{\alpha_j - (\theta_i)_2} = 0 \qquad \text{or} \qquad \sum_{j=1}^{n} \frac{\alpha_j x_{jB}}{\alpha_j - (\theta_k)_2} = 0$$

$(\theta_{BC})_2$ or $(\theta_{B-})_2$
$(\theta_{CD})_2$ or $(\theta_{BC})_2$
$(\theta_{DE})_2$ or $(\theta_{CD})_2$
$(\theta_{EF})_2$ or $(\theta_{DE})_2$

The common roots are found at the feed level. By inspection, the only common roots are $(\Phi_{BC})_F$, $(\Phi_{CD})_F$, and $(\Phi_{DE})_F$. Roots $(\theta_{E-})_1$ and $(\theta_{B-})_2$ are discarded.

3.1.6.3 Treatment of the roots of Equation 3.25

Figure 19 shows the solution of Equation 3.25 for a six component mixture with $\Delta V > 0$. We find six roots. All these roots will be found whether all components distribute or not because they are all present in the feed. Equation 3.25 takes only account of the components present in the feed. Even though all roots can be found, only some of them are valid (common to both sections), following the discussion in Sections 3.1.6.1 and 3.1.6.2.

The only valid roots are those located between α_i of components that distribute. In the two examples given, they are :

- when all 6 components distribute : $(\Phi_{AB})_F$ $(\Phi_{BC})_F$ $(\Phi_{CD})_F$ $(\Phi_{DE})_F$ $(\Phi_{EF})_F$
- when components A and F do not distribute : $(\Phi_{BC})_F$ $(\Phi_{CD})_F$ $(\Phi_{DE})_F$

This rule, as stated, applies to columns with one feed. Application for multiple feed columns will be shown in Section 3.2 of this chapter.

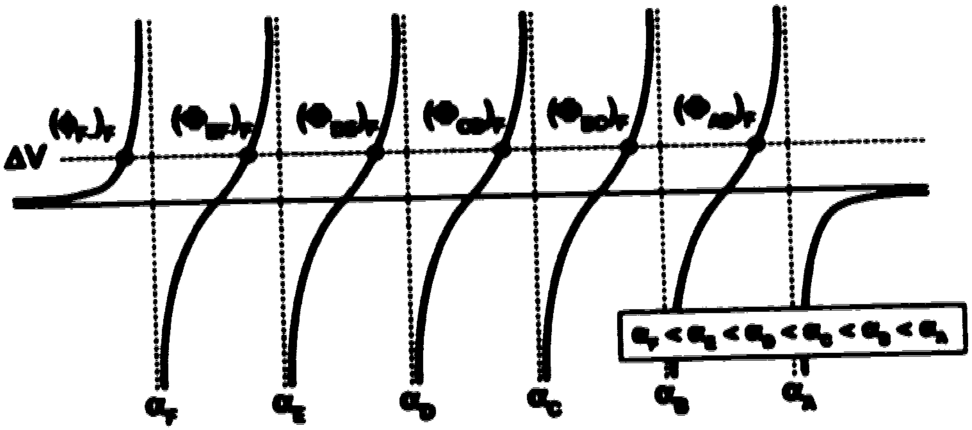

FIGURE 19. Representation of the roots Φ at the feed level. 6 components present in the feed.

3.1.7 Summary of the Equations Taken from Underwood's Work

1° Relationship between the upper plate "u" and the lower plate "l" of any given section of the column. This relationship links the liquid compositions of the plates previously mentioned. The equation is satisfied when either term is equal to zero.

$$\sum_{j=1}^{n} \frac{\alpha_j (x_j)_u}{\alpha_j - (\theta_1)_i} \cdot \sum_{j=1}^{n} \frac{\alpha_j (x_j)_l}{\alpha_j - (\theta_2)_i} = 0 \qquad \text{(U1)}$$

where :
n : number of components
α_j : relative volatility of component 'j'
$(x_j)_u$: liquid mole fraction of component 'j' on the upper plate of section 'i'
$(x_j)_l$: liquid mole fraction of component 'j' on the lower plate of section 'i'
$(\theta_1)_i$ and $(\theta_2)_i$: any roots satisfying Equation U1 for section 'i'
$(\theta_2)_i > (\theta_1)_i$

2° Relationship between the net upward flowrates of the components and the constant vapor flowrate for any given section of the column.

$$\sum_{j=1}^{n} \frac{\alpha_j (d_j)_i}{\alpha_j - (\theta_2)_i} = V_i \qquad \text{(U2)}$$

where :
n : number of components
α_j : relative volatility of component 'j'
$(d_j)_i$: net upward flowrate of component 'j' in section 'i'
$(\theta_2)_i$: any root satisfying Equation U2 for section 'i'
V_i : constant vapor flowrate in section 'i'

3° Intersection of Equation U1 for two adjacent sections, the lower plate of the top section and the upper plate of the bottom section being the feed plate between the two sections.

$$\sum_{j=1}^{n} \frac{\alpha_j (x_j)_f}{\alpha_j - (\theta_k)_f} = 0 \qquad \text{(U3)}$$

where :
n : number of components
α_j : relative volatility of component "j"
$(x_j)_f$: liquid mole fraction of component "j" on the feed plate
$(\theta_k)_f$: any root satisfying Equation U3
f : stands for "feed plate"

4° Subtraction of Equation U2 applied to two adjacent sections. This gives a relationship between the feed composition and the change of vapor flowrate on the feed plate.

$$\sum_{j=1}^{n} \frac{\alpha_j f_j}{\alpha_j - (\theta_k)_F} = \Delta V = V_F \qquad \text{(U4)}$$

where :
n : number of components
α_j : relative volatility of component "j"
f_j : amount of component "j" in the feed
$(\theta_k)_F$: any root satisfying Equation U4
ΔV : change of vapor flowrate on the feed tray
V_F vaporized portion of the feed
F : stands for "feed"

3.1.8 Procedure to Find the Minimum Reflux for Single Feed Columns

1° **Specifications :**

α_j $j = 1, 2, \dots, n$

f_j $j = 1, 2, \dots, n$

ΔV

$\frac{d_j}{f_j}$, $j = LK, HK$

2° Now, we can use Equation U4 to find the common roots $(\Phi_k)_F$, $k = 1, 2, \dots, n-1$. Let us remind that not all $(\Phi_k)_F$ are valid. The only ones valid are those located between relative volatilities of components that distribute. There are $n' - 1$ valid roots, where n' is the number of distributing components.

3° Since Equation U4 was derived from Equation U2 common roots $(\Phi_k)_F$ also apply to Equation U2. The unknowns are p_j and V_1 . The net upward flowrate (p_j) for LK and HK are specified ($p_{LK} = d_{LK}$, $p_{HK} = d_{HK}$) and if one component does not distribute, p_j is known ($p_j = f_j$ or $p_j = 0$, depending on the section). The number of unknown "p_j" is equal to $n' - 2$. The total number or unknowns is then $n' - 1$, when counting V_1 . Since there are $n' - 1$ roots (see step 2°), $n' - 1$ linear Equations U2 are generated to find $n' - 1$ unknowns.

4° The minimum reflux ratio is calculated with these equations :

$$D = \sum_{j=1}^{n} (p_j)_1 \tag{3.26}$$

$$L_1 = V_1 - D \tag{3.27}$$

$$R_m = \frac{L_1}{D} \tag{3.28}$$

3.2 Underwood's Equations Applied to Multiple Feed Columns

3.2.1 Introduction

Barnés, Hanson, and King (1972) applied Underwood's equations to multiple feed columns. This was done by extending the application of Equation U1 to intermediate sections. This application enables us to determine which common roots $(\Phi_k)_F$ are valid for Equation U4 and to find the common roots $(\Phi_k)_I$ for Equation U3. The common roots between sections are found by analysing two adjacent sections at a time.

For single feed columns, the net upward flowrate of each component "j" is positive "+" ($p_j \geq 0$) in the rectifying section, and negative "-" ($p_j \leq 0$) in the stripping section. For multiple feed columns, the same considerations hold for the rectifying (section 1) and the stripping (last section) sections. However, for the intermediate sections, the flow directions are not as obvious. For some components it is positive "+" and, for others, it is negative "-". A reasonable assumption is that the light components including LK have a positive net upward flowrate ($p_j \geq 0$) and that the heavy components including HK have a negative net upward flowrate ($p_j \leq 0$). As for split-key components, p_j may be either positive "+" ($p_j \geq 0$) or negative "-" ($p_j \leq 0$).

One difficulty of multiple feed application is that $(\Phi_k)_F$ for any "k" is found for each feed. For feed 1, it is noted $(\Phi_k)_{F1}$ and for feed 2 , $(\Phi_k)_{F2}$. However, only one $(\Phi_k)_F$ is valid for each "k". The valid root is determined by using Equations U1 and U3.

The other difficulty is that since split-key components may have a positive or negative net upward flowrate in the intermediate sections, different internal flow patterns are generated and must be investigated as potential solutions. Hypothesis on the internal flow directions must be made and, then, Equations U1 and U3 can be used. The way to establish the internal flow patterns and to use Equations U1 and U3 is treated in the next section.

3.2.2 Procedure to Choose the Valid Roots

For cases where there is no split-key component Equations U1 and U3 can be applied directly because there is only one possible internal flow pattern. When split-key components are present, all patterns must first be determined.

The principles involved in the algorithm will be illustrated with four cases :

1 - Column with one feed and adjacent key components
2 - Column with two feeds and adjacent key components
3 - Column with three feeds and adjacent key components
4 - Column with three feeds and one split-key component

All cases are illustrated for a six component mixture and it is assumed that all components distribute. Even though roots $(\Theta_k)_F$ do not satisfy directly Equation U3, the equation can still be used with the valid $(\Theta_k)_F$. This is possible because the valid $(\Theta_k)_F$ form a subset of the roots $(\Theta_k)_j$.

3.2.2.1 Column with one feed and adjacent key components

This case was covered in Section 3.1 of this chapter, but will be treated again to establish the structure that will lead to the analysis of more complex cases.

Table 1 shows how Equations U1 and U3 are utilized. Equation U1 is applied to each section and overlap at the feed plate. This overlap generates Equation U3. In Table 1, on top of each column we have Equations U1 and U3 applied to each end of the two sections and to the feed. Below it, we have the roots $(\Theta_k)_j$ placed so that Equation U1 is satisfied for both sections ($j = 1, 2$). The interest of this exercise is to find the common roots at the feed that satisfy Equation U3. In this case, the first and the third

TABLE 1. Utilization of Equations U1 and U3 to find the common roots $(\phi_{LL})_F$ at the feed level. 1 feed column.

Case : 6 components : A, B, C, D, E, F

1 feed, 2 sections

adjacent key components : LK = C, HK = D

$$\sum_{j=1}^{n} \frac{\alpha_j d_j}{\alpha_j - (\phi_t)_1} = 0 \qquad \sum_{j=1}^{n} \frac{\alpha_j z_j}{\alpha_j - (\phi_{LL})_F} = 0 \qquad \sum_{j=1}^{n} \frac{\alpha_j b_j}{\alpha_j - (\phi_b)_2} = 0$$

	top		feed		bottom
Section 1	$(\phi_{BC})_1$ $(\phi_{CD})_1$ $(\phi_{DE})_1$ $(\phi_{EF})_1$ $(\phi_{F-})_1$	or	$(\phi_{\underline{AB}})_1$ $(\phi_{\underline{BC}})_1$ $(\phi_{\underline{CD}})_1$ $(\phi_{\underline{DE}})_1$ $(\phi_{\underline{EF}})_1$		
Section 2			$(\phi_{\underline{AB}})_2$ $(\phi_{\underline{BC}})_2$ $(\phi_{\underline{CD}})_2$ $(\phi_{\underline{DE}})_2$ $(\phi_{\underline{EF}})_2$	or	$(\phi_{A-})_2$ $(\phi_{AB})_2$ $(\phi_{BC})_2$ $(\phi_{CD})_2$ $(\phi_{DE})_2$

columns are of no interest. The common roots are then $(\Phi_{AB})_F$, $(\Phi_{BC})_F$, $(\Phi_{CD})_F$, $(\Phi_{DE})_F$, and $(\Phi_{EF})_F$. Once these roots are found with Equation U4, $(p_j)_1$ and $(p_j)_2$ $(j = 1, 2, ..., n)$ and V_i $(i = 1, 2)$ are easily found with Equation U2.

3.2.2.2 Column with two feeds and adjacent key components

The basic equations still apply but the solution is more complex because roots $(\Phi_k)_F$ $(k = 1, 2, ..., n - 1)$ can be found from either feed with Equation U4. Even if we find $(\Phi_{AB})_{F1}$ and $(\Phi_{AB})_{F2}$, for example, only one is valid.

Let us recall that :

1° for all components in section 1 (rectifying section), $p_j \geq 0$
2° for light components and LK in section 2 (intermediate section), $p_j \geq 0$ (sign is "+")
3° for heavy components and HK in section 2, $p_j \leq 0$ (sign is "-")
4° for all components in section 3 (stripping section), $p_j \leq 0$

Writing Equation U2 for each section :

section 1 :
$$\sum_{j=1}^{n} \frac{\alpha_j (p_j)_1}{\alpha_j - (\Phi_k)_1} = V_1 \qquad (3.29a)$$

section 2 :
$$\sum_{j=1}^{n} \frac{\alpha_j (p_j)_2}{\alpha_j - (\Phi_k)_2} = V_2 \qquad (3.29b)$$

section 3 :
$$\sum_{j=1}^{n} \frac{\alpha_j (p_j)_3}{\alpha_j - (\Phi_k)_3} = V_3 \qquad (3.29c)$$

The roots of each equation are shown in Figures 20a, 20b, and 20c. We observe that the pattern of section 2 is different. Between the keys, there are two roots. In more general terms, there are two roots where the sign change occurs. In this case it is between the key components because they are adjacent. Since LK is component C and HK is component D, the two roots are noted $(\phi_{CD1})_2$ and $(\phi_{CD2})_2$.

The roots for each section of the column are :

section 1 :	$(\phi_{AB})_1$	$(\phi_{BC})_1$	$(\phi_{CD})_1$	$(\phi_{DE})_1$	$(\phi_{EF})_1$	$(\phi_{F-})_1$
section 2 :	$(\phi_{AB})_2$	$(\phi_{BC})_2$	$(\phi_{CD1})_2$	$(\phi_{CD2})_2$	$(\phi_{DE})_2$	$(\phi_{EF})_2$
section 3 :	$(\phi_{A+})_3$	$(\phi_{AB})_3$	$(\phi_{BC})_3$	$(\phi_{CD})_3$	$(\phi_{DE})_3$	$(\phi_{EF})_3$

Let us write Equation U1 for each section :

section 1 : $$\sum_{j=1}^{n} \frac{\alpha_j (x_j)_{t1}}{\alpha_j - (\phi_i)_1} = 0 \quad \text{or} \quad \sum_{j=1}^{n} \frac{\alpha_j (x_j)_{b1}}{\alpha_j - (\phi_k)_1} = 0 \qquad (3.30a)$$

section 2 : $$\sum_{j=1}^{n} \frac{\alpha_j (x_j)_{t2}}{\alpha_j - (\phi_i)_2} = 0 \quad \text{or} \quad \sum_{j=1}^{n} \frac{\alpha_j (x_j)_{b2}}{\alpha_j - (\phi_k)_2} = 0 \qquad (3.30b)$$

section 3 : $$\sum_{j=1}^{n} \frac{\alpha_j (x_j)_{t3}}{\alpha_j - (\phi_i)_3} = 0 \quad \text{or} \quad \sum_{j=1}^{n} \frac{\alpha_j (x_j)_{b3}}{\alpha_j - (\phi_k)_3} = 0 \qquad (3.30c)$$

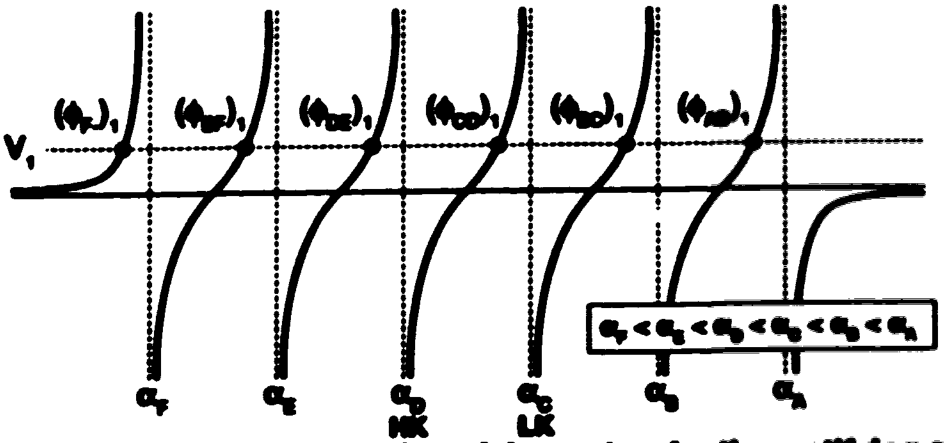

FIGURE 20a. Representation of the roots ϕ for the rectifying section. 6 components, all components distribute. 2 feed column.

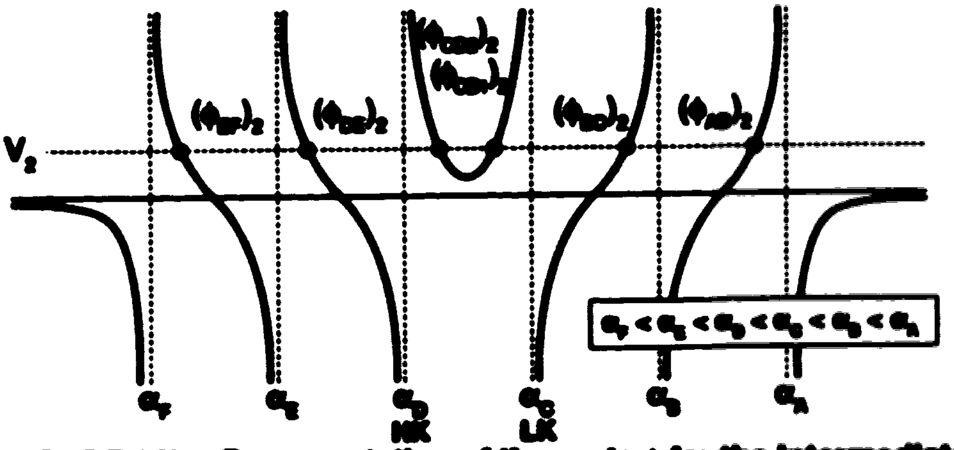

FIGURE 20b. Representation of the roots ϕ for the intermediate section. 6 components, all components distribute. 2 feed column.

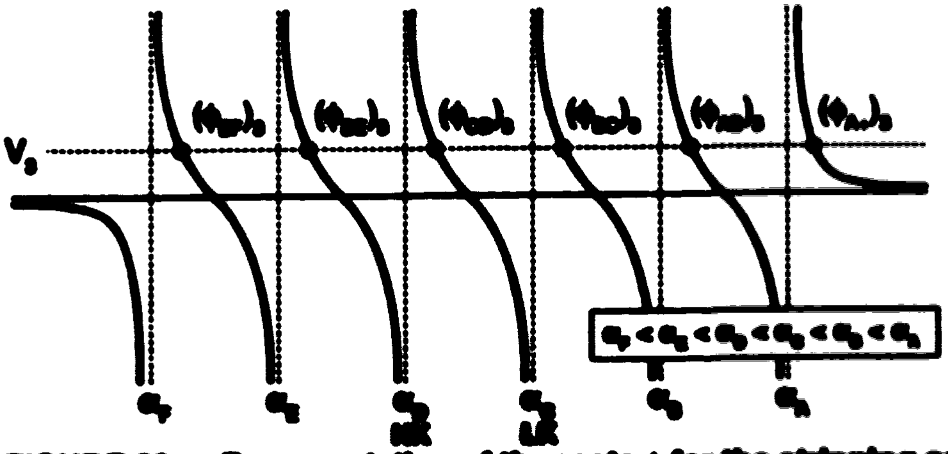

FIGURE 20c. Representation of the roots ϕ for the stripping section. 6 components, all components distribute. 2 feed column.

For each section, Equation 3.30 must be satisfied and, at the same time, all three equations must coincide on the feed plate. Equations 3.30a, 3.30b, and 3.30c are simplified and the remaining equations are :

$$\sum_{j=1}^{n} \frac{\alpha_j (b_j)_{t1}}{\alpha_j - (\Theta_k)_{t1}} = 0 \qquad (3.31a)$$

$$\sum_{j=1}^{n} \frac{\alpha_j (b_j)_{t2}}{\alpha_j - (\Theta_k)_{t2}} = 0 \qquad (3.31b)$$

Equations 3.31a and 3.31b are like Equation U3. $(\Theta_k)_{t1}$ and $(\Theta_k)_{t2}$ are the common roots on feed plate 1 and feed plate 2, respectively. As for the previous case, Equations U1 and U3 are used to determine which $(\Theta_k)_{F1}$ and $(\Theta_k)_{F2}$ are valid for each feed. This is shown in Table 2.

What interests us in Table 2 are the common roots from feed 1 and feed 2 in columns two and three. It appears that section 2 has roots in common with the two other sections at the same time, for example $(\theta_{BC})_1$ and $(\theta_{BC})_3$ .Since there is only one $(\theta_{BC})_2$, see Figure 20b, only one can be common with section 2. By inspection, we find in Table 2 that only a few roots are common at the feed. For feed 1, only $(\Theta_{CD})_{F1}$, $(\Theta_{DE})_{F1}$, and $(\Theta_{EF})_{F1}$ can be common. For feed 2, only $(\Theta_{AB})_{F2}$, $(\Theta_{BC})_{F2}$, and $(\Theta_{CD})_{F2}$ can be common. The roots that are potentially common are underlined. (Θ_{CD}) may come from either feed, and only one is possible. We must solve the system for both cases and determine whether the solutions are physically possible.

TABLE 2. Utilization of Equations U1 and U3 to find the common roots $(\theta_k)_r$ at the feed levels. 2 feed column.

Case : 6 components : A, B, C, D, E, F

2 feeds, 3 sections

adjacent key components : LK = C, HK = D

	$\sum_{j=1}^{6}\frac{\alpha_j x_j}{\alpha_j-(\theta)_1}=0$		$\sum_{j=1}^{6}\frac{\alpha_j x_j}{\alpha_j-(\theta)_{1,2}}=0$		$\sum_{j=1}^{6}\frac{\alpha_j x_j}{\alpha_j-(\theta)_{2,3}}=0$		$\sum_{j=1}^{6}\frac{\alpha_j x_j}{\alpha_j-(\theta)_3}=0$
	top		feed 1		feed 2		bottom
Section 1	$(\theta_{BC})_1$ $(\theta_{CD})_1$ $(\theta_{DE})_1$ $(\theta_{EF})_1$ $(\theta_{F-})_1$	or	$(\theta_{AB})_1$ $(\theta_{BC})_1$ $(\theta_{CD})_1$ $(\theta_{DE})_1$ $(\theta_{EF})_1$				
Section 2			$(\theta_{BC})_2$ $(\theta_{CD1})_2$ $(\theta_{CD2})_2$ $(\theta_{DE})_2$ $(\theta_{EF})_2$	or	$(\theta_{AB})_2$ $(\theta_{BC})_2$ $(\theta_{CD1})_2$ $(\theta_{CD2})_2$ $(\theta_{DE})_2$		
Section 3					$(\theta_{AB})_3$ $(\theta_{BC})_3$ $(\theta_{CD})_3$ $(\theta_{DE})_3$ $(\theta_{EF})_3$	or	$(\theta_{-A})_3$ $(\theta_{AB})_3$ $(\theta_{BC})_3$ $(\theta_{CD})_3$ $(\theta_{DE})_3$

The two sets of common roots that can solve Equation U4 applied to each section are:

$(\Phi_{AB})_{F2}$	$(\Phi_{AB})_{F2}$
$(\Phi_{BC})_{F2}$	$(\Phi_{BC})_{F2}$
$(\Phi_{CD})_{F2}$	$(\Phi_{CD})_{F1}$
$(\Phi_{DE})_{F1}$	$(\Phi_{DE})_{F1}$
$(\Phi_{EF})_{F1}$	$(\Phi_{EF})_{F1}$

We must try each set and discard the solutions through the process of elimination described in the next chapter.

3.2.2.3 Column with three feeds and adjacent key components

This case carries one step further the exercise done for columns with two feeds. Table 3 shows the underlined roots that should satisfy Equation U1 for each section. We find that, for feed 1, only $(\Phi_{CD})_{F1}$, $(\Phi_{DE})_{F1}$, and $(\Phi_{EF})_{F1}$ can be common. For feed 2, only $(\Phi_{CD})_{F2}$ can be common. For feed 3, only $(\Phi_{AB})_{F3}$, $(\Phi_{BC})_{F3}$, and $(\Phi_{CD})_{F3}$ can be common. Root (Φ_{CD}) can be found with Equation U4 applied to any feed, but only one is valid. We have to investigate all three cases.

The three sets of common roots that can solve Equation U4 applied to each section are :

$(\Phi_{AB})_{F3}$	$(\Phi_{AB})_{F3}$	$(\Phi_{AB})_{F3}$
$(\Phi_{BC})_{F3}$	$(\Phi_{BC})_{F3}$	$(\Phi_{BC})_{F3}$
$(\Phi_{CD})_{F3}$	$(\Phi_{CD})_{F2}$	$(\Phi_{CD})_{F1}$
$(\Phi_{DE})_{F1}$	$(\Phi_{DE})_{F1}$	$(\Phi_{DE})_{F1}$
$(\Phi_{EF})_{F1}$	$(\Phi_{EF})_{F1}$	$(\Phi_{EF})_{F1}$

TABLE 3. **Utilization of Equations U1 and U3 to find the common roots $(\theta_k)_F$ at the feed levels. 3 feed column.**

Case : 6 components : A, B, C, D, E, F

3 feeds, 4 sections

adjacent key components : LK = C, HK = D

$$\sum_{j=1}^{6}\frac{\text{[illegible]}}{\alpha_j-\text{[illegible]}_1}=0 \qquad \sum_{j=1}^{6}\frac{\text{[illegible]}}{\alpha_j-\text{[illegible]}_1}=0 \qquad \sum_{j=1}^{6}\frac{\text{[illegible]}}{\alpha_j-\text{[illegible]}_2}=0 \qquad \sum_{j=1}^{6}\frac{\text{[illegible]}}{\alpha_j-\text{[illegible]}_3}=0 \qquad \sum_{j=1}^{6}\frac{\text{[illegible]}}{\alpha_j-\text{[illegible]}_4}=0$$

	top		feed 1		feed 2		feed 3		bottom
Section 1	$(\theta_{BC})_1$ $(\theta_{CD})_1$ $(\theta_{DE})_1$ $(\theta_{EF})_1$ $(\theta_{F-})_1$	or	$(\theta_{AB})_1$ $(\theta_{BC})_1$ $(\theta_{CD})_1$ $(\theta_{DE})_1$ $(\theta_{EF})_1$						
Section 2			$(\theta_{BC})_2$ $(\theta_{CD1})_2$ $(\theta_{CD2})_2$ $(\theta_{DE})_2$ $(\theta_{EF})_2$	or	$(\theta_{AB})_2$ $(\theta_{BC})_2$ $(\theta_{CD1})_2$ $(\theta_{CD2})_2$ $(\theta_{DE})_2$				
Section 3					$(\theta_{BC})_3$ $(\theta_{CD1})_3$ $(\theta_{CD2})_3$ $(\theta_{DE})_3$ $(\theta_{EF})_3$	or	$(\theta_{AB})_3$ $(\theta_{BC})_3$ $(\theta_{CD1})_3$ $(\theta_{CD2})_3$ $(\theta_{DE})_3$		
Section 4							$(\theta_{AB})_4$ $(\theta_{BC})_4$ $(\theta_{CD})_4$ $(\theta_{DE})_4$ $(\theta_{EF})_4$	or	$(\theta_{-A})_4$ $(\theta_{AB})_4$ $(\theta_{BC})_4$ $(\theta_{CD})_4$ $(\theta_{DE})_4$

3.2.2.4 Column with three feeds and one split-key component

It has been found that the sign change determines which roots $(\Theta_h)_F$ may come from more than one feed. The light components and LK have a "+" sign, and the heavy component and HK, a "-" sign, in the intermediate sections. A split-key (SK) component can be either "+" or "-". Both alternatives have to be investigated. For adjacent keys, when LK = C and HK = D, the sign change occurs between components C and D, meaning that $(\Theta_{CD})_F$ can be calculated from more than one feed. With one split-key component, the sign change may occur between LK and SK or between SK and HK. This additional possibility generates other sets of common roots. In this example, SK = C, LK = B, and HK = D.

Table 4a shows the roots when we assume that the sign change occurs between components C and D in both intermediate sections. Table 4b shows the roots when we assume that the sign change occurs between components C and D in the first intermediate section, and between components B and C in the second intermediate section. Table 4c shows the roots when the sign change occurs between components B and C in both intermediate sections. These three flow patterns are summarized in Table 5.

The assumption for which the sign change occurs between components B and C in the first intermediate section and between components C and D in the second intermediate section is not possible. There would be an accumulation of component C on the second feed plate. However it would be possible with a side-cut in either intermediate section.

TABLE 4a. Utilization of Equations U1 and U3 to find the common roots $(\Theta_k)_r$ at the feed levels. 3 feed column and 1 split-key component. Flow level No. 1.

Case : 6 components : A, B, C, D, E, F

3 feeds, 4 sections

one split-key component : LK = B, SK = C, HK = D

flow pattern No. 1 : sign change section 2 : C → D

sign change section 3 : C → D

$$\sum_{j=1}^{6}\frac{\alpha_j x_j}{\alpha_j-\theta_{k1}}=0 \qquad \sum_{j=1}^{6}\frac{\alpha_j x_j}{\alpha_j-\theta_{k,1}}=0 \qquad \sum_{j=1}^{6}\frac{\alpha_j x_j}{\alpha_j-\theta_{k2}}=0 \qquad \sum_{j=1}^{6}\frac{\alpha_j x_j}{\alpha_j-\theta_{k3}}=0 \qquad \sum_{j=1}^{6}\frac{\alpha_j x_j}{\alpha_j-\theta_{k4}}=0$$

	top		feed 1		feed 2		feed 3		bottom
	$(\theta_{BC})_1$	or	$(\theta_{AB})_1$						
	$(\theta_{CD})_1$		$(\theta_{BC})_1$						
Section 1	$(\theta_{DE})_1$		$(\theta_{CD})_1$						
	$(\theta_{EF})_1$		$(\theta_{DE})_1$						
	$(\theta_{F-})_1$		$(\theta_{EF})_1$						
			$(\theta_{BC})_2$	or	$(\theta_{AB})_2$				
			$(\theta_{CD1})_2$		$(\theta_{BC})_2$				
Section 2			$(\theta_{CD2})_2$		$(\theta_{CD1})_2$				
			$(\theta_{DE})_2$		$(\theta_{CD2})_2$				
			$(\theta_{EF})_2$		$(\theta_{DE})_2$				
					$(\theta_{BC})_3$	or	$(\theta_{AB})_3$		
					$(\theta_{CD1})_3$		$(\theta_{BC})_3$		
Section 3					$(\theta_{CD2})_3$		$(\theta_{CD1})_3$		
					$(\theta_{DE})_3$		$(\theta_{CD2})_3$		
					$(\theta_{EF})_3$		$(\theta_{DE})_3$		
							$(\theta_{AB})_4$	or	$(\theta_{A-})_4$
							$(\theta_{BC})_4$		$(\theta_{AB})_4$
Section 4							$(\theta_{CD})_4$		$(\theta_{BC})_4$
							$(\theta_{DE})_4$		$(\theta_{CD})_4$
							$(\theta_{EF})_4$		$(\theta_{DE})_4$

TABLE 4b. Utilization of Equations U1 and U3 to find the common roots $(\theta_k)_F$ at the feed levels. 3 feed column and 1 split-key component. Flow level No. 2.

Case : 6 components : A, B, C, D, E, F

3 feeds, 4 sections

one split-key component : LK = B, SK = C, HK = D

flow pattern No. 2 : sign change section 2 : C → D

sign change section 3 : B → C

	$\sum_{j=1}^{6}\frac{\alpha_j d_j}{\alpha_j-(\theta)_1}=0$		$\sum_{j=1}^{6}\frac{\alpha_j z_{j1}}{\alpha_j-(\theta_k)_1}=0$		$\sum_{j=1}^{6}\frac{\alpha_j z_{j2}}{\alpha_j-(\theta_k)_2}=0$		$\sum_{j=1}^{6}\frac{\alpha_j z_{j3}}{\alpha_j-(\theta_k)_3}=0$		$\sum_{j=1}^{6}\frac{\alpha_j b_j}{\alpha_j-(\theta)_4}=0$
	top		feed 1		feed 2		feed 3		bottom
Section 1	$(\theta_{BC})_1$ $(\theta_{CD})_1$ $(\theta_{DE})_1$ $(\theta_{EF})_1$ $(\theta_{F-})_1$	or	$(\theta_{AB})_1$ $(\theta_{BC})_1$ $(\theta_{CD})_1$ $(\theta_{DE})_1$ $(\theta_{EF})_1$						
Section 2			$(\theta_{BC})_2$ $(\theta_{CD1})_2$ $(\theta_{CD2})_2$ $(\theta_{DE})_2$ $(\theta_{EF})_2$	or	$(\theta_{AB})_2$ $(\theta_{BC})_2$ $(\theta_{CD1})_2$ $(\theta_{CD2})_2$ $(\theta_{DE})_2$				
Section 3					$(\theta_{BC1})_3$ $(\theta_{BC2})_3$ $(\theta_{CD})_3$ $(\theta_{DE})_3$ $(\theta_{EF})_3$	or	$(\theta_{AB})_3$ $(\theta_{BC1})_3$ $(\theta_{BC2})_3$ $(\theta_{CD})_3$ $(\theta_{DE})_3$		
Section 4							$(\theta_{AB})_4$ $(\theta_{BC})_4$ $(\theta_{CD})_4$ $(\theta_{DE})_4$ $(\theta_{EF})_4$	or	$(\theta_{-A})_4$ $(\theta_{AB})_4$ $(\theta_{BC})_4$ $(\theta_{CD})_4$ $(\theta_{DE})_4$

TABLE 4c. Utilization of Equations U1 and U3 to find the common roots $(\theta_k)_F$ at the feed levels. 3 feed column and 1 split-key component. Flow level No. 3.

Case : 6 components : A, B, C, D, E, F
3 feeds, 4 sections
one split-key component : LK = B, SK = C, HK = D
flow pattern No. 3 : sign change section 2 : B → C
sign change section 3 : B → C

$$\sum_{j=1}^{n}\frac{\alpha_j x_{j}}{\alpha_j-(\theta)_{1}}=0 \qquad \sum_{j=1}^{n}\frac{\alpha_j x_{j}}{\alpha_j-(\theta)_{1,2}}=0 \qquad \sum_{j=1}^{n}\frac{\alpha_j x_{j}}{\alpha_j-(\theta)_{2,3}}=0 \qquad \sum_{j=1}^{n}\frac{\alpha_j x_{j}}{\alpha_j-(\theta)_{3,4}}=0 \qquad \sum_{j=1}^{n}\frac{\alpha_j x_{j}}{\alpha_j-(\theta)_{4}}=0$$

	top		feed 1		feed 2		feed 3		bottom
Section 1	$(\theta_{BC})_1$ $(\theta_{CD})_1$ $(\theta_{DE})_1$ $(\theta_{EF})_1$ $(\theta_{F-})_1$	or	$(\theta_{AB})_1$ $(\theta_{BC})_1$ $(\theta_{CD})_1$ $(\theta_{DE})_1$ $(\theta_{EF})_1$						
Section 2			$(\theta_{BC1})_2$ $(\theta_{C1C2})_2$ $(\theta_{CD})_2$ $(\theta_{DE})_2$ $(\theta_{EF})_2$	or	$(\theta_{AB})_2$ $(\theta_{BC1})_2$ $(\theta_{C1C2})_2$ $(\theta_{CD})_2$ $(\theta_{DE})_2$				
Section 3					$(\theta_{BC1})_3$ $(\theta_{C1C2})_3$ $(\theta_{CD})_3$ $(\theta_{DE})_3$ $(\theta_{EF})_3$	or	$(\theta_{AB})_3$ $(\theta_{BC1})_3$ $(\theta_{C1C2})_3$ $(\theta_{CD})_3$ $(\theta_{DE})_3$		
Section 4							$(\theta_{AB})_4$ $(\theta_{BC})_4$ $(\theta_{CD})_4$ $(\theta_{DE})_4$ $(\theta_{EF})_4$	or	$(\theta_{A-})_4$ $(\theta_{AB})_4$ $(\theta_{BC})_4$ $(\theta_{CD})_4$ $(\theta_{DE})_4$

TABLE 5. Flow patterns for a 3 feed column with 1 split-key component.

SECTION	KEYS	COMPONENT	NET UPWARD FLOWRATE, p_j		
			Pattern # 1	Pattern # 2	Pattern # 3
1 (rectifying section)		A	+	+	+
	LK	B	+	+	+
		C	+	+	+
	HK	D	+	+	+
		E	+	+	+
		F	+	+	+
2 (intermediate section # 1)		A	+	+	+
	LK	B	+	+	+
		C	+	+	-
	HK	D	-	-	-
		E	-	-	-
		F	-	-	-
3 (intermediate section # 2)		A	+	+	+
	LK	B	+	+	+
		C	+	-	-
	HK	D	-	-	-
		E	-	-	-
		F	-	-	-
4 (stripping section)		A	-	-	-
	LK	B	-	-	-
		C	-	-	-
	HK	D	-	-	-
		E	-	-	-
		F	-	-	-

Each flow pattern generates many sets of common roots $(\Phi_{ij})_F$. For the first flow pattern, $(\Phi_{DE})_F$ and $(\Phi_{EF})_F$ come from Equation U4 for feed 1, and $(\Phi_{AB})_F$ and $(\Phi_{BC})_F$ come from feed 3. Root $(\Phi_{CD})_F$ may come from feed 1, feed 2, or feed 3. For the second flow pattern, $(\Phi_{DE})_F$ and $(\Phi_{EF})_F$ come from feed 1, and $(\Phi_{AB})_F$ comes from feed 3. Root $(\Phi_{BC})_F$ comes from either feed 2 or 3, and $(\Phi_{CD})_F$ from either feed 1 or 2. For the third flow pattern, $(\Phi_{CD})_F$, $(\Phi_{DE})_F$, and $(\Phi_{EF})_F$ come from feed 1, and $(\Phi_{AB})_F$, from feed 3. Root $(\Phi_{BC})_F$ may come from feed 1, feed 2, or feed 3.

The different sets of common roots generated by each flow pattern are the following :

Flow pattern No. 1	$(\Phi_{AB})_{F3}$	$(\Phi_{AB})_{F3}$	$(\Phi_{AB})_{F3}$	
	$(\Phi_{BC})_{F3}$	$(\Phi_{BC})_{F3}$	$(\Phi_{BC})_{F3}$	
	$(\Phi_{CD})_{F3}$	$(\Phi_{CD})_{F2}$	$(\Phi_{CD})_{F1}$	
	$(\Phi_{DE})_{F1}$	$(\Phi_{DE})_{F1}$	$(\Phi_{DE})_{F1}$	
	$(\Phi_{EF})_{F1}$	$(\Phi_{EF})_{F1}$	$(\Phi_{EF})_{F1}$	
Flow pattern No. 2	$(\Phi_{AB})_{F3}$	$(\Phi_{AB})_{F3}$	$(\Phi_{AB})_{F3}$	$(\Phi_{AB})_{F3}$
	$(\Phi_{BC})_{F3}$	$(\Phi_{BC})_{F3}$	$(\Phi_{BC})_{F2}$	$(\Phi_{BC})_{F2}$
	$(\Phi_{CD})_{F2}$	$(\Phi_{CD})_{F1}$	$(\Phi_{CD})_{F2}$	$(\Phi_{CD})_{F1}$
	$(\Phi_{DE})_{F1}$	$(\Phi_{DE})_{F1}$	$(\Phi_{DE})_{F1}$	$(\Phi_{DE})_{F1}$
	$(\Phi_{EF})_{F1}$	$(\Phi_{EF})_{F1}$	$(\Phi_{EF})_{F1}$	$(\Phi_{EF})_{F1}$
Flow pattern No. 3	$(\Phi_{AB})_{F3}$	$(\Phi_{AB})_{F3}$	$(\Phi_{AB})_{F3}$	
	$(\Phi_{BC})_{F3}$	$(\Phi_{BC})_{F2}$	$(\Phi_{BC})_{F1}$	
	$(\Phi_{CD})_{F1}$	$(\Phi_{CD})_{F1}$	$(\Phi_{CD})_{F1}$	
	$(\Phi_{DE})_{F1}$	$(\Phi_{DE})_{F1}$	$(\Phi_{DE})_{F1}$	
	$(\Phi_{EF})_{F1}$	$(\Phi_{EF})_{F1}$	$(\Phi_{EF})_{F1}$	

By inspection, we find that some sets appear more than one time, leaving only six different sets :

$(\Phi_{AB})_{F3}$	$(\Phi_{AB})_{F3}$	$(\Phi_{AB})_{F3}$	$(\Phi_{AB})_{F3}$	$(\Phi_{AB})_{F3}$	$(\Phi_{AB})_{F3}$
$(\Phi_{BC})_{F3}$	$(\Phi_{BC})_{F3}$	$(\Phi_{BC})_{F3}$	$(\Phi_{BC})_{F2}$	$(\Phi_{BC})_{F2}$	$(\Phi_{BC})_{F1}$
$(\Phi_{CD})_{F3}$	$(\Phi_{CD})_{F2}$	$(\Phi_{CD})_{F1}$	$(\Phi_{CD})_{F2}$	$(\Phi_{CD})_{F1}$	$(\Phi_{CD})_{F1}$
$(\Phi_{DE})_{F1}$	$(\Phi_{DE})_{F1}$	$(\Phi_{DE})_{F1}$	$(\Phi_{DE})_{F1}$	$(\Phi_{DE})_{F1}$	$(\Phi_{DE})_{F1}$
$(\Phi_{EF})_{F1}$	$(\Phi_{EF})_{F1}$	$(\Phi_{EF})_{F1}$	$(\Phi_{EF})_{F1}$	$(\Phi_{EF})_{F1}$	$(\Phi_{EF})_{F1}$

We have to solve the problem six times and then eliminate the solutions that are not physically possible. The procedure to follow in order to solve the problem for multiple feed columns is briefly described in Section 3.2.3.

3.2.2.5 Valid roots with non-distributing components

All demonstrations in Section 3.2.2 were for separation where all components distribute. If component A does not distribute, the sets remain the same with the exception that $(\Phi_{AB})_F$ would not be valid regardless of the feed it comes from. The root is not required to solve the system because $(p_A)_1$ in the rectifying section is then known : $(p_A)_1 = \sum_{i=1}^{N}(f_A)_i$, where N is the number of feeds. If component F does not distribute, $(\Phi_{EF})_F$ is not valid.

Since LK and HK are the components for which the split is specified in the top and bottom products only the components lighter than LK and heavier than HK may not distribute. At the limit, when only the two adjacent keys distribute, there is only one valid common root located between α_{LK} and α_{HK}.

3.2.3 Procedure to Find the Minimum Reflux for Multiple Feed Columns

The procedure presented here is a very short summary of the steps to follow. The complete sequence will be given in the next chapter with the application of the Generalized Underwood model.

1° Specifications : α_j $j = 1, 2, ..., n$
$(f_j)_i$ $j = 1, 2, ..., n$
$i = 1, 2, ..., N$
ΔV_i $i = 1, 2, ..., N$
$d_j / \sum_{i=1}^{N} (f_j)_i$ $j = LK, HK$

where : n : number of components
N : number of feeds

2° Find common roots $(\Phi_k)_{Fi}$ $(i = 1, 2, ..., N)$ with Equation U4 for each feed.

3° Choose valid roots $(\Phi_k)_{Fi}$ following the process of elimination previously demonstrated.

4° Apply selected $(\Phi_k)_{Fi}$ in Equation U2 for sections adjacent to the feed where the root comes from. For example, $(\Phi_{CD})_{F2}$ applies to sections 2 and 3. Unknowns $(p_j)_i$ and V_i can be found for all components 'j' in each section 'i'.

5° Calculate minimum reflux.

Chapter 4
Generalized Underwood Method for Multiple Feed Columns

Nandakumar and Andres (1981a) proposed to replace the assumption of constant molal overflow in Underwood's equations by the assumption of constant liquid (h_i) and vapor (H_i) enthalpies of the components for single feed columns. This is still an approximation, but this approach takes into account the difference of energy content between components. It is called "Generalized Underwood Model". As we are going to see, the format of the new equations is essentially the same as the one of Underwood's equations. In Section 4.1 of this chapter, we derive the Generalized Underwood equations in the same fashion it was done for Underwood's model.

The objective of the present work is the application of the Generalized Underwood method to multiple feed columns. In Section 4.2, we describe the steps and present the block diagram of the computer program written to calculate the minimum reflux for columns with up to five feeds and mixtures containing up to ten components.

4.1 Generalized Underwood Model

4.1.1 Introduction

Underwood's equations are only based on material balances. Constant molal overflow and constant relative volatilities (α_{ij}) are the basic assumptions. Underwood developed a scheme for class 2 separations which is superior to previous class 1 models trying to predict class 2 separations. However, class 2 separation really applies to mixtures with a broad range of relative volatilities. While the model is exact within the assumptions, the assumption of constant molal overflow limits the effectiveness of the application.

The assumption of constant molal overflow in Underwood's equations is replaced by the assumption of constant liquid enthalpy (h_j) and vapor enthalpy (H_j) of the components. Therefore, the latent heat of vaporization (λ_j) is constant for each component "j" :

$$H_j - h_j = \lambda_j = \text{constant} \tag{4.1}$$

Even though constant λ_j are still a limitation, it permits us to take into account energy considerations which are neglected in Underwood's equations. The Generalized Underwood equations still retain the simplicity of the Underwood equations. This idea was proposed by Nandakumar and Andres (1981a).

In the next sections, we derive the basic equations for the Generalized Underwood method. The basic assumptions are : constant relative volatilities (α_j) , constant liquid enthalpies (h_j), constant vapor enthalpies (H_j). From the latter two follows the assumption of constant latent heats of vaporization (λ_j).

4.1.2 Basis for Generalized Underwood Equations

From the energy balance around plate "i", and recalling that plate "i+1" is the adjacent plate below it, we have :

$$L_{i-1}\sum_{j=1}^{n} h_j(x_j)_{i-1} + V_{i+1}\sum_{j=1}^{n} H_j(y_j)_{i+1} = L_i\sum_{j=1}^{n} h_j(x_j)_i + V_i\sum_{j=1}^{n} H_j(y_j)_i \tag{4.2}$$

and from the material balance of component "j" around plate "i" we get :

$$L_{i-1}(x_j)_{i-1} = L_i(x_j)_i + V_i(y_j)_i - V_{i+1}(y_j)_{i+1} \tag{4.3}$$

After substituting Equation 4.3 in 4.2 and using 4.1, we obtain :

$$V_i \sum_{j=1}^{n} (y_j)_i \lambda_j = V_{i+1} \sum_{j=1}^{n} (y_j)_{i+1} \lambda_j = \Gamma = \text{constant} \qquad (4.4)$$

Equation 4.4 can also be written :

$$V_i A_i = V_{i+1} A_{i+1} = \Gamma = \text{constant} \qquad (4.5)$$

when we define A_i as follows :

$$\sum_{j=1}^{n} (y_j)_i \lambda_j = A_i \qquad (4.6)$$

Derivation of Equation 4.4 enables us to derive equations similar to Equations U1, U2, U3, and U4 from Underwood. Recalling Equation 3.3 and substituting Equation 3.4 in it :

$$L_i (x_j)_i + P(z_j)_P = V_{i+1} \cdot \frac{\alpha_j (x_j)_{i+1}}{\sum_{j=1}^{n} \alpha_j (x_j)_{i+1}} \qquad (4.7)$$

Multiplying Equation 4.7 by the latent heat of vaporization, λ_j, and rearranging :

$$\frac{L_i (x_j)_i \lambda_j}{V_{i+1}} + \frac{P(z_j)_P \lambda_j}{V_{i+1}} = \frac{\alpha_j (x_j)_{i+1} \lambda_j}{\sum_{j=1}^{n} \alpha_j (x_j)_{i+1}} \qquad (4.8)$$

Multiplying Equation 4.8 by $\frac{\alpha_j}{\alpha_j - \phi}$ and adding up for all "n" components :

$$\frac{L_i \sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_i}{\alpha_j - \phi}}{V_{i+1}} + \frac{\sum_{j=1}^{n} \frac{P(z_j)_F \alpha_j \lambda_j}{\alpha_j - \phi}}{V_{i+1}} = \frac{\sum_{j=1}^{n} \alpha_j \lambda_j (x_j)_{i+1} \frac{\alpha_j}{\alpha_j - \phi}}{\sum_{j=1}^{n} \alpha_j (x_j)_{i+1}} \qquad (4.9)$$

Now, we can divide Equation 4.9 by $\sum_{j=1}^{n} (y_j)_{i+1} \lambda_j$:

$$\frac{L_i \sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_i}{\alpha_j - \phi}}{V_{i+1} \sum_{j=1}^{n} (y_j)_{i+1} \lambda_j} + \frac{\sum_{j=1}^{n} \frac{P(z_j)_F \alpha_j \lambda_j}{\alpha_j - \phi}}{V_{i+1} \sum_{j=1}^{n} (y_j)_{i+1} \lambda_j} = \frac{\sum_{j=1}^{n} \alpha_j \lambda_j (x_j)_{i+1} \frac{\alpha_j}{\alpha_j - \phi}}{\left(\sum_{j=1}^{n} \alpha_j (x_j)_{i+1}\right) \cdot \left(\sum_{j=1}^{n} (y_j)_{i+1} \lambda_j\right)} \qquad (4.10)$$

We notice that the denominator of the second term is Γ as defined in Equation 4.4. Following Underwood's method, ϕ is choosen so that :

$$\frac{\sum_{j=1}^{n} \frac{P(z_j)_F \alpha_j \lambda_j}{\alpha_j - \phi}}{V_{i+1} \sum_{j=1}^{n} (y_j)_{i+1} \lambda_j} = 1 \qquad (4.11)$$

4.1.3 Derivation of the First Equation

As for Underwood's case, this equation links the liquid compositions of any tray to those of any other tray in the same section. The case of interest is the link between the upper and the lower ends of a given section. Substituting Equation 4.11 in 4.10 :

$$\frac{L_i \sum_{j=1}^{n} \frac{\alpha_j \lambda_j (b_j)_i}{\alpha_j - \phi}}{V_{i+1} \sum_{j=1}^{n} (b_j)_{i+1} \lambda_j} = \frac{\sum_{j=1}^{n} \alpha_j \lambda_j (b_j)_{i+1} \frac{\alpha_j}{\alpha_j - \phi}}{\left(\sum_{j=1}^{n} \alpha_j (b_j)_{i+1}\right) \cdot \left(\sum_{j=1}^{n} (b_j)_{i+1} \lambda_j\right)} - 1 \qquad (4.12)$$

After a few manipulations, we obtain :

$$\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (b_j)_i}{\alpha_j - \phi} = \frac{\phi \sum_{j=1}^{n} \frac{\alpha_j \lambda_j (b_j)_{i+1}}{\alpha_j - \phi}}{\frac{L_i}{V_{i+1}} \sum_{j=1}^{n} \alpha_j (b_j)_{i+1}} \qquad (4.13)$$

Equation 4.13 is of the n^{th} order and n different real roots ϕ satisfy the equation. As for Underwood, we denote them as follows :

$\phi_1, \phi_2, \ldots, \phi_k, \ldots, \phi_n$ where $\phi_1 > \phi_2 > \phi_k > \phi_n$

Applying Equation 4.13 to any two roots ϕ_k and ϕ_l and then dividing one equation by the other enables us to eliminate the factor $\frac{L_i}{V_{i+1}}$ in the denominator :

$$\frac{\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (b_j)_i}{\alpha_j - \phi_l}}{\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (b_j)_i}{\alpha_j - \phi_k}} = \frac{\phi_l}{\phi_k} \cdot \frac{\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (b_j)_{i+1}}{\alpha_j - \phi_l}}{\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (b_j)_{i+1}}{\alpha_j - \phi_k}} \qquad (4.14)$$

Equation 4.14 relates two adjacent plates "I" and "I+1". As it was done for Underwood Equation 4.14 can be generalized for any plates "I" and "I+m" :

$$\frac{\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_I}{\alpha_j - \phi_l}}{\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_I}{\alpha_j - \phi_k}} = \left(\frac{\phi_l}{\phi_k}\right)^m \cdot \frac{\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_{I+m}}{\alpha_j - \phi_l}}{\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_{I+m}}{\alpha_j - \phi_k}} \qquad (4.15)$$

Equation 4.15 is general for any reflux ratio. For minimum reflux calculation, it is written in a more convenient form with the restriction $\phi_k > \phi_l$:

$$\frac{\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_I}{\alpha_j - \phi_l}}{\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_I}{\alpha_j - \phi_k}} \cdot \frac{\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_{I+m}}{\alpha_j - \phi_k}}{\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_{I+m}}{\alpha_j - \phi_l}} = \left(\frac{\phi_l}{\phi_k}\right)^m \qquad (4.16)$$

where : ϕ_k and ϕ_l are any root
$k = 1, 2, \ldots, n$
$l = 1, 2, \ldots, n$
$k < l$ or $\phi_k > \phi_l$

Minimum reflux ratio implies that $m \rightarrow \infty$ and, since $\phi_k > \phi_l$, $\left(\frac{\phi_l}{\phi_k}\right)^{m \rightarrow \infty} \rightarrow 0$

Equation 4.16 reduces to :

$$\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_I}{\alpha_j - \phi_l} \cdot \sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_{I+m}}{\alpha_j - \phi_k} = 0 \qquad (4.17)$$

Equation 4.17 applies to any "l" and "l+m" plates. Finally, the case of interest is when it links the upper tray and the lower tray of a given section of the column. This is noted by the "u" and "l" subscripts :

$$\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_u}{\alpha_j - \phi_u} - \sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_l}{\alpha_j - \phi_l} = 0 \qquad (4.18)$$

4.1.4 Derivation of the Second Equation

This equation describes the relationship between the energy content of the net upward flow, P, and Γ as defined in Equation 4.4. We can recall that Γ is constant for a given section. Rewriting Equation 4.11 and using Equation 4.4 :

$$\sum_{j=1}^{n} \frac{P(x_D)_j \alpha_j \lambda_j}{\alpha_j - \phi} = V_l \sum_{j=1}^{n} (y_l)_j \lambda_j = \Gamma \qquad (4.19)$$

or

$$\sum_{j=1}^{n} \frac{p_j \alpha_j \lambda_j}{\alpha_j - \phi} = V_l \Lambda_l = \Gamma \qquad (4.20)$$

Let us recall that considerations discussed in Sections 3.1.4.1 and 3.1.4.2 of Chapter 3 about distributing and non-distributing components are still valid. The graphs of Equation 4.20 are the same as those shown in Figures 17a, 17b, 18a, and 18b with the exception that the units of the y-axis are not "V_l" but "$V_l \Lambda_l$" for section "l".

4.1.5 Derivation of the Third Equation

Each section has its own roots ϕ when Equation 4.20 is applied. It is found that some of these roots may be common to two adjacent sections. As for Underwood's case, roots for section 'i' are noted $(\phi_k)_i$, roots that are common on the feed plate are noted $(\Phi_k)_f$, and roots common at the feed level are noted $(\Phi_k)_F$.

Writing Equation 4.18 for two adjacent sections :

section 1 : $$\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_1}{\alpha_j - (\phi_k)_1} - \sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_f}{\alpha_j - (\Phi_k)_1} = 0 \qquad (4.21)$$

section 2 : $$\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_f}{\alpha_j - (\Phi_k)_2} - \sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_2}{\alpha_j - (\phi_k)_2} = 0 \qquad (4.22)$$

The second term of Equation 4.21 and the first term of Equation 4.22 describe the same point in the column, the feed plate. As for Underwood, $(\Phi_k)_1$ and $(\Phi_k)_2$ should be the same. Since only one term for each equation must be equal to zero, both equations are satisfied when the common term is zero. These considerations are summarized in one equation :

$$\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_f}{\alpha_j - (\Phi_k)_f} = 0 \qquad (4.23)$$

where : $(x_j)_f$: liquid mole fraction of component 'j' on the feed plate

$(\Phi_k)_f$: common roots on the feed plate

4.1.6 Derivation of the Fourth Equation

Equation 4.19 (or 4.20) can be applied to two adjacent sections. Subtracting the lower section equation from the upper section equation generates a third one which is the intersection at the feed level. As demonstrated for Underwood's equations, roots ϕ must be common to both sections. This is indicated by changing ϕ for Φ. Subscript "i" indicates any plate in the first section and "g" indicates any plate in the second section.

$$\sum_{j=1}^{n} \frac{(p_j)_1 \alpha_j \lambda_j}{\alpha_j - (\Phi_k)_1} - \sum_{j=1}^{n} \frac{(p_j)_2 \alpha_j \lambda_j}{\alpha_j - (\Phi_k)_2} = V_i \sum_{j=1}^{n} (y_j)_i \lambda_j - V_g \sum_{j=1}^{n} (y_j)_g \lambda_j \qquad (4.24)$$

and with $(p_j)_1 - (p_j)_2 = f_j$, we have :

$$\sum_{j=1}^{n} \frac{f_j \alpha_j \lambda_j}{\alpha_j - (\Phi_k)_F} = V_i \sum_{j=1}^{n} (y_j)_i \lambda_j - V_g \sum_{j=1}^{n} (y_j)_g \lambda_j \qquad (4.25)$$

Equation 4.25 can be written in another form. This is done through the following manipulations. The material balance is done for any component "j" around the portion of the column bounded by plate "i" in the upper section and plate "g" in the lower section. This portion includes the feed. Let us recall that plate 1 is at the top.

$$L_{i-1} (x_j)_{i-1} - L_g (x_j)_g = -F(z_j)_F + V_i (y_j)_i - V_{g+1} (y_j)_{g+1} \qquad (4.26)$$

Multiplying Equation 4.26 by λ_j establishes the liquid state as the "zero" for the energy content. Interest of this consideration is shown later. Summing up for all n components yields:

$$L_{f+1}\sum_{j=1}^{n}(x_j)_{f+1}h_j - L_g\sum_{j=1}^{n}(x_j)_g h_j = V_f\sum_{j=1}^{n}(y_j)_f h_j - V_{g+1}\sum_{j=1}^{n}(y_j)_{g+1}h_j - F\sum_{j=1}^{n}(z_j)_F h_j \tag{4.27}$$

Energy balance around plates "f" and "g" :

$$L_{f+1}\sum_{j=1}^{n}(x_j)_{f+1}h_j - L_g\sum_{j=1}^{n}(x_j)_g h_j = V_f\sum_{j=1}^{n}(y_j)_f H_j - V_{g+1}\sum_{j=1}^{n}(y_j)_{g+1}H_j - F\,H_F \tag{4.28}$$

Subtracting Equation 4.27 from 4.28 and using Equation 4.1 :

$$F\,H_F - F\sum_{j=1}^{n}(z_j)_F h_j = V_f\sum_{j=1}^{n}(y_j)_f\lambda_j - V_g\sum_{j=1}^{n}(y_j)_g\lambda_j \tag{4.29}$$

Finally, we combine Equations 4.25 and 4.29 :

$$\sum_{j=1}^{n}\frac{(\alpha_j f_j)\lambda_j}{\alpha_j - (\Theta_s)_F} = F\,H_F - F\sum_{j=1}^{n}(z_j)_F h_j \tag{4.30}$$

or

$$\sum_{j=1}^{n}\frac{(\alpha_j f_j)\lambda_j}{\alpha_j - (\Theta_s)_F} = V_F\sum_{j=1}^{n}(y_j)_{V_F}\lambda_j \tag{4.31}$$

The right hand side expresses the energy of the feed using the saturated liquid state of the feed as reference.

The comparison between Equations 4.31 and 3.14 is easily done. In both equations the right hand side is equal to zero if we have a saturated liquid feed. When the feed is subcooled, the right hand side is negative. When the feed is partially vaporized, only the vapor flow appears in Equation 3.14, whereas the energy of the vaporized portion of the feed appears in Equation 4.31. In both cases, saturated liquid is the reference state. The graph of Equations 4.31 is the same as the one shown in Figure 19 with the exception that the units of the y-axis are not "ΔV" but " $V_F \sum_{j=1}^{n} (y_j) y_F \lambda_j$ ".

4.1.7 Summary of the Equations

1° Relationship between the upper plate "u" and the lower plate "l" of any given section of the column. This relationship links the compositions of the plates previously mentioned. The equation is satisfied when either term is equal to zero.

$$\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_u}{\alpha_j - (\theta_1)_l} \cdot \sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_l}{\alpha_j - (\theta_2)_l} = 0 \qquad \text{(GU1)}$$

where :

n : number of components

α_j : relative volatility of component "j"

λ_j : latent heat of vaporization of component "j" per mole

$(x_j)_u$: liquid mole fraction of component "j" on the upper plate of section "l"

$(x_j)_l$: liquid mole fraction of component "j" liquid on the lower plate of section "l"

$(\theta_1)_l$ and $(\theta_2)_l$: any roots satisfying Equation GU1 for section "l"

$(\theta_2)_l > (\theta_1)_l$

2° Relationship between the net upward flowrates of the components and the energy content of the vapor flow for any section of the column.

$$\sum_{j=1}^{n} \frac{(p_j)_l \alpha_j \lambda_j}{\alpha_j - (\theta_2)_l} = (V_l)_l \sum_{j=1}^{n} (y_{lj})_l \lambda_j = (V_l)_l (\Lambda_l)_l = \eta_l \qquad \text{(GU2)}$$

where :

n : number of components

α_j : relative volatility of component "j"

λ_j : latent heat of vaporization of component "j" per mole

$(p_j)_l$: net upward flowrate of component "j" in section "l" (moles)

$(\theta_2)_l$: any root satisfying Equation GU2 for section "l"

$(V_l)_l$: vapor flowrate on plate "l" in section "l" (moles)

$(y_{lj})_l$: vapor mole fraction of component "j" on plate "l" in section "l"

η_l : constant term for section "l" as defined in Equation GU2

3° Intersection of Equation GU1 for two adjacent sections, the lower plate of the top section and the upper plate of the bottom section being the feed plate between the two sections.

$$\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_{fi}}{\alpha_j - (\Phi_k)_{fi}} = 0 \qquad \text{(GU3)}$$

where :
n : number of components
α_j : relative volatility of component 'j'
λ_j : latent heat of vaporization of component 'j' per mole
$(x_j)_{fi}$: liquid mole fraction of component 'j' on feed plate 'i'
$(\Phi_k)_{fi}$: any root satisfying Equation GU3 for feed plate 'i'

4° Subtraction of Equation GU2 applied to two adjacent sections. This gives a relationship between the feed composition and the energy contribution of the feed entering the column. Saturated liquid is considered as the reference state (zero).

$$\sum_{j=1}^{n} \frac{(f_j)_i \alpha_j \lambda_j}{\alpha_j - (\Phi_k)_{Fi}} = F_i H_{Fi} - F_i \sum_{j=1}^{n} (z_j)_{Fi} h_j = V_{Fi} \sum_{j=1}^{n} (y_j)_{V_{Fi}} \lambda_j = (\Delta HF)_i = (\Delta \Gamma)_i \qquad \text{(GU4)}$$

where :

n : number of components

α_j : relative volatility of component 'j'

λ_j : latent heat of vaporization of component 'j' per mole

$(f_j)_i$: quantity of component 'j' in feed 'i' (moles)

$(\Phi_k)_{Fi}$: any root satisfying Equation GU4 for feed 'i'

F_i : total feed 'i' (moles)

H_{Fi} : enthalpy of feed 'i' per mole

$(z_j)_{Fi}$: fraction of component 'j' in feed 'i'

h_j : liquid enthalpy of component 'j' per mole

V_{Fi} : vaporized portion of feed 'i' (moles)

$(y_j)_{V_{Fi}}$: fraction of component 'j' in the vaporized portion of feed 'i'

$F_i H_{Fi}$: total enthalpy of feed 'i'

$F_i \sum_{j=1}^{n} (z_j)_{Fi} h_j$: total enthalpy of the feed in the saturated liquid state

$(\Delta HF)_i$: total enthalpy of feed 'i' with respect to its saturated liquid state

$(\Delta \Gamma)_i$: difference between Γ values of the two adjacent sections around feed 'i'

4.1.8 Comparison Between Underwood and Generalized Underwood Equations

When compared with Equations U1, U2, U3, and U4, Equations GU1, GU2, GU3, and GU4 are very similar. Underwood's method is a special case of Generalized Underwood method when the latent heats of vaporization are assumed to be the same for all components "j", $\lambda_j = \lambda_{j+1}$.

For Equations U1, U3 and GU1, GU3, the form is exactly the same. For Equations U2 and GU2, the right hand side terms differ, but are constant quantities in their respective equation. In Equation U2 it is the vapor flowrate, V, and in Equation GU2 we define Γ which takes account of the variable vapor flowrate in a section. This comparison shows very well that the Generalized Underwood method removes the assumption of constant molal overflow while keeping the simple form of Underwood's equations. For Equations U4 and GU4, the right hand side terms represent the contribution of the feed. In the first equation it is a material contribution and in the second one it is an energy contribution. In both cases the liquid phase is said to be the "zero"; this is the reason why only the vapor portion of the feed appears in the equations.

The generalized method requires a little more calculation because $(V_j)_i$ has to be calculated from Γ_j, whereas V_j is found directly for Underwood's method. All the steps and equations for the calculation of the minimum reflux are given in detail in Section 4.2 of this chapter.

4.2 Generalized Underwood Method Applied to Multiple Feed Columns

4.2.1 Introduction

In Section 3.1 of Chapter 3, we derived the basic equations established by Underwood to calculate the minimum reflux for distillation of multicomponent mixtures with single feed columns. In Section 3.2 of the same chapter, these equations were extended to multiple feed columns.

In Section 4.1 of this chapter, we derived the basic equations for the Generalized Underwood method. These equations have exactly the same form as those from Underwood. The appearance of the latent heats of vaporization (λ_i) constitutes the only difference. Underwood's equations are based on material balance only. Generalized Underwood equations are based on material and energy balances.

In Section 4.2, we present the contribution of the present work, which consists in the application of the Generalized Underwood method to multiple feed columns. A computer program was developed to calculate the minimum reflux with this method. The necessary steps are described in detail and are followed by a block diagram which summarizes the procedure.

4.2.2 Description of the Computer Program

This program can find the minimum reflux with either Underwood or Generalized Underwood method. It can accept mixtures containing up to ten components and distillation columns with up to five feeds. Each feed must contain all components. For non-present components in a feed, a very small amount should be assigned instead of zero. Also we can choose between partial or total condensers. To simulate the

Underwood model with the present program, we set all the constant latent heats of vaporization to be the same, $\lambda_j = \lambda_{j+1}$. The following explanations cover the generalized method.

The basic idea of this program is threefold :

1- Treatment of the input data
2- Solving the equations and finding all the possible solutions
3- Eliminating the non valid solutions through an eight test procedure.

The assumptions are the following :
- constant α_j
- constant h_j
- constant H_j
- constant λ_j

The specifications that must be provided are :

- constant relative volatility of each component, α_j
- K-value of the heaviest component as a function of temperature
- constant liquid enthalpy of each component, h_j
- constant vapor enthalpy of each component, H_j
- energy content and composition of each feed
- selection of the light key (LK) and the heavy key (HK)
- recovery ratio of LK and HK in the top and the bottom products, respectively
- selection of a partial or a total condenser

Note that component 1 is the most volatile and feed 1 is located at the top of the column.

First, the algorithm is selected and the data are read accordingly. Although there are four ways to specify the feed condition, HF, ΔHF, HF/F and ΔHF/F, only ΔHF is used for the calculation. The other specifications are transformed into ΔHF.

Then, the program calculates the maximum dimension of the linear system to be solved. The sizing is determined by the limits of ten components and five feeds:

- maximum number of sections
- maximum number of intermediate sections
- maximum number of light components
- maximum number of intermediate components
- maximum number of heavy components
- maximum number of roots ϕ
- maximum number of roots ϕ between the lightest component and LK
- maximum number of roots ϕ between LK and HK
- maximum number of roots between HK and the heaviest component
- maximum number of hypothesis (internal flow patterns)
- maximum number of hypothesis for a case
- maximum number of cases
- maximum number of distributions (external distribution)

Also, relative volatilities should be specified from the most volatile to the least volatile components. They can be specified with reference to any component. The program transforms the data in two sets: one with the least volatile component as the reference and the other one with HK as the reference.

The feeds are placed in the right order. This is necessary because they may not be specified in the best order or may be specified so that the separation is impossible. The K-value of the reference component is calculated from the bubble point equation for each feed. Starting from the top, the feed with the lowest K_{ref} is the first one. Once we find the proper order of the feeds, the specifications are transfered accordingly.

The latent heat of vaporization of each component is then found with Equation 4.1 :

$$\lambda_j = H_j - h_j \qquad (4.1)$$

and the energy contribution of each feed (ΔHF), which is equal to the gap between two adjacent sections, is described by Equation GU4 :

$$(\Delta\Gamma)_i = (\Delta HF)_i \tag{GU4}$$

From the specified recovery of the keys in the distillate, p_{LK} and p_{HK} are known for each section of the column. The split location of the net upward flowrate of LK and HK is, then, determined. For example, if d_{LK} =18 moles and the first, the second, and the third feeds contain 10, 6, and 3 moles, respectively, the split of LK occurs on the third feed where 2 moles go up and 1 mole goes down in the bottom product. The same thing is done for HK. Since the upper feed should contain less heavy components and the lower feed, less light components, LK-split and HK-split should occur on the lower and the upper feeds, respectively. There is one limit : LK-split can not be higher than HK-split. Otherwise, the sections located between LK-split and HK-split become a mixer instead of a fractionator and should be removed.

The maximum number of feeds and components enables us to declare the maximum dimensions of the arrays. However, the dimensions of the actual problem can be smaller. The actual dimensions are also calculated in the same fashion. At this point, the solution of the problem starts. First, the common roots $(\Phi_k)_{Fi}$ are found with Equation GU4 :

$$\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (f_j)_i}{\alpha_j - (\Phi_k)_{Fi}} = (\Delta HF)_i \tag{GU4}$$

where α_j, λ_j, $(f_j)_i$ and $(\Delta HF)_i$ are specified. This is done for each feed "i". The roots are labelled $(\Phi_{AB})_{Fi}$, $(\Phi_{BC})_{Fi}$, and $(\Phi_{CD})_{Fi}$ for a four component mixture. The number of potentially valid roots is n'-1, where n' is the number of distributing components. If component A does not distribute, $(\Phi_{AB})_{Fi}$ must be rejected for each feed. The roots are kept in memory for future recalls.

As described in Chapter 3 (Section 3.2), $(\Phi_k)_{Fi}$ may be chosen from any feed 'i'. This generates more than one possible solutions. In order to cover all cases applicable to a given problem, the computer program is structured in the following manner :

1° The external distribution is assumed. The sequence starts with all components distributing and one by one the lightest and the heaviest components are said not to distribute.

2° From the external distribution, the program assumes the internal flow pattern. It generates hypothesis on $(p_j)_i$ for each component 'j' in each section 'i'. As seen in Chapter 3 (Section 3.2) each hypothesis produces many cases. Since different hypothesis may generate the same case, the program finds directly each case in order not to repeat it. The corresponding hypothesis for each case are found later in the testing procedure.

Now, Equation GU2 must be solved for each section 'i' :

$$\sum_{j=1}^{n} \frac{(p_j)_i \alpha_j \lambda_j}{\alpha_j - (\phi_k)_i} = \Gamma_i \qquad \text{(GU2)}$$

where α_j, λ_j and $(\phi_k)_i$ are known. Roots $(\phi_k)_i$ are selected among $(\Phi_k)_{Fi}$ as demonstrated in Chapter 3 (Section 3.2). The unknowns are $(p_j)_i$ and Γ_i. However, $(p_{LK})_i$ and $(p_{HK})_i$ are known for each section 'i'.

Let us illustrate the problem with the separation of six components with a three feed column. Assuming that all components distribute, a selected set of $(\Phi_k)_{Fi}$ would be :

$(\Phi_{AB})_{F3}$ $(\Phi_{BC})_{F3}$ $(\Phi_{CD})_{F2}$ $(\Phi_{DE})_{F2}$ $(\Phi_{EF})_{F1}$. Each $(\Phi_k)_{Fi}$ can apply to the sections adjacent to feed "i". For example, $(\Phi_{AB})_{F3}$ comes from feed 3 and can only be applied to Equation GU2 for sections 3 and 4 of the column. For practical reasons, each $(\Phi_k)_{Fi}$ is used for one section only. This leaves five degrees of freedom to variables $(p_j)_i$. Otherwise we have to verify which equations are linearly dependent from one section to the next. The unknowns and the equations are established as follows :

1° The unknowns are :

$(p_j)_i$	: (4 sections "i") · (6 components "j") :	24
Γ_i	: 4 sections "i" :	4
$(\theta_k)_i$	: (4 sections "i") · (5 roots "k") :	20
total		48

2° The specified variables are :

$(p_{LK})_1$	:	1
$(p_{HK})_4$	:	1
$(\theta_k)_i = (\Phi_k)_{Fi}$	:	5
total		7

which makes a total of 41 unknowns.

3° The equations available are:

Type 1 : from Equation GU2

$$\sum_{j=1}^{n} \frac{(p_j)_i\, q_j}{q_j - (\theta_k)_i} = \Gamma_i \qquad \text{(GU2)}$$

(4 sections "i") · (5 roots "k") : 20

Type 2 :

$$(p_j)_i + \sum_{l=1}^{i-1} (f_j)_l = (p_j)_1 \tag{4.32}$$

(3 sections 'i') · (6 components 'j') : 18

Type 3 :

$$\Gamma_i + \sum_{l=1}^{i-1} (\Delta\Gamma)_l = \Gamma_1 \tag{4.33}$$

3 sections 'i' : 3

total 41

Adding equations of Type 1, Type 2, and Type 3 makes a total of 41 equations available to determine the 41 unknowns. Equation 4.32 is a relationship between the net upward flowrate in any section 'i' and the net upward flowrate in the top section, for any component 'j'. Equation 4.33 links Γ_i for any section 'i' to Γ_1 for the top section by introducing the contribution of the feeds. From Equation GU4, $(\Delta HF)_l = (\Delta\Gamma)_l$.

This linear system of equations can be simplified. Equation GU2 for any section 'i' ($i \neq 1$) can be transfered to section 1 with Equations 4.32 and 4.33. Substituting Equation 4.32 in GU2 yields :

$$\sum_{j=1} \frac{\left[(p_j)_1 - \sum_{l=1}^{i-1} (f_j)_l\right] \alpha_j}{\alpha_j - (\phi_k)_i} = \Gamma_i \tag{4.34}$$

Isolating $(p_j)_1$:

$$\sum_{j=1}^{n}\frac{(p_j)_1\alpha_j\lambda_1}{\alpha_j-(\theta_k)_1}-\Gamma_1=\sum_{j=1}^{n}\frac{\alpha_j\lambda_1\sum_{i=1}^{l-1}(f_j)_i}{\alpha_j-(\theta_k)_1} \tag{4.35}$$

and substituting Equation 4.33 in 4.35 :

$$\sum_{j=1}^{n}\frac{(p_j)_1\alpha_j\lambda_1}{\alpha_j-(\theta_k)_1}-\Gamma_1=\sum_{j=1}^{n}\frac{\alpha_j\lambda_1\sum_{i=1}^{l-1}(f_j)_i}{\alpha_j-(\theta_k)_1}-\sum_{i=1}^{l-1}(\Delta\Gamma)_i \tag{4.36}$$

Basically, all the unknowns appear in the left hand side term. Since $(p_j)_1$ is equal to d_j for LK and HK, and since $(p_j)_1$ is either zero or the amount fed to the column for the non-distributing components, Equation 4.36 becomes :

$$\sum_{\substack{\geq ITC\\ \leq IBC\\ \neq LK\\ \neq HK}}\frac{(p_j)_1\alpha_j\lambda_1}{\alpha_j-(\theta_k)_1}-\Gamma_1=\sum_{j=1}^{n}\frac{\alpha_j\lambda_1\sum_{i=1}^{l-1}(f_j)_i}{\alpha_j-(\theta_k)_1}-\sum_{\substack{< ITC\\ > IBC\\ = LK\\ = HK}}\frac{(p_j)_1\alpha_j\lambda_1}{\alpha_j-(\theta_k)_1}-\sum_{i=1}^{l-1}(\Delta\Gamma)_i \tag{4.37}$$

With six distributing components, the unknowns are :

$(p_j)_1$	:	6 components T - LK - HK	: 4
Γ_1	:	section 1	: 1
total			5

and five Equations 4.37 are generated from the five roots ϕ_{AB} ϕ_{BC} ϕ_{CD} ϕ_{DE} ϕ_{EF}. The problem started with 41 unknowns and is reduced to 5 unknowns. Basically, we solve the system for the rectifying section (section 1) and then we apply Equations 4.32 and 4.33 to find the unknowns in the lower sections. In more general terms, the dimension of the simplified system is equal to n'-1, where n' is number of distributing components.

The solution for this case is found. Now, we have to make sure that the assumptions made prior to the calculation are verified. Eight tests are performed and the order minimizes the additional calculations required to eliminate or keep the case.

Test No. 1 : verify the compatibility of the computed internal flow pattern with Equation GU1. For example, we have a five component mixture fractionated with a two feed column. LK and HK are, respectively, components B and D. Let us say that the actual sign change occurs between components C and D. As demonstrated in Chapter 3 (Section 3.2), application of Equation GU1 for the intermediate section yields :

$$\sum_{j=1}^{n} \frac{\alpha_j (\Delta d_j)_1}{\alpha_j - (\phi_{BC})_2} - \boxed{\sum_{j=1}^{n} \frac{\alpha_j (\Delta d_j)_2}{\alpha_j - (\phi_{AB})_2}} = 0$$

$$\sum_{j=1}^{n} \frac{\alpha_j (\Delta d_j)_1}{\alpha_j - (\phi_{CD1})_2} - \boxed{\sum_{j=1}^{n} \frac{\alpha_j (\Delta d_j)_2}{\alpha_j - (\phi_{BC})_2}} = 0$$

$$\boxed{\sum_{j=1}^{n} \frac{\alpha_j (\Delta d_j)_1}{\alpha_j - (\phi_{CD2})_2} - \sum_{j=1}^{n} \frac{\alpha_j (\Delta d_j)_2}{\alpha_j - (\phi_{CD1})_2}} = 0$$

$$\boxed{\sum_{j=1}^{n} \frac{\alpha_j (\Delta d_j)_1}{\alpha_j - (\phi_{DE})_2}} - \sum_{j=1}^{n} \frac{\alpha_j (\Delta d_j)_2}{\alpha_j - (\phi_{CD2})_2} = 0$$

The terms in a box must satisfy their respective equation. As for the third equation, it may be satisfied by either term. This exercise tells us that ϕ_{AB} and ϕ_{BC} used for the calculation must come from Equation GU4 for feed 2 and be equal to $(\Phi_{AB})_{F2}$ and $(\Phi_{BC})_{F2}$, respectively. In the same fashion, ϕ_{EF} must be equal to $(\Phi_{EF})_{F1}$ coming from feed 1. Root ϕ_{CD} can come from either feed and be equal to $(\Phi_{CD})_{F1}$ or $(\Phi_{CD})_{F2}$. The origin (feed number) of each root is compared with the possible origin of the roots generated with the actual flow pattern. If the original ϕ_{BC} comes from feed 1, $(\Phi_{BC})_{F1}$, it is not compatible with $(\Phi_{BC})_{F2}$ deducted from the internal flow pattern. Only the feed indexes are required to perform this test.

Test No. 2 : verify the overall material balance for each component "j", where N is the number of feeds :

$$\sum_{i=1}^{N} (f_j)_i = d_j + b_j \qquad (4.38)$$

where : $d_j \geq 0$, $b_j \geq 0$, $(f_j)_i > 0$

Test No. 3 : verify internal flowrates. This procedure requires several steps.

Step 1 : The first step is to find the roots $(\Phi_k)_k$ valid on the feed trays "k". They should satisfy Equation GU3 :

$$\sum_{j=1}^{n} \frac{\alpha_j (f_j)_k}{\alpha_j - (\Phi_k)_k} = 0 \qquad (GU3)$$

One must distinguish these roots from the roots $(\Phi_k)_{Fi}$ already determined with Equation GU4. The latter are potentially valid roots. Among them, only the set generating the good solution is a subset of the roots valid on the feed trays. However,

$(\Phi_{lk})_{fi}$ cannot be found with Equation GU3 because the liquid concentrations on the feed trays, $(x_j)_{fi}$, are not known. The roots $(\Phi_{lk})_{fi}$ must be found with Equation GU2 applied to the adjacent sections of a given feed plate "fi".

$$\sum_{j=1}^{n} \frac{(p_j)_k \alpha_j \lambda_j}{\alpha_j - (\phi_{lk})_i} = \Gamma_i \tag{GU2}$$

where $(p_j)_k$, α_j, λ_j, and Γ_i are known. There are roots $(\phi_{lk})_i$ to be found. We now explain the relationship between $(\phi_{lk})_i$ and $(\Phi_{lk})_{fi}$.

Table 6 displays the application of Equations GU1 and GU3 for a six component mixture fractionated with a three feed column. The sign change occurs between components B and C in both intermediate sections. The underlined roots satisfy Equation GU1 for each section (horizontal axis). With the double roots, $(\phi_{BC1})_3$, and $(\phi_{BC2})_3$, for example, only one is necessary. The set of common roots $(\Phi_{lk})_{Fi}$ generating this case is : $(\Phi_{AB})_{F3}$ $(\Phi_{BC})_{F3}$ $(\Phi_{CD})_{F1}$ $(\Phi_{DE})_{F1}$ $(\Phi_{EF})_{F1}$, where "i" is the feed index. These common roots are indicated by the stars. At this point, the latter are the only roots known.

Now the selection of the double roots can be done. As indicated by the stars, $(\phi_{BC1})_3$ and $(\phi_{BC})_4$ are the same. This is a common root and must be choosen. Therefore, $(\phi_{BC2})_3$ is not required to satisfy Equation GU1. Starting form the top, $(\phi_{BC})_1$ and $(\phi_{BC2})_2$ are not common. The latter is eliminated because $(\phi_{BC})_1$ is required to satisfy Equation GU1 in section 1. Since $(\phi_{BC2})_2$ is eliminated, $(\phi_{BC1})_2$ is kept. This is in concordance with the previous elimination of $(\phi_{BC2})_3$.

TABLE 6. Utilization of Equations GU1 and GU3 to find the common roots $(\Phi_{i,j})_f$ on the feed plates. 3 feed column and 2 split-key components.

Case : 6 components : A, B, C, D, E, F,
3 feeds, 4 sections
two split-key components : LK = B, HK = E
flow pattern : sign change section 2 : B → C
sign change section 3 : B → C

$$\sum_{j=1}^{n} \frac{\alpha_j \Delta (q z_j)_{f1}}{\alpha_j - (\Phi_{i,j})_{f1}} = 0 \qquad \sum_{j=1}^{n} \frac{\alpha_j \Delta (q z_j)_{f2}}{\alpha_j - (\Phi_{i,j})_{f2}} = 0 \qquad \sum_{j=1}^{n} \frac{\alpha_j \Delta (q z_j)_{f3}}{\alpha_j - (\Phi_{i,j})_{f3}} = 0$$

	feed 1		feed 2		feed 3
section 1	$(\phi_{\underline{AB}})_1$ $(\phi_{\underline{BC}})_1$ $(\phi_{\underline{CD}})_1^*$ $(\phi_{\underline{DE}})_1^*$ $(\phi_{\underline{EF}})_1^*$				
section 2	$(\phi_{BC1})_2$ $(\phi_{\underline{BC2}})_2$ $(\phi_{\underline{CD}})_2^*$ $(\phi_{\underline{DE}})_2^*$ $(\phi_{\underline{EF}})_2^*$	or	$(\phi_{\underline{AB}})_2$ $(\phi_{\underline{BC1}})_2$ $(\phi_{BC2})_2$ $(\phi_{CD})_2$ $(\phi_{DE})_2$		
section 3			$(\phi_{BC1})_3$ $(\phi_{\underline{BC2}})_3$ $(\phi_{\underline{CD}})_3$ $(\phi_{\underline{DE}})_3$ $(\phi_{\underline{EF}})_3$	or	$(\phi_{\underline{AB}})_3^*$ $(\phi_{\underline{BC1}})_3^*$ $(\phi_{BC2})_3$ $(\phi_{CD})_3$ $(\phi_{DE})_3$
section 4					$(\phi_{\underline{AB}})_4^*$ $(\phi_{\underline{BC}})_4^*$ $(\phi_{\underline{CD}})_4$ $(\phi_{\underline{DE}})_4$ $(\phi_{\underline{EF}})_4$

In summary, we have :

feed 1 : $(\Phi_{AB})_{f1} = (\phi_{AB})_1$

$(\Phi_{BC})_{f1} = (\phi_{BC})_1$

$(\Phi_{CD})_{f1} = (\phi_{CD})_1 = (\phi_{CD})_2 = (\Phi_{CD})_{F1}$

$(\Phi_{DE})_{f1} = (\phi_{DE})_1 = (\phi_{DE})_2 = (\Phi_{DE})_{F1}$

$(\Phi_{EF})_{f1} = (\phi_{EF})_1 = (\phi_{EF})_2 = (\Phi_{EF})_{F1}$

feed 2 : $(\Phi_{AB})_{f2} = (\phi_{AB})_2$

$(\Phi_{BC})_{f2} = (\phi_{BC1})_2$

$(\Phi_{CD})_{f2} = (\phi_{CD})_3$

$(\Phi_{DE})_{f2} = (\phi_{DE})_3$

$(\Phi_{EF})_{f2} = (\phi_{EF})_3$

feed 3 : $(\Phi_{AB})_{f3} = (\phi_{AB})_3 = (\phi_{AB})_4 = (\Phi_{AB})_{F3}$

$(\Phi_{BC})_{f3} = (\phi_{BC1})_3 = (\phi_{BC})_4 = (\Phi_{BC})_{F3}$

$(\Phi_{CD})_{f3} = (\phi_{CD})_4$

$(\Phi_{DE})_{f3} = (\phi_{DE})_4$

$(\Phi_{EF})_{f3} = (\phi_{EF})_4$

Roots $(\phi_k)_i$ are found with Equation GU2 for each section which provides us with roots $(\Phi_k)_{fi}$. The valid common roots $(\Phi_k)_{Fi}$ do not have to be determined again. If all roots cannot be found, the case must be rejected.

Step 2 : Once all $(\Phi_k)_{fi}$ are found, Equation GU3 is solved for the liquid fractions $(x_j)_{fi}$ on each feed plate "fi". On each feed plate, there are five roots generating five Equations GU3. The system of equations is the following :

$$\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (x_j)_{fi}}{\alpha_j - (\Phi_k)_{fi}} = 0 \tag{4.39}$$

with $(\Phi_k)_{fi} = (\Phi_{AB})_{fi}, (\Phi_{BC})_{fi}, (\Phi_{CD})_{fi}, (\Phi_{DE})_{fi}, (\Phi_{EF})_{fi}$

and

$$\sum_{j=1}^{n} (x_j)_{fi} = 1 \tag{4.40}$$

Step 3 : Other quantities related to the feed plate are calculated. The vapor fractions $(y_j)_{fi}$ on each feed plate "fi" are found from Equation 3.4 and V_{fi} and L_{fi} from Equation GU2 :

$$(y_{HK})_{fi} = \frac{1}{\sum_{j=1}^{n} \alpha_j \left(\frac{x_j}{x_{HK}}\right)_{fi}} \tag{4.41}$$

$$(y_j)_{fi} = \alpha_j \, (y_{HK})_{fi} \left(\frac{x_j}{x_{HK}}\right)_{fi} \tag{4.42}$$

$$V_{fi} = \frac{\Gamma_{fi}}{\sum_{j=1}^{n} (y_j)_{fi} \lambda_j} \tag{4.43}$$

$$L_{fl} = \frac{r_l - \sum_{j=1}^{n} (p_j)_l \lambda_j}{\sum_{j=1}^{n} (x_j)_{fl} \lambda_j} \tag{4.44}$$

where subscripts are :

fl : feed plate 'f'
u : section above a given feed
l : section below a given feed

Step 4 : Calculation of the vapor and liquid fractions as well as the vapor and liquid flowrates at the top and the bottom of the rectifying section. The basic relationships used are Equations 3.2, 3.3, 3.4, and GU2.

- Top of the section with a total condenser :

$$((y_j)_t)_l = d_j/D \tag{4.45}$$

$$((x_j)_t)_l = d_j/D \tag{4.46}$$

$$(V_t)_l = \frac{r_l}{\sum_{j=1}^{n} ((y_j)_t)_l \lambda_j} \tag{4.47}$$

$$(L_t)_l = (V_t)_l - \sum_{j=1}^{n} (p_j)_l \tag{4.48}$$

- Top of the section with a partial condenser :

$$(y_j)_c = d_j/D \tag{4.49}$$

$$(x_{HK})_c = \frac{1}{\sum_{j=1}^{n} \frac{1}{\alpha_j}\cdot\left(\frac{y_j}{y_{HK}}\right)_c} \qquad (4.50)$$

$$((x_j)_t)_i = (x_j)_c = \frac{1}{\alpha_j}\cdot(x_{HK})_c\cdot\left(\frac{y_j}{y_{HK}}\right)_c \qquad (4.51)$$

$$(L_t)_i = \frac{r_i - \sum_{j=1}^{n}(p_j)_i\,\lambda_j}{\sum_{j=1}^{n}((x_j)_t)_i\,\lambda_j} \qquad (4.52)$$

$$(V_t)_i = (L_t)_i + \sum_{j=1}^{n}(p_j)_i \qquad (4.53)$$

$$((y_j)_t)_i = \frac{(L_t)_i\,((x_j)_t)_i + (p_j)_i}{(V_t)_i} \qquad (4.54)$$

- Bottom of the section :

$$(V_b)_i = (V_t)_b \qquad (4.55)$$

$$(L_b)_i = (V_b)_i - \sum_{j=1}^{n}(p_j)_i \qquad (4.56)$$

$$((y_j)_b)_i = ((y_j)_t)_b \qquad (4.57)$$

$$((x_j)_b)_i = \frac{(V_b)_i\,((y_j)_b)_i - (p_j)_i}{(L_b)_i} \qquad (4.58)$$

where subscripts are :

i : section 'i'

t : top of the section
b : bottom of the section
fi : "feed plate i"
c : "condenser"

Step 5 : Calculation of the vapor and liquid fractions as well as the vapor and liquid flowrates at the top and bottom of all intermediate sections. The basic relationships used are Equations 3.2, 3.3, and GU2.

- Top of the section :

$$(L_t)_i = (L_{fi})_t \qquad (4.59)$$

$$(V_t)_i = (L_t)_i + \sum_{j=1}^{n} (p_j)_i \qquad (4.60)$$

$$((x_j)_t)_i = ((x_j)_{fi})_t \qquad (4.61)$$

$$((y_j)_t)_i = \frac{(L_t)_i \, ((x_j)_t)_i + (p_j)_i}{(V_t)_i} \qquad (4.62)$$

- Bottom of the section :

$$(V_b)_i = (V_{fi})_b \qquad (4.63)$$

$$(L_b)_i = (V_b)_i - \sum_{j=1}^{n} (p_j)_i \qquad (4.64)$$

$$((y_j)_b)_i = ((y_j)_{fi})_b \qquad (4.65)$$

$$((x_j)_{fi})_i = \frac{(V_{fi})_i\,((y_j)_{fi})_i - (p_j)_i}{(L_{fi})_i} \qquad (4.66)$$

where subscripts are :

i : section "i"
t : top of the section
b : bottom of the section
fi : "feed plate i"

Step 6 : Calculation of the vapor and liquid fractions as well as the vapor and liquid flowrates at the top and bottom of the stripping section. The basic relationships used are Equations 3.2, 3.3, 3.4, and GU2.

- Top of the section :

$$(L_t)_i = (L_{fi})_i \qquad (4.67)$$

$$(V_t)_i = (L_t)_i + \sum_{j=1}^{n} (p_j)_i \qquad (4.68)$$

$$((x_j)_t)_i = ((x_j)_{fi})_i \qquad (4.69)$$

$$((y_j)_t)_i = \frac{(L_t)_i\,((x_j)_t)_i + (p_j)_i}{(V_t)_i} \qquad (4.70)$$

- Bottom of the section :

$$(x_j)_R = b_j / B \qquad (4.71)$$

$$(K_{HK})_R = \frac{1}{\displaystyle\sum_{j=1}^{n} x_j \left(\frac{K_j}{K_{HK}}\right)_R} \qquad (4.72)$$

$$((y_j)_b)_i = (y_j)_R = \alpha_j (y_{HK})_R \left(\frac{x_j}{x_{HK}}\right)_R \qquad (4.73)$$

$$(V_b)_i = \frac{\Gamma_i}{\sum_{j=1}^{n} ((y_j)_b)_i \lambda_j} \qquad (4.74)$$

$$(L_b)_i = (V_b)_i - \sum_{j=1}^{n} (b_j)_i \qquad (4.75)$$

$$((x_j)_b)_i = \frac{(V_b)_i ((y_j)_b)_i - (b_j)_i}{(L_b)_i} \qquad (4.76)$$

where subscripts are :

i : section "i"
t : top of the section
b : bottom of the section
fi : "feed plate i"
R : "reboiler"

Step 7 : Verify all flowrates :

$$V \geq 0 \qquad (4.77)$$

$$L \geq 0 \qquad (4.78)$$

Test No. 4 : Verify if there are any negative fractions around the feed plates, two plates up and two plates down. The fractions on the feed plates are already known. All fractions should be greater than or equal to zero. The basic relationships are Equations 3.2, 3.3, 3.4, and GU2.

- The equations when moving up are :

$$(L_i)_k = (V_{i-1})_k - \sum_{j=1}^{n} (p_j)_k \tag{4.79}$$

$$((x_j)_i)_k = \frac{(V_{i-1})\,((y_j)_{i-1})_k - (p_j)_k}{(L_i)_k} \tag{4.80}$$

$$((y_{HK})_i)_k = \frac{1}{\displaystyle\sum_{j=1}^{n} \alpha_j \left(\left(\frac{x_j}{x_{HK}}\right)_i\right)_i} \tag{4.81}$$

$$((y_j)_i)_k = \alpha_j\,((y_{HK})_i)_k \left(\left(\frac{x_j}{x_{HK}}\right)_i\right)_i \tag{4.82}$$

$$(V_i)_k = \frac{\Gamma_i}{\displaystyle\sum_{j=1}^{n} ((y_j)_i)_k\,\lambda_j} \tag{4.83}$$

- The equations when moving down are :

$$(V_i)_k = (L_{i+1})_k + \sum_{j=1}^{n} (p_j)_k \tag{4.84}$$

$$((y_j)_i)_k = \frac{(L_{i+1})\,((x_j)_{i+1})_k + (p_j)_k}{(V_i)_k} \tag{4.85}$$

$$(D_{HK\,adj})_i = \frac{1}{\sum_{j=1}^{n} \frac{1}{\alpha_j} \cdot \left(\left(\frac{x_j}{x_{HK}}\right)_{\lambda}\right)_i} \qquad (4.86)$$

$$(D_j)_i = \frac{1}{\alpha_j} (D_{HK\,adj})_i \left(\left(\frac{x_j}{x_{HK}}\right)_{\lambda}\right)_i \qquad (4.87)$$

$$(L_D)_i = \frac{r_i - \sum_{j=1}^{n} (d_j)_i \lambda_j}{\sum_{j=1}^{n} (D_j)_i \lambda_j} \qquad (4.88)$$

where subscripts are :

i : section "i"

j : any plate "j"

Test No. 5 : Verify the following equation for each intermediate section.

$$(\Phi_{SC})_t \leq (\Phi_{SC})_b \qquad (4.89)$$

Φ_{SC} stands for the root which corresponds to the location of the "sign change" in the section. For example, when the flowrates of components C and D are, respectively, +80 and -80, the root is Φ_{CD}. Roots Φ_{SC} determined with Equation GU4 should be smaller for the feed at the top of the section. Subscripts "t" and "b" stand for "top feed" and "bottom feed" of a section.

Test No. 6 : We already said that the sets of roots $(\Phi_k)_{Fi}$ are generated from the hypothesis made on the internal flow patterns. By inspection of these sets, it is possible to build them without knowing the hypothesis. Since more than one hypothesis may generate the same set, sets of roots are directly applied to avoid repetition.

For a given set, we can find all the corresponding hypothesis. Now, we have to verify if the actual (calculated) internal flow pattern matches with at least one hypothesis generating the set of roots $(\Phi_k)_{Fi}$ selected for the calculation.

Test No. 7 : Find the pinch region for each section. If only one pinch cannot be found, the case is rejected. Superscript "∞" indicates the pinch region. The equations and the procedure to follow are :

From Equations GU2 and 3.2 :

$$V_i^{\infty}\sum_{j=1}^{n}(y_j)_i^{\infty}\lambda_j = \sum_{j=1}^{n}(v_j)_i^{\infty}\lambda_j = \Gamma_i \tag{4.90}$$

$$(l_j)_i^{\infty} = (v_j)_i^{\infty} - (d_j)_i \tag{4.91}$$

With Equation 3.4 and knowing that for a pinch region,

$$(x_j)^{\infty} = (x_j)_i = (x_j)_{i+1} \tag{4.92}$$

$$(y_j)^{\infty} = (y_j)_i = (y_j)_{i+1} \tag{4.93}$$

we have :

$$\alpha_j = \frac{(v_j)^{\infty}/(l_j)^{\infty}}{(v_{HK})^{\infty}/(l_{HK})^{\infty}} \tag{4.94}$$

$$(v_j)_i^{\infty} = \frac{\alpha_j (v_{HK})_i^{\infty} (p_j)_i}{(\alpha_j - 1) \cdot (v_{HK})_i^{\infty} + (p_{HK})_i} \qquad (4.95)$$

Substituting Equation 4.95 in 4.90 :

$$\sum_{j=1}^{n} \frac{\alpha_j \lambda_j (p_j)_i (v_{HK})_i^{\infty}}{(\alpha_j - 1) \cdot (v_{HK})_i^{\infty} + (p_{HK})_i} = \Gamma_i \qquad (4.96)$$

Now, we solve Equation 4.96 for $(v_{HK})_i^{\infty}$. Once this is done, we can replace it in Equation 4.95 and find the vapor flows of each component $(v_j)_i^{\infty}$ at the pinch. The liquid flows $(l_j)_i^{\infty}$ are easily found with Equation 4.91. All concentrations at the pinch must be greater than or equal to zero and are calculated with these equations:

$$(y_j)_i^{\infty} = \frac{(v_j)_i^{\infty}}{\sum_{j=1}^{n} (v_j)_i^{\infty}} \qquad (4.97)$$

$$(x_j)_i^{\infty} = \frac{(l_j)_i^{\infty}}{\sum_{j=1}^{n} (l_j)_i^{\infty}} \qquad (4.98)$$

where subscripts are :

i : section 'i'
j : any plate 'j'

Test No. 8 : Starting from the feed, we calculate the concentrations on each plate until we reach the pinch concentrations found in Test No.7. This is done going up and down from each feed. Also no negative concentrations should be encountered. If the pinch concentrations are not correct or if any concentration is negative, the case must be rejected. The necessary equations are exactly the same as the ones used in Test No.4.

In fact, Test No.8 is an extension of Test No.4. In Test No.4, only two plates are calculated because, most of the time, negative concentrations appear after one or two plates.

At this point, the testing procedure is completed. When the case passes all the tests, complementary calculations are performed. The temperature profile is found with the bubble point equation applied to the liquid phase. We find the temperature at the top, on all pinch plates, on all feed plates, and at the bottom. Finally, the minimum reflux ratio is calculated. This completes all the calculation for one case. The program returns at the beginning and goes through the same procedure for the next case. All cases are tried even if a valid solution is already determined.

The block diagram of the program appears in Figure 21.

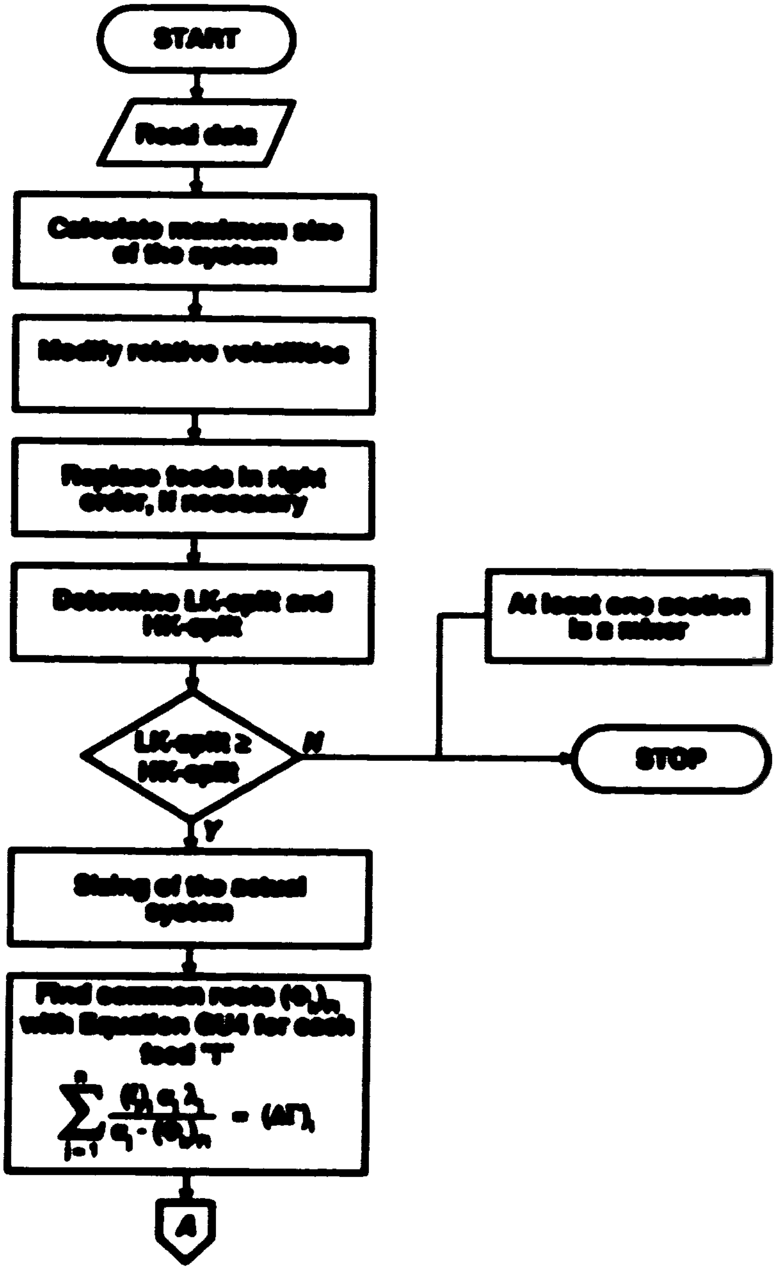

FIGURE 21. Block diagram of the computer program. — *(Part 1 of 3)*

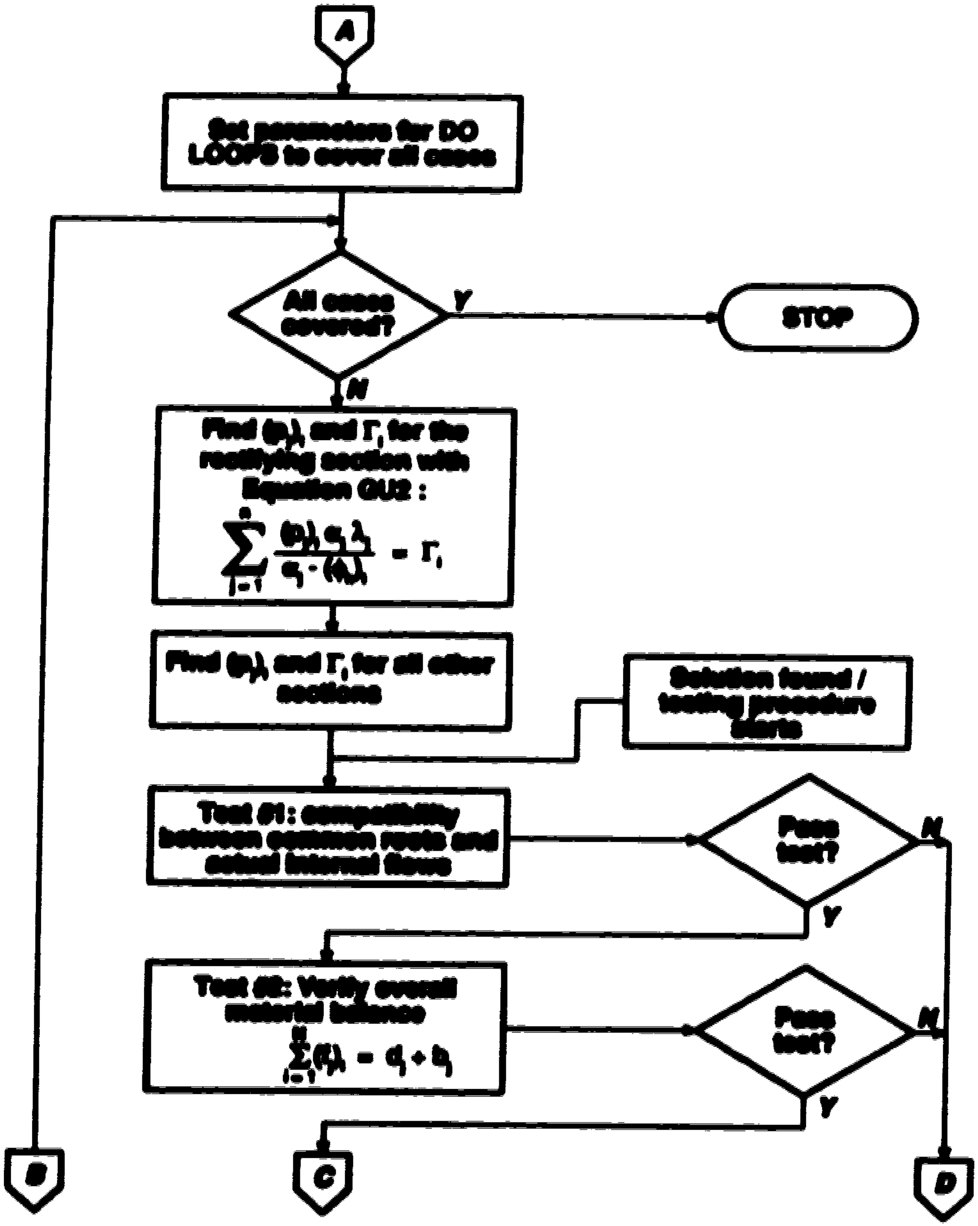

FIGURE 21. Block diagram of the computer program. — *(Part 2 of 3)*

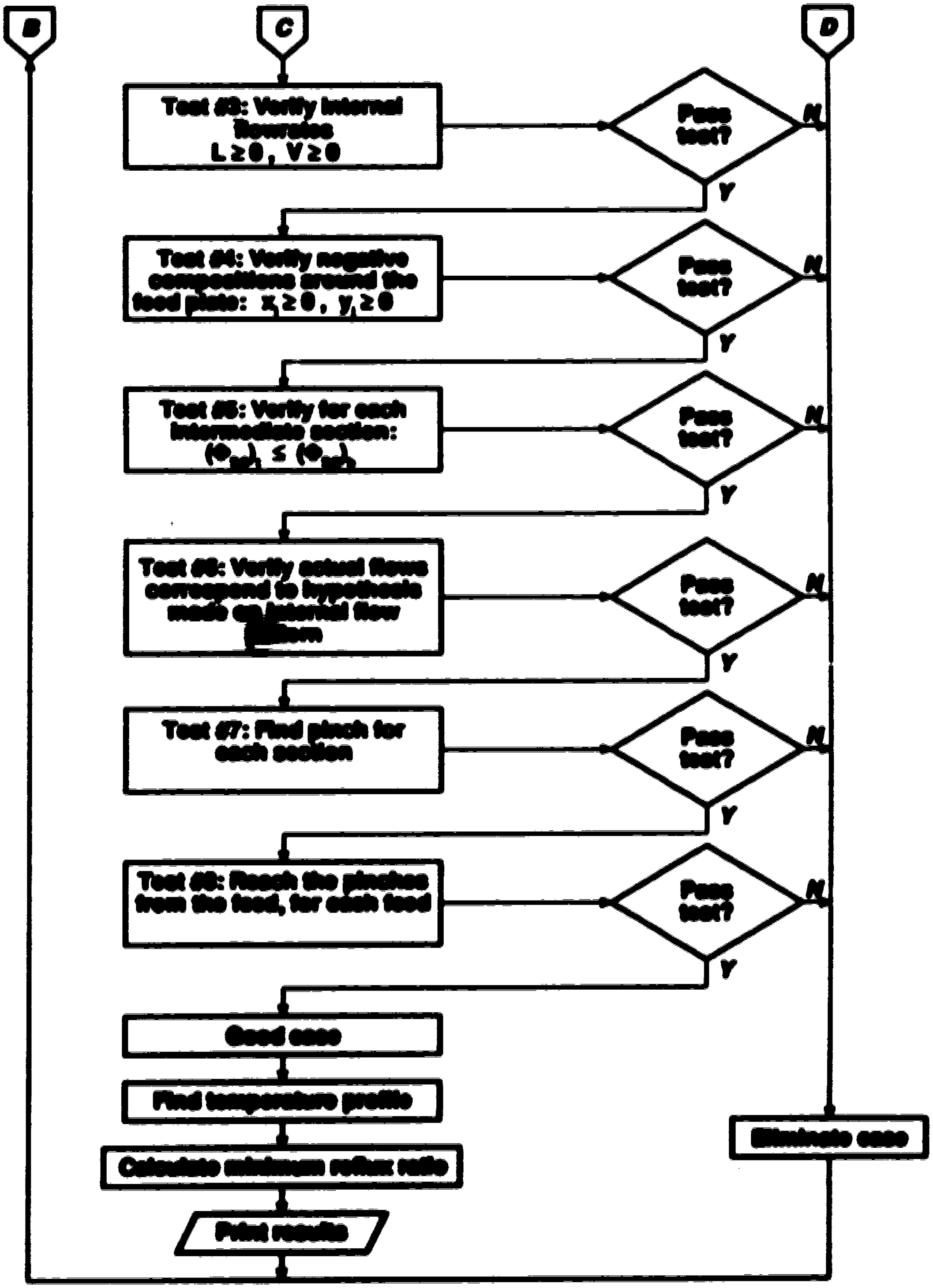

FIGURE 21. Block diagram of the computer program. — *(Part 3 of 3)*

Chapter 5

Evaluation of the New Method

5.1 Method of Comparison

In the previous chapters we have shown the development of the necessary equations for the calculation of the minimum reflux ratio with the Generalized Underwood model applied to multiple feed columns. Also, we explained the utilization of these equations and the sequence observed to eliminate the multiple solutions generated.

The evaluation of the method is twofold. Firstly, results obtained with the model are compared with those obtained with a plate-by-plate algorithm using the same basic assumptions. In other words, both methods should generate exactly the same results. This ensures that the model is correct within the assumptions made. The evaluation is made for different conditions including single and multiple feed columns and for different mixtures. Plate-by-plate calculation is performed with the algorithm of Ishii and Otto (1973).

Secondly, we want to evaluate the minimum reflux ratio value predicted by the model. The results are compared with those of a rigorous plate-by-plate algorithm based on Peng-Robinson's equations. The rigorous simulation is considered as the reference. Also, the Generalized Underwood model is compared with Underwood's model to assess the contribution of the latent heats of vaporization (λ_j). These comparisons are made for single feed columns and for narrow and wide boiling mixtures.

5.2 Verification of the Model

5.2.1 Methodology

The first step is to determine the assumed properties for each component. As required by the Generalized Underwood model, the properties (α_j, h_j, H_j, λ_j) are constant throughout the column. They are estimated at the feed conditions. For multiple feed columns, they are estimated with the geometric mean of the values of each feed. Correlations for the K-values and the enthalpies are taken from Holland (1983). Knowing V_F/F, the temperature is easily determined from a flash calculation. The temperature is then inserted in the correlations. Relative volatilities are calculated from the K-values. Any component may be the reference, but, in this work, we choose the heaviest so that $\alpha_i \geq 1$ for all i.

Ishi's plate-by-plate algorithm can account for pressure drops and accepts rigorous correlations for K-values and enthalpies. However, in this exercise, vapor and liquid enthalpies are set constant to the values estimated earlier. Also, since the calculations require K-values, we must provide the K-value correlation of the reference component. It enables the program to calculate the K-values of the other components from the relative volatilities. The specifications required by this program are the feed degree of vaporization, the top product, and the reflux ratio. We have to make sure that the number of plates is large enough to observe pinch regions. This ensures that minimum reflux conditions are reached. Once all the specifications are established, we can run Ishi's program.

In the last step, we run the Generalized Underwood model to reproduce exactly the results generated by the plate-by-plate simulation. We use the same properties. One must note that the algorithm requires relative volatilities and not K-values. However, providing the K-value correlation of the reference component enables the program to determine the temperature at different locations in the column. The specifications required are the recovery ratio of the amount of LK in the top product over the amount fed, the recovery ratio of the HK recovered in the bottom product over the amount fed, and the energy content of the feed. These three specifications are taken from the results of the plate-by-plate simulation. Then, the algorithm provides us with these outputs :

- Input data
- Composition of the top and bottom products
- Composition of the net upward flowrates in the intermediate sections
- Liquid and vapor traffic at the top, the pinch and the bottom of each section
- Liquid and vapor flow changes on the feed trays
- External minimum reflux ratio (L/D)
- Internal minimum reflux ratio (L/V)
- Feed trays composition
- Pinch regions composition
- Temperature profile

The results selected for the verification with the plate-by-plate algorithm are the composition of the top and bottom products, the composition of the feed trays, the composition of the pinch regions, and the minimum reflux ratio.

5.2.2 Examples and Results

We present here three examples (Examples 1 to 3). In all examples, there are six components which differ for each case. Also, we vary the number of feeds and the key components. In these examples, LK and HK are the lightest and heaviest components that distribute, respectively. However, this program allows the selection of any two components for the keys.

In Example 1, only the key components (C and D) distribute. The separation is performed with a single feed column. A summary of the input data for the plate-by-plate algorithm and the Generalized Underwood model appear in Tables 7a and 7b, respectively. A comparison of the results is shown in Table 8 and a complementary analysis of the pinch regions for the plate-by-plate simulation in Table 9. The complete inputs and outputs for both methods appear in Appendix 1.

TABLE 7a. Specifications for Example 1.
Plate-by-plate method for a 1 feed column.

PLATE-BY-PLATE SIMULATION WITH [illegible] PROGRAM

6 components : C_3H_8, i-C_4, i-C_5, n-C_6, n-C_7, n-C_8

1 feed

Feed : 100 lb-mole

Composition : A=0.15 B=0.15 C=0.20 D=0.20 E=0.15 F=0.15

Liquid feed (L_F/F) : 0.5

Feed plate : Plate #60

Number of plates : 120

Top product : 50 lb-mole

Reflux ratio : 2.2

Condenser : Total

Pressure in the column : 300 PSIA

Properties of the components :

Component		α	h	H	λ = H-h
			BTU/lb-mole		
A	(C_3H_8)	17.38	16204	18932	2728
B	(i-C_4)	11.36	19155	23207	4052
C	(i-C_5)	6.11	22804	28708	5904
D	(n-C_6)	5.41	23506	29367	5861
E	(n-C_7)	1.77	30384	40942	10558
F	(n-C_8)	1.00	33714	46397	12682

TABLE 7b. Specifications for Example 1. Generalized Underwood method for a 1 feed column.

GENERALIZED UNDERWOOD MODEL

6 components : C_3H_8, i-C_4, i-C_5, n-C_5, n-C_7, n-C_8

1 feed : 100 lb-mole

Composition : A=0.15 B=0.15 C=0.20 D=0.20 E=0.15 F=0.15

Energy content of the feed (HF) : 2891868.79 BTU

LK = C

HK = D

LK recovery in the top product $(d/f)_{LK}$: 0.9079815

HK recovery in the bottom product $(b/f)_{HK}$: 0.9079815

Condenser : Total

Pressure in the column : 300 PSIA

Properties of the components :

Component		α	h	H	λ = H-h
			BTU/lb-mole		
A	(C_3H_8)	17.38	16204	18932	2728
B	(i-C_4)	11.36	19155	23207	4052
C	(i-C_5)	6.11	22904	28708	5804
D	(n-C_5)	5.41	23506	29367	5861
E	(n-C_7)	1.77	30384	40942	10558
F	(n-C_8)	1.00	33714	46367	12682

TABLE 8. Results from Example 1.
Comparison of the liquid mole fractions at selected locations in the column obtained with the plate-by-plate and Generalized Underwood methods.

Location in the column	Algorithm	Component liquid mole fraction							Reflux ratio
		A	B	C	D	E	F	TOTAL	
Top product	plate-by-plate	0.3000	0.3000	0.2432	0.1568	0.0000	0.0000	1.0000	2.20
	G. UND.	0.3000	0.3000	0.2432	0.1568	0.0000	0.0000	1.0000	2.20
Top pinch	plate-by-plate	0.0586	0.1119	0.3880	0.4416	0.0000	0.0000	1.0000	
	G. UND.	0.0586	0.1119	0.3880	0.4416	0.0000	0.0000	1.0000	
Feed plate	plate-by-plate	0.0478	0.0871	0.2727	0.3004	0.1542	0.1378	1.0000	
	G. UND.	0.0478	0.0871	0.2727	0.3004	0.1542	0.1378	1.0000	
Bottom pinch	plate-by-plate	0.0000	0.0000	0.3309	0.3540	0.1672	0.1479	1.0000	
	G. UND.	0.0000	0.0000	0.3309	0.3540	0.1672	0.1479	1.0000	
Bottom product	plate-by-plate	0.0000	0.0000	0.1568	0.2432	0.3000	0.3000	1.0000	
	G. UND.	0.0000	0.0000	0.1568	0.2432	0.3000	0.3000	1.0000	

TABLE 9. Results from Example 1.
Locations of the pinch regions for the plate-by-plate calculation.

Location in the column	Component liquid mole fraction		Plates with same mole fractions	Plates constituting the pinch
	component	x		
Top pinch	A	0.0586	16 to 54	32 to 40
	B	0.1119	21 to 53	
	C	0.3880	31 to 40	
	D	0.4416	32 to 52	
	E	0.0000	1 to 50	
	F	0.0000	1 to 54	
Bottom pinch	A	0.0000	60 to 120	74 to 85
	B	0.0000	60 to 120	
	C	0.3309	80 to 92	
	D	0.3540	76 to 85	
	E	0.1672	75 to 100	
	F	0.1479	74 to 112	

Number of plates : 120
Location of the feed : Plate #60

In Example 2, components B, C, D, and E distribute. Components B and E are the keys. The separation is performed with a two feed column. A summary of the input data appears in Tables 10a and 10b. The results and the analysis of the pinch regions are shown in Tables 11 and 12, respectively. The complete inputs and outputs for both methods appear in Appendix 2.

In Example 3, all six components distribute. Components A and F are the keys. The separation is performed with a three feed column. A summary of the input data appear in Tables 13a and 13b. The results and the analysis of the pinch regions are shown in Tables 14 and 15, respectively.

In Table 16, we complete these results with a comparison of the time required to run each algorithm.

TABLE 10a. Specifications for Example 2.
Plate-by-plate method for a 2 feed column.

PLATE-BY-PLATE SIMULATION WITH [illegible] PROGRAM

6 components : C_3H_8, $n\text{-}C_4$, $i\text{-}C_5$, $n\text{-}C_5$, $n\text{-}C_6$, $n\text{-}C_7$
2 feeds
Feed #1 : 100 lb-mole
Feed #2 : 100 lb-mole
Composition feed #1: A=0.25 B=0.20 C=0.20 D=0.20 E=0.10 F=0.05
Composition feed #2: A=0.05 B=0.10 C=0.20 D=0.20 E=0.20 F=0.25
Liquid feed #1 (L_F/F) : 0.4
Liquid feed #2 (L_F/F) : 0.6
Feed plate #1 : 60
Feed plate #2 : 120
Number of plates : 180
Top product : 110 lb-mole
Reflux ratio : 0.85
Condenser : Total
Pressure in the column : 300 PSIA

Properties of the components:

Component		α	h	H	$\lambda = H\text{-}h$
			BTU/lb-mole		
A	(C_3H_8)	11.04	15425	18425	3000
B	($n\text{-}C_4$)	5.96	18672	23025	4353
C	($i\text{-}C_5$)	3.08	21708	28011	6303
D	($n\text{-}C_5$)	3.24	22375	28716	6341
E	($n\text{-}C_6$)	1.77	25703	34283	8580
F	($n\text{-}C_7$)	1.00	28905	40006	11101

TABLE 10b. Specifications for Example 2.
Generalized Underwood method for a 2 feed column.

GENERALIZED UNDERWOOD MODEL

6 components : C_3H_8, n-C_4, i-C_5, n-C_5, n-C_6, n-C_7

2 feeds

Feed #1 : 100 lb-mole

Feed #2 : 100 lb-mole

Composition feed #1: A=0.25 B=0.20 C=0.20 D=0.20 E=0.10 F=0.05

Composition feed #2: A=0.05 B=0.10 C=0.20 D=0.20 E=0.20 F=0.25

Energy content feed #1 (HF) : 2254430.11 BTU

Energy content feed #2 (HF) : 2655110.58 BTU

LK = B

HK = E

LK recovery in the top product $(d/f)_{LK}$: 0.9143714

HK recovery in the bottom product $(b/f)_{HK}$: 0.8853846

Condenser : Total

Pressure in the column : 300 PSIA

Properties of the components :

Component		α	h	H	λ = H-h
			BTU/lb-mole		
A	(C_3H_8)	11.04	15425	18425	3000
B	(n - C_4)	5.96	18972	23025	4053
C	(i - C_5)	3.68	21703	28011	6308
D	(n - C_5)	3.24	22375	28716	6341
E	(n - C_6)	1.77	25763	34363	8600
F	(n - C_7)	1.00	28905	40006	11101

TABLE 11. Results from Example 2. Comparison of the liquid mole fractions at selected locations in the column obtained with the plate-by-plate and Generalized Underwood methods.

Location in the column	Algo-rithm	Component liquid mole fraction							Reflux ratio
		A	B	C	D	E	F	TOTAL	
Top product	plate-by-plate	0.2727	0.2494	0.2338	0.2074	0.0367	0.0000	1.0000	0.550
	G. UND.	0.2727	0.2494	0.2338	0.2074	0.0367	0.0000	1.0000	0.550
Top pinch	plate-by-plate	0.0767	0.1487	0.2726	0.2956	0.2033	0.0000	0.9999	
	G. UND.	0.0767	0.1487	0.2726	0.2956	0.2033	0.0000	0.9999	
Feed plate #1	plate-by-plate	0.0751	0.1414	0.2830	0.2722	0.1706	0.0578	1.0001	
	G. UND.	0.0751	0.1414	0.2830	0.2722	0.1706	0.0578	1.0001	
Inter-mediate pinch	plate-by-plate	0.0223	0.0889	0.2774	0.3322	0.1855	0.0937	1.0000	
	G. UND.	0.0223	0.0889	0.2772	0.3323	0.1855	0.0937	0.9999	
Feed plate #2	plate-by-plate	0.0180	0.0714	0.1940	0.2136	0.2475	0.2555	1.0000	
	G. UND.	0.0180	0.0714	0.1940	0.2136	0.2475	0.2555	1.0000	
Bottom pinch	plate-by-plate	0.0000	0.0743	0.1885	0.2171	0.2513	0.2688	1.0000	
	G. UND.	0.0000	0.0743	0.1885	0.2171	0.2513	0.2688	1.0000	
Bottom product	plate-by-plate	0.0000	0.0285	0.1687	0.1910	0.2894	0.3223	0.9999	
	G. UND.	0.0000	0.0285	0.1687	0.1910	0.2894	0.3223	0.9999	

TABLE 12. Results from Example 2.
Locations of the pinch regions for the plate-by-plate calculation.

Location in the column	Component liquid mole fraction		Plates with same mole fractions	Plates constituting the pinch
	component	x		
Top pinch	A	0.0767	12 to 30	19 to 25
	B	0.1487	19 to 38	
	C	0.2726	19 to 34	
	D	0.2986	16 to 32	
	E	0.2033	19 to 28	
	F	0.0000	1 to 25	
Intermediate pinch	A	0.0823	75 to 110	none
	B	0.0880	81 to 104	
	C	0.2774	98 to 101	
	D	0.2822	90 to 100	
	E	0.1855	76 to 93	
	F	0.0857	78 to 104	
Bottom pinch	A	0.0000	140 to 180	140 to 162
	B	0.0743	132 to 162	
	C	0.1886	135 to 163	
	D	0.2171	140 to 166	
	E	0.2513	134 to 164	
	F	0.2688	135 to 167	

Number of plates : 180
Location of the feeds : Plate #60, Plate #120

TABLE 13a. Specifications for Example 3.
Plate-by-plate method for a 3 feed column.

PLATE-BY-PLATE SIMULATION WITH ISHII'S PROGRAM

6 components : C_3H_8, i-C_4, i-C_4H_8, n-C_4, i-C_5, n-C_5
3 feeds
Feed #1 : 100 lb-mole
Feed #2 : 100 lb-mole
Feed #3 : 100 lb-mole
Composition feed #1: A=0.30 B=0.25 C=0.20 D=0.10 E=0.10 F=0.05
Composition feed #2: A=0.20 B=0.20 C=0.15 D=0.15 E=0.15 F=0.15
Composition feed #3: A=0.10 B=0.10 C=0.10 D=0.20 E=0.25 F=0.25
Liquid feed #1 (L_F/F) : 0.40
Liquid feed #2 (L_F/F) : 0.60
Liquid feed #3 (L_F/F) : 0.80
Feed plate #1 : 30
Feed plate #2 : 100
Feed plate #3 : 175
Number of plates : 200
Top product : 140 lb-mole
Reflux ratio : 0.15
Condenser : Total
Pressure in the column : 300 PSIA

Properties of the components :

Component		α	h	H	$\lambda = H - h$
			BTU/lb-mole		
A	(C_3H_8)	4.64	12029	16085	4056
B	(i - C_4)	2.64	14192	19472	5280
C	(i - C_4H_8)	2.40	14192	19753	5561
D	(n - C_4)	2.14	14778	20659	5881
E	(i - C_5)	1.17	16999	24900	7901
F	(n - C_5)	1.00	17435	25692	8257

**TABLE 13b. Specifications for Example 3.
Generalized Underwood method for a 3 feed column.**

GENERALIZED UNDERWOOD MODEL

6 components : C_3H_8, i-C_4, i-C_4H_8, n-C_4, i-C_5, n-C_5

3 feeds

Feed #1 : 100 lb-mole

Feed #2 : 100 lb-mole

Feed #3 : 100 lb-mole

Composition feed #1: A=0.30 B=0.25 C=0.20 D=0.10 E=0.10 F=0.05

Composition feed #2: A=0.20 B=0.20 C=0.15 D=0.15 E=0.15 F=0.15

Composition feed #3: A=0.10 B=0.10 C=0.10 D=0.20 E=0.25 F=0.25

Energy content feed #1 (HF) : 1716351.13 BTU

Energy content feed #2 (HF) : 1696969.05 BTU

Energy content feed #3 (HF) : 1680344.83 BTU

LK = A

HK = F

LK recovery in the top product $(d/f)_{LK}$: 0.8708043

HK recovery in the bottom product $(b/f)_{HK}$: 0.9118061

Condenser : Total

Pressure in the column : 300 PSIA

Properties of the components :

Component		α	h	H	λ = H-h
			BTU/lb-mole		
A	(C_3H_8)	4.64	12029	16095	4066
B	(i - C_4)	2.64	14192	19472	5280
C	(i - C_4H_8)	2.40	14192	19753	5561
D	(n - C_4)	2.14	14778	20659	5881
E	(i - C_5)	1.17	16899	24800	7901
F	(n - C_5)	1.00	17435	25692	8257

TABLE 14. Results from Example 3.
Comparison of the liquid mole fractions at selected locations in the column obtained with the plate-by-plate and Generalized Underwood methods.

Location in the column	Algorithm	Component liquid mole fraction							Reflux ratio
		A	B	C	D	E	F	TOTAL	
Top product	plate-by-plate	0.3506	0.2443	0.1906	0.1136	0.0643	0.0366	1.0000	0.150
	G. UND.	0.3506	0.2443	0.1906	0.1136	0.0643	0.0366	1.0000	0.150
Top pinch	plate-by-plate	0.1783	0.2397	0.2002	0.1360	0.1624	0.0835	1.0001	
	G. UND.	0.1783	0.2397	0.2002	0.1360	0.1624	0.0835	1.0001	
Feed plate #1	plate-by-plate	0.1783	0.2397	0.2002	0.1360	0.1624	0.0835	1.0001	
	G. UND.	0.1783	0.2397	0.2002	0.1360	0.1624	0.0835	1.0001	
Inter-mediate pinch #1	plate-by-plate	0.1396	0.1938	0.1518	0.1598	0.2471	0.1078	0.9999	
	G. UND.	0.1396	0.1938	0.1518	0.1598	0.2475	0.1078	1.0001	
Feed plate #2	plate-by-plate	0.1364	0.1875	0.1484	0.1533	0.1901	0.1842	0.9999	
	G. UND.	0.1364	0.1875	0.1484	0.1533	0.1901	0.1842	0.9999	
Inter-mediate pinch #2	plate-by-plate	0.0911	0.2033	0.1565	0.1620	0.1958	0.1913	1.0000	
	G. UND.	0.0910	0.2033	0.1565	0.1620	0.1958	0.1913	0.9999	
Feed plate #3	plate-by-plate	0.0816	0.1255	0.1175	0.1915	0.2426	0.2412	0.9999	
	G. UND.	0.0816	0.1255	0.1175	0.1915	0.2426	0.2412	0.9999	
Bottom pinch	plate-by-plate	0.0816	0.1255	0.1175	0.1915	0.2426	0.2412	0.9999	
	G. UND.	0.0816	0.1255	0.1175	0.1915	0.2426	0.2412	0.9999	
Bottom product	plate-by-plate	0.0514	0.1133	0.1080	0.1880	0.2677	0.2717	1.0000	
	G. UND.	0.0514	0.1133	0.1080	0.1880	0.2677	0.2717	1.0000	

TABLE 15. Results from Example 3.
Locations of the pinch regions for the plate-by-plate calculation.

Location in the column	Component liquid mole fraction		Plates with same mole fractions	Plates constituting the pinch
	component	x		
Top pinch	A	0.1783	6 to 30	7 to 30
	B	0.2387	6 to 30	
	C	0.2002	6 to 30	
	D	0.1380	6 to 30	
	E	0.1624	7 to 30	
	F	0.0836	7 to 30	
Intermediate pinch #1	A	0.1396	55 to 67	60 and 61
	B	0.1936	59 to 66	
	C	0.1518	60 to 69	
	D	0.1598	60 to 66	
	E	0.2471	58 to 65	
	F	0.1078	60 to 61	
Intermediate pinch #2	A	0.0911	151 to 157	151 to 157
	B	0.2033	140 to 157	
	C	0.1585	144 to 158	
	D	0.1620	143 to 158	
	E	0.1958	141 to 163	
	F	0.1913	147 to 165	
Bottom pinch	A	0.0816	175 to 192	175 to 192
	B	0.1285	175 to 192	
	C	0.1175	175 to 194	
	D	0.1915	175 to 192	
	E	0.2406	175 to 193	
	F	0.2412	175 to 193	

Number of plates : 200
Location of the feeds : Plate #50, Plate #100, Plate #175

TABLE 16. Results from Examples 1, 2, and 3.
Comparison of the time required by the plate-by-plate and the Generalized Underwood methods.

Plate-by-plate ([illegible])	Example	Time (sec)	Number of plates	Number of iterations	Residuals
	1	330	120	37	0.31×10^{-13}
	2	1216	180	48	0.15×10^{-12}
	3	1275	200	36	0.66×10^{-11}

Generalized Underwood	Example	Time (sec)	Number of feeds	Number of distributing components	Number of cases
	1	0.243	1	2	9
	2	0.507	2	4	16
	3	0.9[illegible]	3	6	21

5.2.3 Discussion

Example 1. - Table 8 shows a complete comparison of the liquid mole fractions in the top and bottom products, on the feed plate, and in the pinch regions. Both methods yield exactly the same results. Also, the reflux ratio specified in the plate-by-plate calculation is verified by the value obtained from the model.

Table 9 shows in more detail the pinch regions for the plate-by-plate calculation. We can see the number of plates on which the mole fractions remain the same for a given component. For example, in the top pinch, the fraction of A is 0.0596 from plates 16 to 54. Fraction of B is 0.1119 from plates 21 to 53. Each component has its own pinch region, but the boundaries of the pinch, as defined in Chapter 2, must only consider the intersection of all these individual regions. In the case of the top pinch, there are no concentration changes from plates 32 to 49. They constitute the pinch region. The top and bottom pinches spread over 18 and 12 plates, respectively. In both cases, they are easily identified because they are fully developed. For this separation, 120 plates are adequate to meet minimum reflux conditions.

Example 2. - Table 11 shows the comparison of the results. As in Example 1, there are pinch regions in the rectifying and the stripping sections. However, since there are two feeds, a third pinch is present in the intermediate section. For the top and bottom pinches, concentrations correspond exactly. However, concentrations of components C and D do not exactly match in the intermediate pinch. This pinch is not fully developed. It is pointed out in Table 12. Each component has its pinch region but there is no common one. A few additional plates would be required in the intermediate section to meet full minimum reflux conditions. Finally, as in Example 1, the minimum reflux ratio calculated with the model corresponds to the plate-by-plate algorithm specification.

Example 3. - Table 14 shows the comparison of the results. Since there is one more feed, there is another intermediate section with a pinch. As in Example 2, concentrations in the top and bottom products, on the feed plates, and in the top and bottom pinches obtained with the model are verified by the plate-by-plate simulation. On the other hand, the pinches do not exactly match. However, Table 15 shows that they are defined even though they are not developed. Intermediate pinch #1 and intermediate pinch #2 spread over 2 and 7 plates, respectively. As previously mentioned, adding a few plates would increase their definition. As in Examples 1 and 2, the minimum reflux ratio predicted is verified.

The comparisons made in the three examples show that the model is correct within the limitations of its assumptions. Even if we mention that intermediate pinches would be more defined with additional plates for the plate-by-plate simulation, in practice the precision obtained in these examples is adequate.

As discussed in Chapter 2, we observe that the top and bottom pinches occur away from the feeds in Examples 1 and 2 (class 2 separation), and that they touch the feed trays in Example 3 (class 1 separation). This is done by comparing the pinch and feed trays concentrations in Tables 8, 11, and 14. We also notice that, for Examples 2 and 3, the intermediate pinch regions are away from the feeds. Intermediate pinches may be located anywhere between two feeds regardless of the class of separation.

Finally, Table 16 presents the comparison of the computer time required by each method for all three examples. With the plate-by-plate simulation, the times are 398, 1216, and 1275 seconds. The time required depends, for one part, on the number of iterations which depends in turn on the convergence criteria. In these cases, the residuals are

$r \leq 1.0 \times 10^{-11}$ which is tight. This precision was required for the comparison with the Generalized Underwood model.

However, to make a fair comparison, we divide the numbers cited by three which makes 110, 405, and 425 seconds. If we compare these times to the 0.988 seconds required by the Generalized Underwood model in Example 3, we find that the time required by the model is smaller by at least two orders of magnitude.

We must state that the computer time increases according to different parameters depending on the method. With the plate-by-plate algorithm, it increases with the number of components and the number of plates which increases with the number of feeds.

As for the model, it increases with the number of components and the number of cases to cover. The latter depends on the number of feeds because of the different ϕ-values generated for each one, and on the number of non-distributing components generating different distributions to investigate. The most important characteristic differentiating the two methods is the requirement of infinite number of plates built in the model whereas with the plate-by-plate simulation one must assume a number of plates large enough to meet the same requirement.

5.3 Accuracy of the Model

5.3.1 Methodology

In this section, we evaluate the accuracy of the Generalized Underwood model. This is accomplished by comparing its predictions of the top product and the minimum reflux ratio to those of a rigorous plate-by-plate simulation using the Peng-Robinson correlations. This simulation is considered as the reference. For a more complete analysis, we also compare the results obtained with Underwood's model to the plate-by-plate simulation. Constant relative volatilities and constant molal overflow are the basic assumptions of Underwood's model. Note that constant relative volatilities and constant liquid and vapor enthalpies (or constant latent heats of vaporization) are the assumptions of the Generalized Underwood model. By introducing energy considerations, the constant molal overflow assumption is removed in comparison with Underwood's model. Since the two cited models have the same basic form, we are able to observe the difference made by the replacement of the assumption of constant molal overflow in Underwood's model by the assumption of constant liquid and vapor enthalpies of the components in the Generalized Underwood model.

The plate-by-plate simulation is performed first. The specifications are the feed temperature, the amount of top product, and the reflux ratio. In each simulation, enough plates are provided to develop well defined pinch zones. From the results, we can extract the specifications necessary to run the two models.

The specifications required by Underwood's model are the constant relative volatilities, the vaporized feed and the recovery ratios of LK and HK in the top and bottom products, respectively. The volatilities are evaluated with the Peng-Robinson correlations at the feed temperature of the plate-by-plate simulation. Since fractions in the liquid and vapor feed are not readily available with the plate-by-plate simulation, they are taken on the feed tray. For class 1 separation with a single feed column it is correct because the feed enters the column at the pinch conditions. The examples are built so that the class 1 separation proceeds the class 2 separation of the same feed. The properties found in the class 1 example are used directly in the class 2 example. The plate-by-plate simulation provides us with the vaporized feed which is, also, used directly. The recovery ratios are easily calculated with the compositions of the top product and the feed.

The specifications required by the Generalized Underwood model are the constant relative volatilities, the constant liquid and vapor enthalpies, the energy content of the feed, and the recovery ratios as described earlier. The volatilities and the recovery ratios are exactly the same as for Underwood's model. The enthalpies are evaluated at the feed temperature of the plate-by-plate simulation with the correlations taken from Holland (1963). Once the enthalpies are estimated, the feed condition must be given in terms of its energy content instead of its vaporized portion. Since this program utilizes Holland's (1963) correlations for the reference component, one determines the composition of the liquid and vapor feed with a flash calculation based on the relative volatilities and the vaporized portion of the feed. The energy content is then easily calculated.

As in Section 5.5.2 of this chapter, LK and HK are chosen as the lightest and heaviest components that distribute. The results selected for this comparison with the plate-by-plate algorithm are the top product and the reflux ratio.

5.3.2 Examples and Results

We present here four examples (Examples 4 to 7). They are separated in two groups corresponding to two mixtures : narrow-boiling and wide-boiling. For each mixture, we present an example where all components distribute (class 1 separation) and another one where one or more components do not distribute (class 2 separation). All examples are based on a five component mixture and a single feed column.

In Examples 4 and 5, we have the same narrow-boiling mixture composed of C_3H_8, i-C_4, n-C_4, i-C_5, and n-C_5. Example 4 exhibits the class 1 separation and Example 5, the class 2 separation. Tables 17 and 18 show a summary of the input data of each example. Each table contains the data for the three methods. Tables 19 and 20 show the corresponding comparisons of the top product and the minimum reflux ratio.

In Examples 6 and 7, we have a wide-boiling mixture composed of C_3H_8, i-C_5, n-C_5, n-C_6, and n-C_8. Examples 6 and 7 exhibit class 1 and class 2 separations, respectively. Tables 21 and 22 show the input data of each example. Each table shows the data for the three methods compared. Tables 23 and 24 show the corresponding comparisons of the top product and the minimum reflux ratio.

Tables 25 and 26 summarize the results of the four examples for the top product and the reflux ratio, respectively.

TABLE 17. **Specifications for Example 4.
Plate-by-plate, Underwood, and Generalized Underwood methods. Narrow-boiling mixture and class 1 separation.**

PLATE-BY-PLATE SIMULATION WITH THE PENG - ROBINSON CORRELATIONS

5 Components : C_3H_8, i-C_4, n-C_4, i-C_5, n-C_5
1 feed : 100 lb-mole
Composition : A=0.20 B=0.20 C=0.20 D=0.20 E=0.20
Feed temperature : 250° F
Feed plate : Plate #35
Number of plates : 80
Top product : 47 lb-mole
Reflux ratio : 1.35
Condenser : Partial
Pressure in the column : 300 PSIA

UNDERWOOD AND GENERALIZED UNDERWOOD MODELS

LK : A
HK : E
LK recovery ratio in the top product : 0.9610
HK recovery ratio in the bottom product : 0.9185
Vaporized feed* (V_F/F) : 0.5082
Energy content of the feed (HF) : 1048946.38 BTU**
Pressure in the column : 300 PSIA

Properties of the components :

Component		α	h**	H**	λ** = H-h
			BTU/lb-mole		
A	(C_3H_8)	2.96	13410	16940	3530
B	(i-C_4)	1.96	14645	19749	5104
C	(n-C_4)	1.70	15051	20927	5876
D	(i-C_5)	1.11	17442	25119	7677
E	(n-C_5)	1.00	17594	25999	8405

* Applies to Underwood's model only

** Applies to Generalized Underwood model only

TABLE 18. Specifications for Example 5. Plate-by-plate, Underwood, and Generalized Underwood methods. Narrow-boiling mixture and class 2 separation.

PLATE-BY-PLATE SIMULATION WITH THE PENG - ROBINSON CORRELATIONS

5 Components :	C_3H_8, i-C_4, n-C_4, i-C_5, n-C_5
1 feed :	100 lb-mole
Composition :	A=0.20 B=0.20 C=0.20 D=0.20 E=0.20
Feed temperature :	250° F
Feed plate :	Plate #20
Number of plates :	80
Top product :	50 lb-mole
Reflux ratio :	1.90
Condenser :	Partial
Pressure in the column :	300 PSIA

UNDERWOOD AND GENERALIZED UNDERWOOD MODELS

LK : B

HK : E

LK recovery ratio in the top product : 0.9995

HK recovery ratio in the bottom product : 0.9980

Vaporized feed* (V_F/F) : 0.5822

Energy content of the feed** (HF) : 1048846.38 BTU

Pressure in the column : 300 PSIA

Properties of the components :

Component		α	h**	H**	λ^{**} = H-h
			BTU/lb-mole		
A	(C_3H_8)	2.96	13410	16940	3530
B	(i-C_4)	1.96	14645	19749	5104
C	(n-C_4)	1.70	15951	20827	5876
D	(i-C_5)	1.11	17442	25119	7677
E	(n-C_5)	1.00	17804	25869	8065

* Applies to Underwood's model only

** Applies to Generalized Underwood model only

TABLE 19. Results from Example 4.
Comparison between the three methods for the top product composition and the minimum reflux ratio.

		METHOD OF CALCULATION					
		PLATE-BY-PLATE PENG-ROBINSON		UNDER-WOOD'S MODEL		GENERALIZED UNDERWOOD MODEL	
	COMPONENT	mole	x	mole	x	mole	x
TOP PRODUCT COMPOSITION	LK A (C_3H_8)	19.22	0.4089	19.22	0.4084	19.22	0.4084
	B (i-C_4)	12.62	0.2685	12.66	0.2690	12.66	0.2690
	C (n-C_4)	10.28	0.2187	10.30	0.2189	10.30	0.2189
	D (i-C_5)	3.27	0.0696	3.27	0.0695	3.27	0.0695
	HK E (n-C_5)	1.61	0.0343	1.61	0.0343	1.61	0.0342
	TOTAL	47.00	1.0000	47.06	1.0000	47.06	1.0000
MINIMUM REFLUX RATIO		1.35		1.27		1.49	

TABLE 20. Results from Example 5.
Comparison between the three methods for the top product composition and the minimum reflux ratio.

			METHOD OF CALCULATION					
			PLATE-BY-PLATE PENG-ROBINSON		UNDER-WOOD'S MODEL		GENERALIZED UNDERWOOD MODEL	
		COMPONENT	mole	x	mole	x	mole	x
TOP PRODUCT COMPOSITION		A (C_3H_8)	20.00	0.3390	20.00	0.3391	20.00	0.3387
	LK	B (i-C_4)	16.01	0.2714	16.01	0.2714	16.01	0.2711
		C (n-C_4)	13.31	0.2256	13.29	0.2253	13.34	0.2259
		D (i-C_5)	5.72	0.0969	5.72	0.0970	5.74	0.0972
	HK	E (n-C_5)	3.96	0.0671	3.96	0.0671	3.96	0.0671
		TOTAL	59.00	1.0000	58.98	0.9999	59.05	1.0000
MINIMUM REFLUX RATIO			1.00		0.983		1.08	

TABLE 21. Specifications for Example 6.
Plate-by-plate, Underwood, and Generalized Underwood methods. Wide-boiling mixture and class 1 separation.

PLATE-BY-PLATE SIMULATION WITH THE PENG - ROBINSON CORRELATIONS

5 Components :	C_3H_8, i-C_5, n-C_5, n-C_6, n-C_8
1 feed :	100 lb-mole
Composition :	A=0.20 B=0.20 C=0.20 D=0.20 E=0.20
Feed temperature :	350° F
Feed plate :	Plate #25
Number of plates :	55
Top product :	49.1 lb-mole
Reflux ratio :	0.55
Condenser :	Partial
Pressure in the column :	300 PSIA

UNDERWOOD AND GENERALIZED UNDERWOOD MODELS

LK : A

HK : E

LK recovery ratio in the top product : 0.9585

HK recovery ratio in the bottom product : 0.9985

Vaporized feed* (Vp/F) : 0.4414

Energy content of the feed** (HF) : 2709400.71 BTU

Pressure in the column : 300 PSIA

Properties of the components :

Component		α	h**	H**	λ** = H-h
			BTU/lb-mole		
A	(C_3H_8)	7.98	16075	18842	2767
B	(i-C_5)	3.60	[illegible]	[illegible]	[illegible]
C	(n-C_5)	3.33	[illegible]	[illegible]	[illegible]
D	(n-C_6)	2.21	[illegible]	[illegible]	[illegible]
E	(n-C_8)	1.00	[illegible]	[illegible]	[illegible]

* Applies to Underwood's model only

** Applies to Generalized Underwood model only

TABLE 22. Specifications for Example 7. Plate-by-plate, Underwood, and Generalized Underwood methods. Wide-boiling mixture and class 2 separation.

PLATE-BY-PLATE SIMULATION WITH THE PENG - ROBINSON CORRELATIONS

5 Components :	C_3H_8, i-C_5, n-C_5, n-C_6, n-C_8
1 feed :	100 lb-mole
Composition :	A=0.20 B=0.20 C=0.20 D=0.20 E=0.20
Feed temperature :	350° F
Feed plate :	Plate #40
Number of plates :	80
Top product :	50.0 lb-mole
Reflux ratio :	1.20
Condenser :	Partial
Pressure in the column :	300 PSIA

UNDERWOOD AND GENERALIZED UNDERWOOD MODELS

LK : B

HK : D

LK recovery ratio in the top product : 0.6770

HK recovery ratio in the bottom product : 0.7825

Vaporized feed* (V_F/F) : 0.4414

Energy content of the feed** (HF) : 2768480.71 BTU

Pressure in the column : 300 PSIA

Properties of the components :

Component		α	h**	H**	λ** = H-h
			BTU/lb-mole		
A	(C_3H_8)	7.98	16075	18842	2767
B	(i-C_5)	3.60	20004	28570	8566
C	(n-C_5)	3.33	20021	28848	8827
D	(n-C_6)	2.21	25989	34993	9004
E	(n-C_8)	1.00	28444	41203	12759

* Applies to Underwood's model only

** Applies to Generalized Underwood model only

TABLE 23. Results from Example 6.
Comparison between the three methods for the top product composition and the minimum reflux ratio.

		METHOD OF CALCULATION					
		PLATE-BY-PLATE PENG-ROBINSON		UNDER-WOOD'S MODEL		GENERALIZED UNDERWOOD MODEL	
	COMPONENT	mole	x	mole	x	mole	x
TOP PRODUCT COMPOSITION	LK A (C_3H_8)	19.13	0.3896	19.13	0.3895	19.13	0.3895
	B (i-C_4)	11.60	0.2363	11.60	0.2362	11.60	0.2362
	C (n-C_4)	10.84	0.2208	10.83	0.2205	10.83	0.2205
	D (n-C_5)	6.90	0.1405	6.92	0.1409	6.92	0.1409
	HK E (n-C_6)	0.63	0.0128	0.63	0.0128	0.63	0.0128
	TOTAL	49.10	1.0000	49.11	0.9999	49.11	0.9999
MINIMUM REFLUX RATIO		0.550		0.431		0.558	

TABLE 24. Results from Example 7.
Comparison between the three methods for the top product composition and the minimum reflux ratio.

			METHOD OF CALCULATION					
			PLATE-BY-PLATE PENG-ROBINSON		UNDERWOOD'S MODEL		GENERALIZED UNDERWOOD MODEL	
		COMPONENT	mole	x	mole	x	mole	x
TOP PRODUCT COMPOSITION		A (C_3H_8)	20.00	0.4000	20.00	0.4007	20.00	0.4000
	LK	B (i-C_4)	13.54	0.2708	13.54	0.2713	13.54	0.2708
		C (n-C_4)	12.11	0.2422	12.02	0.2408	12.11	0.2422
	HK	D (n-C_5)	4.35	0.0870	4.35	0.0872	4.35	0.0870
		E (n-C_6)	0.00	0.0000	0.00	0.0000	0.00	0.0000
		TOTAL	50.00	1.0000	49.91	1.0000	50.00	1.0000
MINIMUM REFLUX RATIO			1.20		1.01		1.20	

TABLE 25. Results from Examples 4, 5, 6, and 7. Comparison between the three methods for the top product in relation with the type of mixture.

	NARROW-BOILING		WIDE-BOILING	
Example	4	5	6	7
Method	class 1 separation	class 2 separation	class 1 separation	class 2 separation
Plate-by-plate (P.-P.)	47.00	59.00	49.10	50.00
Underwood	47.06	58.98	49.11	49.91
Gen. Underwood	47.06	59.05	49.11	50.00
1 Underwood vs plate-by-plate	+ 0.13 %	- 0.03 %	+ 0.02 %	- 0.18 %
2 Gen. Underwood vs plate-by-plate	+ 0.13 %	+ 0.08 %	+ 0.02 %	0.00 %

$$1 = \frac{(\text{UND}) - (\text{P.-by-P.})}{(\text{P.-by-P.})} \qquad 2 = \frac{(\text{G. UND}) - (\text{P.-by-P.})}{(\text{P.-by-P.})}$$

TABLE 26. Results from Examples 4, 5, 6, and 7.
Comparison between the three methods for the minimum reflux ratio in relation with the type of mixture.

Method \ Example	NARROW-BOILING		WIDE-BOILING	
	4	5	6	7
	class 1 separation	class 2 separation	class 1 separation	class 2 separation
Plate-by-plate (P.-P.)	1.35	1.00	0.550	1.20
Underwood	1.27	0.963	0.431	1.01
Gen. Underwood	1.49	1.08	0.556	1.30
1 Underwood vs plate-by-plate	- 5.9 %	- 3.7 %	- 22 %	- 16 %
2 Gen. Underwood vs plate-by-plate	+ 10 %	+ 8.0 %	+ 1.1 %	+ 8.3 %

$$1 = \frac{(\text{UND.}) - (\text{P.-by-P.})}{(\text{P.-by-P.})} \qquad 2 = \frac{(\text{G. UND.}) - (\text{P.-by-P.})}{(\text{P.-by-P.})}$$

5.3.3 Discussion

Example 4. - Table 19 shows the comparison of the top product and the minimum reflux ratio for the class 1 separation of a narrow-boiling mixture. We first notice that, since components A and E are the keys, the respective amounts recovered in the top product, 19.22 and 1.61 moles, are the same for the three methods. We notice no significant differences between the top product distributions predicted by the three methods. This class 1 separation corresponds to a flash calculation and the split is only a function of the equilibrium data. Both models predict the same product because they use the same relative volatilities. However, when comparing the reflux ratios we can observe the effect of the latent heats of vaporization in the Generalized Underwood model. The specification is 1.35. Underwood predicts a lower value of 1.27. Generalized Underwood predicts a higher value of 1.49.

Example 5. - Table 20 shows the comparison of the top product and the minimum reflux ratio for the class 2 separation of the same narrow-boiling mixture. Since component A does not distribute, components B and E are the keys. Again, the amounts of keys in the top product are the same for the three methods. As in Example 4, we notice no significant differences between the top product distributions predicted by the three methods. The specified reflux ratio is 1.00. Underwood predicts a lower value of 0.943. Generalized Underwood predicts a higher value of 1.08.

Example 6. - Table 23 shows the comparison of the top product and the minimum reflux ratio for the class 1 separation of a wide-boiling mixture. All components distribute and components A and E are the keys. As for the two previous cases, we notice no significant differences between the top product distributions predicted by the three methods. For the reflux ratio, the specification is 0.550. Underwood predicts a lower value of 0.431. Generalized Underwood predicts a higher value of 0.558.

Example 7. - Table 24 shows the comparison of the top product and the minimum reflux ratio for the class 2 separation of the same wide-boiling mixture. Components A and E do not distribute, therefore B and D are the key components. Again, we notice no significant differences between the top product distributions predicted by the three methods. The reference reflux ratio is 1.20. Underwood predicts a lower value of 1.01. The value predicted by Generalized Underwood is higher with 1.30.

All this analysis of Examples 4, 5, 6, and 7 is summarized in Table 25 for the top product and in Table 26 for the reflux ratio. In all four cases presented, the predictions of the top product distribution by the Underwood and Generalized Underwood methods show no significant differences with the Peng-Robinson simulation.

On the other hand, Generalized Underwood predicts significantly higher reflux ratios than Underwood in all four cases examined. This result can be generalized. The constant molal overflow of Underwood's model implies that all components have the same energy properties. The assumption of constant latent heats of vaporization in the Generalized Underwood model removes the assumption of constant molal overflow. Although latent heats of vaporization are not constant in reality, their application accounts for the fact that, for a given energy exchange, more moles of volatile components are vaporized than moles of heavy components condensed. In Underwood's case, all components have the same latent heat so that the vaporization of 1 mole of any component corresponds to the condensation of 1 mole of any other component, which requires less reflux.

For the same reason, Underwood is expected to underestimate the reflux ratio predicted by the Peng-Robinson plate-by-plate simulation. In all four cases presented, the reflux ratio is underestimated. However, this result cannot be generalized since the performance of Underwood is dependant upon the estimate of the constant relative volatilities.

As for Generalized Underwood, in all four cases, the method overestimated the reflux ratio predicted by the Peng-Robinson plate-by-plate simulation. This result cannot be generalized because of the estimates of the constant relative volatilities and the enthalpies.

By inspecting Table 28 in more detail, we find that Underwood underestimates the reflux ratio by a range of 3.7% to 22%. Generalized Underwood overestimates the reflux ratio by a range of 1.1% to 10%. Since we are looking for a minimum limit for a distillation process, the usage of the Generalized Underwood appears to be safer when predicting the minimum reflux ratio.

In the four case studies examined, we find that Underwood predicts a more accurate reflux ratio for the narrow-boiling mixture. We also find that Generalized Underwood predicts a more accurate reflux ratio for the wide-boiling mixture. Even though we cannot generalize from only four examples, one should expect better results from the Generalized Underwood model as the boiling range of a mixture increases because of the increasing differences of latent heats of vaporization between components.

It is important to mention that a model cannot be more accurate than the assumptions and the estimates of the properties. But since the Generalized Underwood model is a shortcut method, these limitations are part of the method.

Although this program is primarily designed to estimate the minimum reflux ratio required for a separation, it can serve other purposes. In particular, it is very useful to establish the initial guess of a rigorous simulation. And since it requires little computer time it becomes very handy when conducting preliminary sensitivity studies of the parameters. It can also be utilized to determine the most promising combinations of distillation columns constituting a network.

Conclusions

We have developed a computationally efficient method for the calculation of the minimum reflux for multiple feed columns.

It is shown that this shortcut multiple feed algorithm based on the "Generalized Underwood Model" is correct within the assumptions of constant relative volatilities and constant liquid and vapor enthalpies of the components.

When compared with Ishii's plate-by-plate algorithm and using the same assumptions to obtain the same results, it is found that the computer time required by the shortcut method is smaller by two orders of magnitude.

In the case studies examined in this work, the comparisons made with a rigorous plate-by-plate simulation using Peng-Robinson correlations indicate that Underwood's model tends to underestimate the minimum reflux ratio, whereas the Generalized Underwood model tends to overestimate it. They also indicate that Underwood tends to predict more accurate values of the minimum reflux ratio for narrow-boiling mixtures. In opposition, Generalized Underwood tends to predict more accurate values for wide-boiling mixtures. It is also shown that, for the prediction of the top product, the two shortcut methods are in close agreement with the plate-by-plate simulation.

This model is simple and the program requires little computer time. This shortcut algorithm predicts the minimum reflux ratio but can serve other purposes. It may be used to find an initial guess for a rigorous simulation. It may also be used to conduct preliminary sensitivity studies of the parameters before performing a rigorous simulation. Finally, one can establish the most promising configurations of a network of columns to optimize the fractionation.

List of References

ACRIVOS, A. and AMUNDSON, N.R. On the Steady-State Fractionation of Multicomponent and Complex Mixtures in an Ideal Cascade. Part 2. – The calculation of the minimum reflux ratio. Chem. Eng. Sci., 4, 2, pp. 68-74 (1955)

BACHELOR, J.B. How to Figure Minimum reflux. Petroleum Refiner, 36, 6, pp. 161-170 (1957)

BARNES, F.J., HANSON, D.N., and KING, C.J. Calculation of Minimum Reflux for Distillation Columns with Multiple Feeds. Ind. Eng. Chem. Process Des. Develop., 11, 1, pp. 136-140 (1972)

BROWN, G. G. and HOLCOMB, D. E. Vapor-Liquid Phase Equilibria in Hydrocarbon Systems. Part VIII Calculation of the approximate minimum reflux required. Petroleum Engr., 11, pp. 23-26 (August 1940a)

BROWN, G. G. and HOLCOMB, D. E. Vapor-Liquid Phase Equilibria in Hydrocarbon Systems. Part IX Calculations of the minimum reflux. Petroleum Engr., 11, pp. 27-30 (Sept. 1940b)

CERDA, J. and WESTERBERG, W. Shortcut Methods for Complex Distillation Columns. 1. Minimum Reflux. Ind. Eng. Chem. Process Des. Dev., 20, 3, pp. 546-557 (1981)

CHIEN, H.H.Y. A Rigorous Method for Calculating of Minimum Reflux Rates in Distillation. AIChE J., 24, 4, pp. 606-613 (1978)

ERBAR, R.C. and MADDOX, R.N. Minimum Reflux Rate for Multicomponent Distillation Systems by Rigorous Plate Calculations. Can. J. Chem. Eng., 40, pp. 25-30 (Feb. 1962)

FENSKE, M.R. Fractionation of Straight-Run Pennsylvania Gasoline. Ind. and Eng. Chem., 24, 5, pp. 482-485 (1932)

GILLILAND, E. R. Multicomponent Rectification. Minimum Reflux Ratio. Ind. and Eng. Chem., 32, 8, pp. 1101-1106 (1940)

GLINOS, K. and MALONE, M.F. Minimum Reflux, Product Distribution, and Lumping Rules for Multicomponent Distillation. Ind. Eng. Chem. Process Des. Dev., 23, 4, pp. 764-768 (1984)

HOLLAND, C. D., *Multicomponent Distillation*. Prentice Hall, Inc., Englewood Cliffs, N.J, pp. 486,487 (1963)

ISHII, Y. and OTTO, F.D. A General Algorithm for Multistage Multicomponent Separation Calculations. Can. J. Chem. Eng., 51, pp. 601-606 (1973)

JENNY, F. J. Graphical Solution of Problems in Multicomponent Fractionation. Trans. Am. Inst. Chem. Engrs., 35, pp. 635-677 (1939)

LEE, E.S. Estimation of Minimum Reflux in Distillation and Multipoint Boundary Value Problems. Chem. Eng. Sci., 29, 3, pp. 871-875 (1974)

LEWIS, W.K. and MATHESON, G.L. Studies in Distillation. Design of Rectifying Columns for Natural and Refinery Gasoline. Ind. and Eng. Chem., 24, 5, pp. 494-498 (1932)

McDONOUGH, J.A. and HOLLAND C.D. Figure Separations This New Way. Part 9 – How to Figure Minimum Reflux. Hydroc. Processing and Petroleum Refiner, 41, 3, pp. 153-160 (1962a)

McDONOUGH, J.A. and HOLLAND C.D. Figure Separations This New Way. Part 10 – Minimum Reflux for Complex Columns. Hydroc. Processing and Petroleum Refiner, 41, 4, pp. 135-140 (1962b)

NANDAKUMAR, K. and ANDRES, R.P. Minimum Reflux Conditions. Part I: Theory. AIChE J., 27, 3, pp. 450-460 (1981a)

NANDAKUMAR, K. and ANDRES, R.P. Minimum Reflux Conditions. Part II: Numerical Solution. AIChE J., 27, 3, pp. 460-465 (1981b)

PETLYUK, F.B., AVET'YAN, V.S. and, PLATONOV, V.M. Fractionation of Multicomponent Mixtures at Minimum Reflux. Translated from Teoreticheskie Osnovy Khimicheskoi Tekhnologii, 2, 2, pp. 155-160 (March-April 1968)

RAMKRISHNA, D. and AMUNDSON, N.R. Self-adjoint operators from selected nonsymmetric matrices : application to kinetics and rectification. Chem. Eng. Sci., 28, 2, pp. 601-605 (1973)

SHIRAS, R.N., HANSON, D.N., and GIBSON, C.H. Calculation of Minimum Reflux in Distillation Columns. Ind. and Eng. Chem., 42, 5, pp. 871-876 (1950)

SUGIE, H. and LU B. C.-Y. On the determination of minimum reflux ratio for a multicomponent distillation column with any number of side-cut streams. Chem. Eng. Sci., 25, 12, pp. 1837-1846 (1970)

THIELE, E.W. and GEDDES, R.L. Computation of Distillation Apparatus for Hydrocarbon Mixtures. Ind. and Eng. Chem., 25, 3, pp. 289-295 (1933)

TSUO, F.-M., YANG, C.L., and CHENG, J.-S. Minimum Reflux for Sidestream Columns. Chem. Eng., 85, 14, pp. 49-58 (1978)

UNDERWOOD, A.J.V. The Theory and Practice of Testing Stills. Trans. Inst. Chem. Engrs. (London), 10, pp. 112-158 (1932)

UNDERWOOD, A.J.V. Fractional Distillation of Ternary Mixtures. Part I. J. Inst. Petroleum (London), 31, 256, pp. 111-118 (1945)

UNDERWOOD, A.J.V. Fractional Distillation of Ternary Mixtures. Part II. J. Inst. Petroleum (London), 32, 274, pp. 598-613 (1946a)

UNDERWOOD, A.J.V. Fractional Distillation of Multi-Component Mixtures – Calculation of Minimum Reflux Ratio. J. Inst. Petroleum (London), 32, 274, pp. 614-626 (1946b)

UNDERWOOD, A.J.V. Fractional Distillation of Multicomponent Mixtures. Chem. Eng. Progress, 44, 8, pp. 603-614 (1948)

UNDERWOOD, A.J.V. Fractional Distillation of Multicomponent Mixtures. A Numerical Example. Chem. Eng. Progress, 45, 10, pp. 609-618 (1949)

APPENDIX 1.

EXAMPLE 1. COMPUTER INPUTS AND OUTPUTS

–Generalized Underwood method

–Plate-by-plate method (ISHII)

```
'EXAMPLE 1'
'GENERALIZED UNDERWOOD'
'TOTAL CONDENSER'
'ALPHA'
'KCONSTANT'
'LB-MOLE/TIME', 'BTU/LB-MOLE', 'F'
6
'C3H8'
'i-C4'
'i-C5'
'n-C5'
'n-C7'
'n-C8'
1
100.0
0.15, 0.15, 0.20, 0.20, 0.15, 0.15
'NF'
2001000.70
3, 4
0.0075815, 0.0075815
17.36, 11.38, 6.11, 5.41, 1.77, 1.0
0
    7.1714400D-2, -52.0085300D-5, 103.72034D-8,   -406.40581D-12
0.0, 570.0
15594.0
19155.0
22594.0
22596.0
23504.0
25716.0
16282.0
22597.0
25768.0
28867.0
40848.0
40887.0
```

```
MINIMUM REFLUX CALCULATION FOR MULTIPLE FEED COLUMN

METHOD: GENERALIZED UNDERWOOD
        TOTAL CONDENSER

MAXIMUM NUMBER OF COMPONENTS: 10
MAXIMUM NUMBER OF FEEDS: 5



********************************
SECTION 1: DATA
********************************
NDATA: EXAMPLE 1


[illegible]:
NUMBER OF COMPONENTS:  6
NUMBER OF FEEDS: 1

RECOVERY OF LIGHT KEY AT THE TOP:    99.79815 %
RECOVERY OF HEAVY KEY AT THE BOTTOM: 99.79815 %

COMPONENTS: C3H8
            i-C4
            i-C5
            n-C5
            n-C7
            n-C8


PROPERTIES OF COMPONENTS:

COMP  KEYS  ALPHA        HL             HV             LAMBDA
                         BTU/LB-MOLE    BTU/LB-MOLE    BTU/LB-MOLE
----  ----  ------------------------------------------------------
 1          [illegible]  [illegible]    [illegible]    [illegible]
 2          11.3000      10155.0000     23007.0000      4082.0000
 3    LK     6.1100      22004.0000     30709.0000      5904.0000
 4    HK     5.4100      22906.0000     30307.0000      5951.0000
 5           1.7700      30004.0000     40942.0000     10938.0000
 6           1.0000      35716.0000     46307.0000     12082.0000
```

```
DATA ON FEEDS:

FEED   FEED RATE     HFBP          HPBP          HF            DHF
----   LB-MOLE/TIME  BTU/TIME      BTU/TIME      BTU/TIME      BTU/TIME
 1       100.0000       3416070.05    3100070.05    3051088.75     273780.75

TOTAL FEED:

COMP   T. FEED RATE  MOLE FRAC
----   LB-MOLE/TIME  ---------
 1        15.0000    0.150000
 2        15.0000    0.150000
 3        20.0000    0.200000
 4        20.0000    0.200000
 5        15.0000    0.150000
 6        15.0000    0.150000
       ----------    --------
         100.0000    1.000000

FEED NO.1: FLASHED FEED

COMP   RATE          MOLE FRAC
----   LB-MOLE/TIME  ---------
 1        15.0000    0.150000
 2        15.0000    0.150000
 3        20.0000    0.200000
 4        20.0000    0.200000
 5        15.0000    0.150000
 6        15.0000    0.150000
       ----------    --------
         100.0000    1.000000
```

```
********************************
SECTION 2: RESULTS
********************************

DISTILLATE:

COMP  KEYS   RATE                MOLE FRAC    FRAC/FEED
             LB-MOLE/TIME
----  ----   ------------        ---------    ---------
 1             15.0000           0.300000     1.000000
 2             15.0000           0.300000     1.000000
 3     LK      12.1596           0.243192     0.607981
 4     HK       7.8404           0.156807     0.392019
 5               0.0             0.0          0.0
 6               0.0             0.0          0.0
             ---------           --------
               50.0000           1.000000

BOTTOM PRODUCT:

COMP  KEYS   RATE                MOLE FRAC    FRAC/FEED
             LB-MOLE/TIME
----  ----   ------------        ---------    ---------
 1               0.0             0.0          0.0
 2               0.0             0.0          0.0
 3     LK       7.8404           0.156807     0.392019
 4     HK      12.1596           0.243192     0.607981
 5             15.0000           0.300000     1.000000
 6             15.0000           0.300000     1.000000
             ---------           --------
               50.0000           1.000000
```

```
LIQUID AND VAPOR FLOWRATES:

SECTION                       LIQUID        VAPOR
                           LB-MOLE/TIME  LB-MOLE/TIME

RECTIFYING      :  TOP      109.9967      159.9967
                   PINCH     87.8821      137.8821
                   BOT       78.1225      128.1225

STRIPPING       :  TOP      123.7347       73.7347
                   PINCH    116.6447       66.6447
                   BOT      108.3840       58.3840


FLOWRATE CHANGES (FEED TRAYS):

FEED  DL            DV            TOTAL
      LB-MOLE/TIME  LB-MOLE/TIME  LB-MOLE/TIME
 1        45.6123       54.3877      100.0000


MINIMUM REFLUX:

EXTERNAL REFLUX RATIO (L/D):  2.199934867

INTERNAL REFLUX RATIO (L/V):  0.687493640
```

```
********************************
SECTION 3: ADDITIONAL RESULTS
********************************

FEED TRAYS COMPOSITION:

FEED TRAY NO.1

COMP  LQ MOLE FRAC  VP MOLE FRAC
  1   0.047535      0.[illegible]
  2   0.007071      0.178117
  3   0.273665      0.301706
  4   0.[illegible]      0.304350
  5   0.154667      0.049427
  6   0.137630      0.084567
       --------      --------
       1.000000      1.000000
```

```
PINCH ZONE COMPOSITION:

PINCH, RECTIFYING SECTION

COMP  LQ MOLE FRAC  VP MOLE FRAC
 1    [illegible]   [illegible]
 2    [illegible]   [illegible]
 3    [illegible]   [illegible]
 4    0.441[illegible]   [illegible]
 5    0.0           0.0
 6    0.0           0.0
      --------      --------
      1.000000      1.000000

PINCH, STRIPPING SECTION

COMP  LQ MOLE FRAC  VP MOLE FRAC
 1    0.0           0.0
 2    0.0           0.0
 3    [illegible]   0.481475
 4    [illegible]   0.407210
 5    [illegible]   [illegible]
 6    0.147[illegible]   [illegible]
      --------      --------
      1.000000      1.000000
```

```
TEMPERATURE PROFILE:

DISTILLATE:       282.80 F
PINCH(1):         310.40 F
FEED TRAY(1):     342.06 F
PINCH(2):         388.82 F
BOTTOM PRODUCT:   408.37 F
```

```
EXAMPLE 1
[illegible]  (PLATE-BY-PLATE ALGORITHM)

6,1,                              > NCP, JCASE
6-component, constant alpha, constant enthalpy model.
1[illegible],3,1,0,0,0,50,0,1,0,2,20,0,1,  > NPLT,TYPE,JF,JBL,JBV,J0,D,ZN,REF,IVAL,JPRINT
0,1,1                        > NPRINT,NCALC,JCALC
2, 1.0E-3, 45.0               > IDATHE, DATEL, DASLO
300.0,0,0,300.0,415.0,300.0,    > PP(1), PD, TT(1), TT(NPLT), PP(2)
50,2,300.0,345.0,0.5,345.0,   > NF(J),JFEED(J),PF(J),TF(J),ZLF(J),TFWH(J)
15.0, 15.0, 20.0, 20.0, 15.0, 15.0   > ZF(I,J)
.1D-14,50,                   > TOL, LIMIT
1.,1.,1.,1.,1.,1.             > EFFI on tray 1
1.,1.,1.,1.,1.,1.             > EFFI on tray 2 to nplt-1
1.,1.,1.,1.,1.,1.             > EFFI on tray nplt

[illegible]
1-C4
1-C5
n-C6
n-C7
n-C8
  -14.[illegible]D-2,   50.[illegible]D-5,  -3.[illegible]D-8,  -173.[illegible]D-12
  -13.[illegible]D-2,   61.[illegible]D-5, -17.[illegible]D-8,   -80.[illegible]D-12
   -7.[illegible]D-2,    3.[illegible]D-5,  55.[illegible]D-8,  -414.[illegible]D-12
   -7.[illegible]D-2,    2.[illegible]D-5,  50.[illegible]D-8,  -413.[illegible]D-12
    5.[illegible]D-2,  -30.[illegible]D-5, 112.[illegible]D-8,  -574.[illegible]D-12
    7.[illegible]D-2,  -32.[illegible]D-5, 100.[illegible]D-8,  -406.[illegible]D-12
[illegible].0,0.,0.,
[illegible].0,0.,0.,
[illegible].0,0.,0.,
[illegible].0,0.,0.,
[illegible].0,0.,0.,
[illegible].0,0.,0.,
[illegible].0,0.,0.,
[illegible].0,0.,0.,
[illegible].0,0.,0.,
[illegible].0,0.,0.,
[illegible].0,0.,0.,
[illegible].0,0.,0.,
.T.
17.38, 11.38, 6.11, 5.41, 1.77, 1.00
```

```
***** EQUILIBRIUM AND ENTHALPY DATA *****
-0.1451047+000     0.[illegible]-005      -0.[illegible]5100-007    -0.17[illegible]-009
-0.[illegible]+000     0.61[illegible]-005      -0.17[illegible]-005    -0.[illegible]1-010
-0.7[illegible]-001     0.[illegible]-004       0.[illegible]724-005    -0.41[illegible]-009
-0.7[illegible]-001     0.[illegible]-004       0.[illegible]-005    -0.4131241-009
 0.[illegible]-001    -0.[illegible]7-005       0.1121734-005    -0.57[illegible]-009
 0.717[illegible]-001    -0.[illegible]-005       0.[illegible]-005    -0.4[illegible]-009
 0.[illegible]+000     0.[illegible]+000       0.0000000+000
 0.[illegible]+000     0.[illegible]+000       0.0000000+000
 0.[illegible]+000     0.[illegible]+000       0.0000000+000
 0.[illegible]+000     0.[illegible]+000       0.0000000+000
 0.[illegible]+000     0.[illegible]+000       0.0000000+000
 0.[illegible]+000     0.[illegible]+000       0.0000000+000
 0.[illegible]+000     0.[illegible]+000       0.0000000+000
 0.[illegible]+000     0.[illegible]+000       0.0000000+000
 0.[illegible]+000     0.[illegible]+000       0.0000000+000
 0.[illegible]+000     0.[illegible]+000       0.0000000+000
 0.[illegible]+000     0.[illegible]+000       0.0000000+000
 0.[illegible]+000     0.[illegible]+000       0.0000000+000
 0.17[illegible]+002     0.11[illegible]+002       0.6110000+001     0.5410000+001
 0.177[illegible]+001     0.1000000+001
```

```
6-COMPONENT, CONSTANT ALPHA, CONSTANT ENTHALPY MODEL.

TYPE OF COLUMN................. 3
NO. OF PLATES..................**
PRESSURE AT TOP PLATE (PSIA)..    300.00
PRESSURE DROP PER PLATE (PSIA)    0.0000

NO. OF FEEDS................... 1

   INFEEDING PLATE OF FEED 1......60
   FEED QUANTITY.................. 0.10000+003
   PRESSURE OF FEED...............    300.00
   LIQUID RATIO OF FEED...........  0.5000

REFLUX RATIO...................        2.200
LIQUID RATIO OF TOP PRODUCT...    1.0000
SPECIFIED TOP PRODUCT......... 0.50000+002

EFFICIENCIES

PLATE  1.....  1.00  1.00  1.00  1.00  1.00  1.00
PLATE 2 ON...  1.00  1.00  1.00  1.00  1.00  1.00
PLATE100.....  1.00  1.00  1.00  1.00  1.00  1.00
```

```
**************************************************
*         CONVERGENCE OF ITERATION               *
**************************************************

 0   SUM OF SQUARES OF RESIDUALS  0.13805+003 (MAT. BAL.   0.13804+003   HEAT BAL.   0.77716-003)
 TEMPERATURE ([illegible])    0.73967+003 0.74080+003 0.74194+003 0.74307+003 0.74421+003 0.74534+003 0.74648+003
 TEMPERATURE ([illegible])    0.74761+003 0.74875+003 0.74988+003 0.75101+003 0.75215+003 0.75328+003 0.75442+003
 TEMPERATURE ([illegible])    [illegible] [illegible] 0.75782+003 0.75895+003 0.76009+003 0.76122+003 0.76236+003
 TEMPERATURE ([illegible])    [illegible] 0.76463+003 0.76576+003 0.76690+003 0.76803+003 0.76917+003 0.77030+003
 TEMPERATURE ([illegible])    0.77143+003 0.77257+003 0.77370+003 0.77484+003 0.77597+003 0.77711+003 0.77824+003
 TEMPERATURE ([illegible])    [illegible] 0.78051+003 0.78164+003 0.78278+003 0.78391+003 0.78505+003 0.78618+003
 TEMPERATURE ([illegible])    0.78732+003 [illegible] 0.78959+003 0.79072+003 0.79186+003 0.79299+003 0.79412+003
 TEMPERATURE ([illegible])    [illegible] [illegible] 0.79753+003 0.79866+003 0.79980+003 0.80093+003 0.80206+003
 TEMPERATURE ([illegible])    [illegible] [illegible] 0.80547+003 0.80660+003 0.80774+003 0.80887+003 0.81001+003
 TEMPERATURE ([illegible])    0.81114+003 [illegible] 0.81341+003 0.81454+003 0.81568+003 0.81681+003 0.81795+003
 TEMPERATURE ([illegible])    [illegible] [illegible] 0.82135+003 0.82249+003 0.82362+003 0.82476+003 0.82589+003
 TEMPERATURE ([illegible])    [illegible] [illegible] [illegible] 0.83043+003 0.83156+003 0.83270+003 0.83383+003
 TEMPERATURE ([illegible])    [illegible] [illegible] [illegible] 0.83837+003 0.83950+003 0.84064+003 0.84177+003
 TEMPERATURE ([illegible])    [illegible] [illegible] 0.84517+003 0.84631+003 0.84744+003 0.84858+003 0.84971+003
 TEMPERATURE ([illegible])    [illegible] [illegible] 0.85312+003 0.85425+003 0.85538+003 0.85652+003 0.85765+003
 TEMPERATURE ([illegible])    [illegible] [illegible] 0.86106+003 0.86219+003 0.86333+003 0.86446+003 0.86560+003
 TEMPERATURE ([illegible])    [illegible] 0.86786+003 [illegible] 0.87013+003 0.87127+003 0.87240+003 0.87354+003
 TEMPERATURE ([illegible])    [illegible]
 VAPOR FLOW RATE      [illegible] [illegible] 0.10000+003 0.10000+003 0.10000+003 0.10000+003 0.10000+003
 VAPOR FLOW RATE      [illegible] [illegible] 0.10000+003 0.10000+003 0.10000+003 0.10000+003 0.10000+003
 VAPOR FLOW RATE      [illegible] [illegible] 0.10000+003 0.10000+003 0.10000+003 0.10000+003 0.10000+003
 VAPOR FLOW RATE      [illegible] [illegible] 0.10000+003 0.10000+003 0.10000+003 0.10000+003 0.10000+003
 VAPOR FLOW RATE      [illegible] [illegible] 0.10000+003 0.10000+003 0.10000+003 0.10000+003 0.10000+003
 VAPOR FLOW RATE      [illegible] [illegible] 0.10000+003 0.10000+003 0.10000+003 0.10000+003 0.10000+003
 VAPOR FLOW RATE      [illegible] [illegible] 0.10000+003 0.10000+003 0.10000+003 0.10000+003 0.10000+003
 VAPOR FLOW RATE      [illegible] [illegible] 0.10000+003 0.10000+003 0.10000+003 0.10000+003 0.10000+003
 VAPOR FLOW RATE      [illegible] [illegible] [illegible] [illegible] 0.11000+003 0.11000+003 0.11000+003
 VAPOR FLOW RATE      0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003
 VAPOR FLOW RATE      0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003
 VAPOR FLOW RATE      0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003
 VAPOR FLOW RATE      0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003
 VAPOR FLOW RATE      0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003
 VAPOR FLOW RATE      0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003
 VAPOR FLOW RATE      0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003
 VAPOR FLOW RATE      0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003 0.11000+003
 VAPOR FLOW RATE      0.11000+003
```

```
37    SUM OF SQUARES OF RESIDUALS  0.31177-013 (MAT. BAL.  0.22250-015   HEAT BAL.  0.30864-013)
TEMPERATURE (R)    0.73824+003 0.75830+003 0.76882+003 0.77481+003 0.77713+003 0.77809+003 0.77854+003
TEMPERATURE (R)    0.77876+003 0.77889+003 0.77898+003 0.77901+003 0.77906+003 0.77907+003 0.77908+003
TEMPERATURE (R)    0.77911+003 0.77912+003 0.77913+003 0.77914+003 0.77914+003 0.77915+003 0.77915+003
TEMPERATURE (R)    0.77915+003 0.77916+003 0.77916+003 0.77916+003 0.77916+003 0.77916+003 0.77916+003
TEMPERATURE (R)    0.77916+003 0.77916+003 0.77916+003 0.77916+003 0.77916+003 0.77916+003 0.77916+003
TEMPERATURE (R)    0.77916+003 0.77916+003 0.77916+003 0.77916+003 0.77916+003 0.77916+003 0.77916+003
TEMPERATURE (R)    0.77916+003 0.77916+003 0.77916+003 0.77916+003 0.77916+003 0.77916+003 0.77916+003
TEMPERATURE (R)    0.77916+003 0.77917+003 0.77917+003 0.77918+003 0.77922+003 0.77931+003 0.77956+003
TEMPERATURE (R)    0.78022+003 0.78219+003 0.78796+003 0.80233+003 0.81071+003 0.81636+003 0.81986+003
TEMPERATURE (R)    0.82227+003 0.82373+003 0.82467+003 0.82526+003 0.82566+003 0.82595+003 0.82613+003
TEMPERATURE (R)    0.82625+003 0.82633+003 0.82638+003 0.82642+003 0.82644+003 0.82646+003 0.82647+003
TEMPERATURE (R)    0.82648+003 0.82648+003 0.82648+003 0.82648+003 0.82648+003 0.82648+003 0.82648+003
TEMPERATURE (R)    0.82648+003 0.82649+003 0.82649+003 0.82649+003 0.82649+003 0.82649+003 0.82649+003
TEMPERATURE (R)    0.82649+003 0.82649+003 0.82649+003 0.82649+003 0.82649+003 0.82649+003 0.82649+003
TEMPERATURE (R)    0.82649+003 0.82650+003 0.82650+003 0.82650+003 0.82650+003 0.82650+003 0.82651+003
TEMPERATURE (R)    [illegible] 0.82652+003 0.82654+003 0.82656+003 0.82657+003 0.82660+003 0.82663+003
TEMPERATURE (S)    [illegible] 0.82677+003 0.82692+003 0.82726+003 0.82816+003 0.83080+003 0.83872+003
TEMPERATURE (R)    0.86804+003
VAPOR FLOW RATE    0.00000+000 0.16000+003 0.14713+003 0.14162+003 0.13943+003 0.13858+003 0.13823+003
VAPOR FLOW RATE    0.13809+003 0.13802+003 0.13800+003 0.13798+003 0.13798+003 0.13797+003 0.13797+003
VAPOR FLOW RATE    0.13797+003 0.13797+003 0.13797+003 0.13796+003 0.13796+003 0.13796+003 0.13796+003
VAPOR FLOW RATE    0.13796+003 0.13796+003 0.13796+003 0.13796+003 0.13796+003 0.13796+003 0.13796+003
VAPOR FLOW RATE    0.13796+003 0.13796+003 0.13796+003 0.13796+003 0.13796+003 0.13796+003 0.13796+003
VAPOR FLOW RATE    0.13796+003 0.13796+003 0.13796+003 0.13796+003 0.13796+003 0.13796+003 0.13796+003
VAPOR FLOW RATE    0.13796+003 0.13796+003 0.13796+003 0.13796+003 0.13796+003 0.13796+003 0.13796+003
VAPOR FLOW RATE    0.13796+003 0.13796+003 0.13796+003 0.13795+003 0.13793+003 0.13788+003 0.13777+003
VAPOR FLOW RATE    0.13749+003 0.13657+003 0.13416+003 0.12812+003 0.73735+002 0.70687+002 0.68348+002
VAPOR FLOW RATE    0.68383+002 0.67743+002 0.67360+002 0.67116+002 0.66896+002 0.66854+002 0.66785+002
VAPOR FLOW RATE    0.66730+002 0.66708+002 0.66688+002 0.66674+002 0.66664+002 0.66658+002 0.66654+002
VAPOR FLOW RATE    0.66651+002 0.66649+002 0.66648+002 0.66647+002 0.66646+002 0.66646+002 0.66646+002
VAPOR FLOW RATE    0.66645+002 0.66645+002 0.66645+002 0.66645+002 0.66645+002 0.66645+002 0.66645+002
VAPOR FLOW RATE    0.66645+002 0.66645+002 0.66645+002 0.66645+002 0.66645+002 0.66645+002 0.66645+002
VAPOR FLOW RATE    0.66645+002 0.66645+002 0.66645+002 0.66645+002 0.66644+002 0.66644+002 0.66644+002
VAPOR FLOW RATE    0.66644+002 0.66644+002 0.66643+002 0.66642+002 0.66642+002 0.66640+002 0.66638+002
VAPOR FLOW RATE    0.66638+002 0.66627+002 0.66608+002 0.66550+002 0.66370+002 0.65788+002 0.63924+002
VAPOR FLOW RATE    0.56384+002
```

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

NUMBER OF ITERATIONS  37

REFLUX RATIO        2.2000000000

PRESSUR . TEMPERATUR . ENTHALPY AND LIQUID FRACTION OF FEED

 0.30000+003 PSIA    0.35332+003 F    0.208188879+007 B.T.U.      0.50000

*** STAGE VARIABLES ***

   PLATE NO.    PRESSURE      TEMPERATURE    LIQ. F. R.     VAP. F. R.     FEED RATE      HEAT DUTY
                  PSIA             F         LB MOL/TIME    LB MOL/TIME    LB MOL/TIME     BTU/TIME
        1       0.30000+003   0.27957+003   0.11000+003    0.00000+000    0.00000+000   -0.70222+006
        2       0.30000+003   0.29963+003   0.97128+002    0.16000+003    0.00000+000    0.00000+000
        3       0.30000+003   0.31015+003   0.91616+002    0.14713+003    0.00000+000    0.00000+000
        4       0.30000+003   0.31524+003   0.89434+002    0.14162+003    0.00000+000    0.00000+000
        5       0.30000+003   0.31746+003   0.88576+002    0.13943+003    0.00000+000    0.00000+000
        6       0.30000+003   0.31842+003   0.88230+002    0.13858+003    0.00000+000    0.00000+000
        7       0.30000+003   0.31887+003   0.88086+002    0.13823+003    0.00000+000    0.00000+000
        8       0.30000+003   0.31909+003   0.88024+002    0.13809+003    0.00000+000    0.00000+000
        9       0.30000+003   0.31922+003   0.87996+002    0.13802+003    0.00000+000    0.00000+000
       10       0.30000+003   0.31929+003   0.87982+002    0.13800+003    0.00000+000    0.00000+000
       11       0.30000+003   0.31934+003   0.87975+002    0.13798+003    0.00000+000    0.00000+000
       12       0.30000+003   0.31938+003   0.87971+002    0.13798+003    0.00000+000    0.00000+000
       13       0.30000+003   0.31940+003   0.87969+002    0.13797+003    0.00000+000    0.00000+000
       14       0.30000+003   0.31942+003   0.87967+002    0.13797+003    0.00000+000    0.00000+000
       15       0.30000+003   0.31944+003   0.87966+002    0.13797+003    0.00000+000    0.00000+000
       16       0.30000+003   0.31945+003   0.87965+002    0.13797+003    0.00000+000    0.00000+000
       17       0.30000+003   0.31946+003   0.87964+002    0.13797+003    0.00000+000    0.00000+000
       18       0.30000+003   0.31947+003   0.87964+002    0.13796+003    0.00000+000    0.00000+000
       19       0.30000+003   0.31947+003   0.87964+002    0.13796+003    0.00000+000    0.00000+000
       20       0.30000+003   0.31948+003   0.87963+002    0.13796+003    0.00000+000    0.00000+000
       21       0.30000+003   0.31948+003   0.87963+002    0.13796+003    0.00000+000    0.00000+000
       22       0.30000+003   0.31948+003   0.87963+002    0.13796+003    0.00000+000    0.00000+000
       23       0.30000+003   0.31948+003   0.87963+002    0.13796+003    0.00000+000    0.00000+000
       24       0.30000+003   0.31948+003   0.87962+002    0.13796+003    0.00000+000    0.00000+000
       25       0.30000+003   0.31948+003   0.87962+002    0.13796+003    0.00000+000    0.00000+000
       26       0.30000+003   0.31948+003   0.87962+002    0.13796+003    0.00000+000    0.00000+000
       27       0.30000+003   0.31948+003   0.87962+002    0.13796+003    0.00000+000    0.00000+000
       28       0.30000+003   0.31948+003   0.87962+002    0.13796+003    0.00000+000    0.00000+000
```

29	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
30	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
31	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
32	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
33	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
34	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
35	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
36	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
37	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
38	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
39	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
40	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
41	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
42	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
43	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
44	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
45	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
46	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
47	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
48	0.30000+003	0.31940+003	0.87962+002	0.13796+003	0.00000+000	0.00000+000
49	0.30000+003	0.31940+003	0.87961+002	0.13796+003	0.00000+000	0.00000+000
50	0.30000+003	0.31940+003	0.87960+002	0.13796+003	0.00000+000	0.00000+000
51	0.30000+003	0.31950+003	0.87958+002	0.13796+003	0.00000+000	0.00000+000
52	0.30000+003	0.31950+003	0.87951+002	0.13796+003	0.00000+000	0.00000+000
53	0.30000+003	0.31951+003	0.87939+002	0.13796+003	0.00000+000	0.00000+000
54	0.30000+003	0.31955+003	0.87889+002	0.13795+003	0.00000+000	0.00000+000
55	0.30000+003	0.31964+003	0.87768+002	0.13789+003	0.00000+000	0.00000+000
56	0.30000+003	0.31989+003	0.87446+002	0.13777+003	0.00000+000	0.00000+000
57	0.30000+003	0.32056+003	0.86867+002	0.13745+003	0.00000+000	0.00000+000
58	0.30000+003	0.32246+003	0.84164+002	0.13657+003	0.00000+000	0.00000+000
59	0.30000+003	0.32789+003	0.78123+002	0.13416+003	0.00000+000	0.00000+000
60	0.30000+003	0.34288+003	0.12373+003	0.13612+003	0.00000+000	0.00000+000
61	0.30000+003	0.35104+003	0.12100+003	0.73736+002	0.10000+003	0.00000+000
62	0.30000+003	0.35888+003	0.11936+003	0.70887+002	0.00000+000	0.00000+000
63	0.30000+003	0.36081+003	0.11836+003	0.68946+002	0.00000+000	0.00000+000
64	0.30000+003	0.36380+003	0.11774+003	0.68383+002	0.00000+000	0.00000+000
65	0.30000+003	0.36406+003	0.11736+003	0.67743+002	0.00000+000	0.00000+000
66	0.30000+003	0.36600+003	0.11712+003	0.67380+002	0.00000+000	0.00000+000
67	0.30000+003	0.36651+003	0.11696+003	0.67116+002	0.00000+000	0.00000+000
68	0.30000+003	0.36601+003	0.11686+003	0.66888+002	0.00000+000	0.00000+000
69	0.30000+003	0.36628+003	0.11678+003	0.66854+002	0.00000+000	0.00000+000
70	0.30000+003	0.36646+003	0.11674+003	0.66786+002	0.00000+000	0.00000+000
71	0.30000+003	0.36658+003	0.11671+003	0.66736+002	0.00000+000	0.00000+000
72	0.30000+003	0.36666+003	0.11669+003	0.66708+002	0.00000+000	0.00000+000

```
 73     0.30000+003   0.38671+003   0.11667+003   0.88688+002   0.00000+000   0.00000+000
 74     0.30000+003   0.38675+003   0.11666+003   0.88674+002   0.00000+000   0.00000+000
 75     0.30000+003   0.38677+003   0.11666+003   0.88664+002   0.00000+000   0.00000+000
 76     0.30000+003   0.38679+003   0.11666+003   0.88658+002   0.00000+000   0.00000+000
 77     0.30000+003   0.38680+003   0.11666+003   0.88654+002   0.00000+000   0.00000+000
 78     0.30000+003   0.38681+003   0.11665+003   0.88651+002   0.00000+000   0.00000+000
 79     0.30000+003   0.38681+003   0.11665+003   0.88649+002   0.00000+000   0.00000+000
 80     0.30000+003   0.38681+003   0.11665+003   0.88648+002   0.00000+000   0.00000+000
 81     0.30000+003   0.38682+003   0.11665+003   0.88647+002   0.00000+000   0.00000+000
 82     0.30000+003   0.38682+003   0.11665+003   0.88646+002   0.00000+000   0.00000+000
 83     0.30000+003   0.38682+003   0.11665+003   0.88646+002   0.00000+000   0.00000+000
 84     0.30000+003   0.38682+003   0.11665+003   0.88646+002   0.00000+000   0.00000+000
 85     0.30000+003   0.38682+003   0.11665+003   0.88645+002   0.00000+000   0.00000+000
 86     0.30000+003   0.38682+003   0.11665+003   0.88645+002   0.00000+000   0.00000+000
 87     0.30000+003   0.38682+003   0.11665+003   0.88645+002   0.00000+000   0.00000+000
 88     0.30000+003   0.38682+003   0.11665+003   0.88645+002   0.00000+000   0.00000+000
 89     0.30000+003   0.38682+003   0.11665+003   0.88645+002   0.00000+000   0.00000+000
 90     0.30000+003   0.38682+003   0.11664+003   0.88645+002   0.00000+000   0.00000+000
 91     0.30000+003   0.38682+003   0.11664+003   0.88645+002   0.00000+000   0.00000+000
 92     0.30000+003   0.38682+003   0.11664+003   0.88645+002   0.00000+000   0.00000+000
 93     0.30000+003   0.38682+003   0.11664+003   0.88645+002   0.00000+000   0.00000+000
 94     0.30000+003   0.38682+003   0.11664+003   0.88645+002   0.00000+000   0.00000+000
 95     0.30000+003   0.38682+003   0.11664+003   0.88645+002   0.00000+000   0.00000+000
 96     0.30000+003   0.38682+003   0.11664+003   0.88645+002   0.00000+000   0.00000+000
 97     0.30000+003   0.38682+003   0.11664+003   0.88645+002   0.00000+000   0.00000+000
 98     0.30000+003   0.38682+003   0.11664+003   0.88645+002   0.00000+000   0.00000+000
 99     0.30000+003   0.38682+003   0.11664+003   0.88645+002   0.00000+000   0.00000+000
100     0.30000+003   0.38683+003   0.11664+003   0.88645+002   0.00000+000   0.00000+000
101     0.30000+003   0.38683+003   0.11664+003   0.88645+002   0.00000+000   0.00000+000
102     0.30000+003   0.38683+003   0.11664+003   0.88645+002   0.00000+000   0.00000+000
103     0.30000+003   0.38683+003   0.11664+003   0.88644+002   0.00000+000   0.00000+000
104     0.30000+003   0.38683+003   0.11664+003   0.88644+002   0.00000+000   0.00000+000
105     0.30000+003   0.38684+003   0.11664+003   0.88644+002   0.00000+000   0.00000+000
106     0.30000+003   0.38685+003   0.11664+003   0.88644+002   0.00000+000   0.00000+000
107     0.30000+003   0.38686+003   0.11664+003   0.88644+002   0.00000+000   0.00000+000
108     0.30000+003   0.38687+003   0.11664+003   0.88643+002   0.00000+000   0.00000+000
109     0.30000+003   0.38688+003   0.11664+003   0.88642+002   0.00000+000   0.00000+000
110     0.30000+003   0.38690+003   0.11664+003   0.88642+002   0.00000+000   0.00000+000
111     0.30000+003   0.38693+003   0.11664+003   0.88640+002   0.00000+000   0.00000+000
112     0.30000+003   0.38696+003   0.11663+003   0.88638+002   0.00000+000   0.00000+000
113     0.30000+003   0.38701+003   0.11663+003   0.88636+002   0.00000+000   0.00000+000
114     0.30000+003   0.38710+003   0.11661+003   0.88627+002   0.00000+000   0.00000+000
115     0.30000+003   0.38725+003   0.11655+003   0.88608+002   0.00000+000   0.00000+000
116     0.30000+003   0.38758+003   0.11637+003   0.88580+002   0.00000+000   0.00000+000
```

117	0.30000+003	0.38848+003	0.11579+003	0.66370+002	0.00000+000	0.00000+000
118	0.30000+003	0.37123+003	0.11382+003	0.65788+002	0.00000+000	0.00000+000
119	0.30000+003	0.38005+003	0.10838+003	0.63824+002	0.00000+000	0.00000+000
120	0.30000+003	0.40837+003	0.90000+002	0.58384+002	0.00000+000	0.42842+006

```
**************************
*    MATERIAL BALANCES   *
**************************

FEEDS

                         PLATE NO.  60               PLATE NO.
                   LB MOL/TIME      MOL FRC.     LB MOL/TIME      MOL FRC.
C3H8               0.15000+002    0.15000+000
I-C4               0.15000+002    0.15000+000
I-C5               0 20000+002    0.20000+000
N-C5               0.70000+002    0.20000+000
N-C7               0.15000+002    0.15000+000
N-C8               0.15000+002    0.15000+000
TOTAL              0.10000+003

PRODUCTS

                       VAPOR DISTILLATE             LIQUID DISTILLATE              BOTTOM PRODUCT
                   LB MOL/TIME      MOL FRC.     LB MOL/TIME      MOL FRC.     LB MOL/TIME      MOL FRC.
C3H8               0.00000000+000 0.30000000+000 0.15000000+002 0.30000000+000 0.77836804-021 0.15567361-022
I-C4               0.00000000+000 0.30000000+000 0.15000000+002 0.30000000+000 0.13087307-009 0.26174613-011
I-C5               0.00000000+000 0.24319260+000 0.12159630+002 0.24319260+000 0.78403700+001 0.15680740+000
N-C5               0.00000000+000 0.15680740+000 0.78403700+001 0.15680740+000 0.12159630+002 0.24319260+000
N-C7               0.00000000+000 0.98012087-025 0.49006044-023 0.98012087-025 0.15000000+002 0.30000000+000
N-C8               0.00000000+000 0.22226106-038 0.11113053-037 0.22226106-038 0.15000000+002 0.30000000+000
TOTAL              0.00000000+000                0.50000000+002                0.50000000+002
```

```
***** COMPOSITION PROFILE *****

*** LIQUID PHASE ***

C3H8
  0.300000  0.159482  0.081617  0.070442  0.063463  0.061160  0.060363  0.060037  0.059886  0.059803
  0.059782  0.059717  0.059691  0.059672  0.059657  0.059646  0.059637  0.059630  0.059624  0.059620
  0.059617  0.059614  0.059612  0.059611  0.059609  0.059608  0.059608  0.059607  0.059607  0.059606
  0.059606  0.059605  0.059605  0.059605  0.059605  0.059605  0.059605  0.059605  0.059605  0.059605
  0.059605  0.059605  0.059605  0.059605  0.059605  0.059605  0.059605  0.059605  0.059605  0.059604
  0.059605  0.059600  0.059592  0.059571  0.059516  0.059370  0.058971  0.057896  0.054830  0.047820
  0.023464  0.011075  0.005102  0.002314  0.001040  0.000464  0.000206  0.000092  0.000041  0.000018
  0.000008  0.000004  0.000002  0.000001  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
I-C4
  0.300000  0.224832  0.177881  0.143841  0.127087  0.119175  0.115618  0.113817  0.113009  0.112584
  0.112372  0.112241  0.112158  0.112100  0.112059  0.112036  0.112006  0.111987  0.111972  0.111962
  0.111955  0.111946  0.111941  0.111937  0.111934  0.111931  0.111930  0.111928  0.111927  0.111926
  0.111925  0.111925  0.111924  0.111924  0.111924  0.111924  0.111923  0.111923  0.111923  0.111923
  0.111923  0.111923  0.111923  0.111923  0.111923  0.111923  0.111923  0.111922  0.111922  0.111921
  0.111916  0.111911  0.111904  0.111849  0.111730  0.111415  0.110686  0.108177  0.101748  0.087071
  0.066864  0.047302  0.036365  0.023088  0.015871  0.010842  0.007377  0.005006  0.003391  0.002284
  0.001551  0.001046  0.000708  0.000478  0.000323  0.000218  0.000147  0.000099  0.000067  0.000045
  0.000031  0.000021  0.000014  0.000009  0.000006  0.000004  0.000003  0.000002  0.000001  0.000001
  0.000001  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
I-C5
  0.349189  [illegible]  0.406382  0.422716  0.423884  0.419224  0.413711  0.408526  0.404088  0.400475
  0.397570  [illegible]  0.393447  0.392017  0.390886  0.390017  0.389329  0.388780  0.388388  0.388088
  0.387780  0.387578  0.387420  0.387296  0.387200  0.387124  0.387065  0.387019  0.386982  0.386954
  0.386932  0.386915  0.386901  0.386891  0.386882  0.386876  0.386871  0.386867  0.386864  0.386861
  0.386860  0.386857  0.386857  0.386856  0.386855  0.386855  0.386854  0.386853  0.386850  0.386845
  0.386838  0.386790  0.386712  0.386480  0.385811  0.384380  0.380296  [illegible]  0.339198  0.272686
  0.332196  0.326856  0.313802  0.316866  0.323336  0.328824  0.327463  0.328864  0.329340  0.329841
  0.330179  0.330407  0.330880  0.330664  0.330724  0.330781  0.330813  0.330834  0.330846  0.330886
  0.330864  0.330880  0.330871  0.330873  0.330873  0.330873  0.330872  0.330871  0.330866  0.330866
  0.330862  0.330886  0.330840  0.330836  0.330825  0.330807  0.330783  0.330752  0.330708  0.330653
  0.330576  0.330478  0.330844  0.330167  0.329830  0.329615  0.329196  0.329636  0.327884  0.326806
  0.329887  0.323830  0.321480  0.318308  0.313833  0.307583  0.297462  0.278649  0.238875  0.196807
```

```
N-C6
  0.188807  0.287741  0.334220  0.362801  0.388627  0.400421  0.410408  0.417619  0.423012  0.427128
  0.430808  0.432777  0.434705  0.436210  0.437388  0.438308  0.439030  0.439584  0.440085  0.440380
  0.440550  0.440862  0.441027  0.441186  0.441257  0.441336  0.441388  0.441446  0.441484  0.441513
  0.441537  0.441555  0.441568  0.441580  0.441588  0.441595  0.441600  0.441604  0.441608  0.441610
  0.441612  0.441614  0.441615  0.441616  0.441617  0.441617  0.441617  0.441617  0.441614  0.441608
  0.441582  0.441550  0.441441  0.441162  0.440434  0.438611  0.433342  0.419287  0.382281  0.300386
  0.318814  0.330746  0.338879  0.343888  0.347258  0.349807  0.351001  0.352000  0.352880  0.353118
  0.353422  0.353686  0.353764  0.353857  0.353930  0.353962  0.353991  0.354010  0.354023  0.354032
  0.354038  0.354042  0.354046  0.354048  0.354050  0.354052  0.354054  0.354056  0.354058  0.354062
  0.354066  0.354072  0.354079  0.354088  0.354102  0.354120  0.354143  0.354174  0.354216  0.354271
  0.354344  0.354442  0.354573  0.354746  0.354978  0.355286  0.355686  0.356242  0.356980  0.357936
  0.358810  0.360819  0.363157  0.366057  0.369675  0.373704  0.376801  0.371872  0.340467  0.243183

N-C7
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000001  0.000001  0.000003  0.000008  0.000022
  0.000005  0.000140  0.000386  0.000808  0.002291  0.005785  0.014534  0.038851  0.081061  0.154207
  0.158686  0.161880  0.163771  0.164661  0.165722  0.166216  0.166540  0.166754  0.166887  0.166983
  0.167057  0.167100  0.167130  0.167148  0.167162  0.167171  0.167177  0.167181  0.167184  0.167186
  0.167187  0.167188  0.167188  0.167189  0.167189  0.167189  0.167189  0.167189  0.167190  0.167190
  0.167190  0.167190  0.167190  0.167190  0.167190  0.167191  0.167191  0.167191  0.167192  0.167193
  0.167194  0.167196  0.167197  0.167200  0.167203  0.167208  0.167214  0.167223  0.167234  0.167250
  0.167273  0.167314  0.167386  0.167556  0.168186  0.169845  0.175024  0.190388  0.230830  0.300000

N-C8
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000001  0.000006  0.000036  0.000118  0.000636  0.002342  0.010142  0.040830  0.137820
  0.141802  0.143880  0.145681  0.146183  0.146773  0.147147  0.147383  0.147584  0.147662  0.147734
  0.147762  0.147815  0.147837  0.147851  0.147861  0.147868  0.147873  0.147876  0.147878  0.147879
  0.147880  0.147881  0.147881  0.147881  0.147881  0.147882  0.147882  0.147882  0.147882  0.147882
  0.147882  0.147882  0.147882  0.147882  0.147882  0.147882  0.147883  0.147883  0.147883  0.147883
  0.147884  0.147885  0.147886  0.147887  0.147888  0.147891  0.147894  0.147897  0.147903  0.147910
  0.147920  0.147937  0.147968  0.148040  0.148237  0.148808  0.151013  0.158079  0.180438  0.300000
```

```
*** VAPOR PHASE ***

C3H8
   0.[illegible]  0.300000  0.203381  0.165330  0.152760  0.148821  0.147565  0.147134  0.146966  0.146886
   0.146848  0.146814  0.146794  0.146779  0.146768  0.146759  0.146752  0.146747  0.146743  0.146740
   0.146737  0.146735  0.146734  0.146733  0.146732  0.146731  0.146731  0.146730  0.146730  0.146730
   0.146730  0.146730  0.146729  0.146729  0.146729  0.146729  0.146729  0.146729  0.146729  0.146729
   0.146729  0.146729  0.146729  0.146729  0.146729  0.146729  0.146729  0.146729  0.146729  0.146729
   0.146729  0.146730  0.146732  0.146738  0.146754  0.146795  0.146906  0.147216  0.148088  0.150502
   0.[illegible]  0.[illegible]  0.018080  0.008834  0.004023  0.001812  0.000810  0.000361  0.000160  0.000071
   0.[illegible]  0.000014  0.000006  0.000003  0.000001  0.000001  0.000000  0.000000  0.000000  0.000000
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000

I-C4
   0.300000  0.300000  0.258979  0.220808  0.198802  0.188483  0.184862  0.182317  0.181283  0.180758
   0.[illegible]  0.[illegible]  0.180284  0.180232  0.180195  0.180170  0.180151  0.180136  0.180125  0.180116
   0.180110  0.180104  0.180100  0.180097  0.180094  0.180092  0.180091  0.180090  0.180089  0.180088
   0.[illegible]  0.180087  0.180087  0.180087  0.180086  0.180086  0.180086  0.180086  0.180086  0.180086
   0.[illegible]  0.[illegible]  0.180086  0.180086  0.180086  0.180086  0.180085  0.180085  0.180085  0.180085
   0.[illegible]  0.[illegible]  0.180084  0.180081  0.180075  0.180060  0.180016  0.179915  0.179665  0.179117
   0.146116  0.111987  0.081234  0.057898  0.040130  0.027851  0.018819  0.012666  0.008749  0.005829
   0.004013  0.002714  0.001694  0.001230  0.000897  0.000566  0.000361  0.000257  0.000174  0.000117
   0.[illegible]  0.[illegible]  0.000036  0.000024  0.000016  0.000011  0.000007  0.000005  0.000003  0.000002
   0.[illegible]  0.000001  0.000001  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000

I-C5
   0.349100  0.349100  0.316800  0.348798  0.358640  0.358808  0.358850  0.351898  0.348639  0.346798
   0.348482  0.341686  0.340155  0.338894  0.338083  0.337367  0.336805  0.336367  0.336023  0.335754
   0.335544  0.335379  0.335250  0.335140  0.335071  0.335000  0.334961  0.334923  0.334893  0.334870
   0.334852  0.334838  0.334827  0.334818  0.334812  0.334806  0.334802  0.334799  0.334797  0.334795
   0.334793  0.334792  0.334791  0.334790  0.334790  0.334789  0.334789  0.334788  0.334787  0.334786
   0.334782  0.334773  0.334748  0.334687  0.334536  0.334114  0.333019  0.330073  0.322107  0.301708
   0.351608  0.387476  0.412881  0.430616  0.439730  0.446046  0.451737  0.454834  0.457073  0.458810
   0.459476  0.460127  0.460606  0.460861  0.461081  0.461196  0.461266  0.461340  0.461389  0.461416
   0.461436  0.461447  0.461455  0.461460  0.461463  0.461465  0.461465  0.461463  0.461461  0.461457
   0.461452  0.461445  0.461436  0.461422  0.461404  0.461381  0.461350  0.461308  0.461253  0.461178
   0.461080  0.460948  0.460774  0.460541  0.460230  0.459817  0.459266  0.458533  0.457567  0.456286
   0.454888  0.452226  0.449157  0.446087  0.438540  0.431983  0.421167  0.404361  0.373851  0.308886
```

```
N-C6
   0.189807  0.189807  0.223440  0.265112  0.288888  0.303184  0.312302  0.318581  0.323130  0.326958
   0.329173  0.331166  0.332760  0.333806  0.334883  0.335703  0.336290  0.336749  0.337106  0.337389
   0.337690  0.337761  0.337816  0.338021  0.338103  0.338167  0.338216  0.338257  0.338288  0.338312
   0.338331  0.338346  0.338357  0.338366  0.338373  0.338378  0.338382  0.338385  0.338386  0.338381
   0.338392  0.338390  0.338385  0.338386  0.338386  0.338386  0.338387  0.338387  0.338386  0.338384
   0.338390  0.338377  0.338346  0.338263  0.338051  0.337407  0.336003  0.332086  0.321467  0.284280
   0.369165  0.371730  0.388871  0.408827  0.416158  0.424605  0.428706  0.431506  0.433377  0.434632
   0.435475  0.436043  0.436436  0.436664  0.436886  0.436876  0.437066  0.437108  0.437148  0.437170
   0.437186  0.437196  0.437206  0.437212  0.437216  0.437220  0.437223  0.437226  0.437230  0.437236
   0.437241  0.437246  0.437256  0.437271  0.437288  0.437312  0.437342  0.437383  0.437436  0.437510
   0.437607  0.437736  0.437907  0.438136  0.438440  0.438845  0.439385  0.440104  0.441061  0.442334
   0.444027  0.446276  0.446256  0.453163  0.458367  0.464702  0.473025  0.477817  0.472522  0.423758

N-C7
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000001  0.000002  0.000005
   0.000014  0.000065  0.000060  0.000236  0.000575  0.001480  0.003887  0.009213  0.022306  0.049427
   0.066044  0.066690  0.066913  0.064130  0.066890  0.066051  0.066990  0.066980  0.067100  0.067247
   0.067345  0.067412  0.067467  0.067487  0.067507  0.067521  0.067530  0.067536  0.067540  0.067543
   0.067545  0.067547  0.067547  0.067548  0.067548  0.067549  0.067549  0.067549  0.067549  0.067549
   0.067549  0.067550  0.067550  0.067550  0.067550  0.067551  0.067551  0.067552  0.067552  0.067553
   0.067555  0.067556  0.067558  0.067562  0.067565  0.067572  0.067580  0.067590  0.067606  0.067632
   0.067640  0.067685  0.067792  0.067883  0.068303  0.069069  0.071781  0.080040  0.104672  0.171067

N-C8
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
   0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
   0.000000  0.000000  0.000001  0.000004  0.000017  0.000075  0.000336  0.001468  0.006362  0.024687
   0.087046  0.088880  0.081230  0.082166  0.083666  0.083036  0.083276  0.083436  0.083541  0.083611
   0.083669  0.083690  0.083712  0.083726  0.083736  0.083743  0.083747  0.083750  0.083752  0.083753
   0.083754  0.083755  0.083755  0.083756  0.083756  0.083756  0.083756  0.083756  0.083756  0.083756
   0.083756  0.083756  0.083756  0.083756  0.083757  0.083757  0.083757  0.083757  0.083757  0.083758
   0.083758  0.083758  0.083760  0.083762  0.083763  0.083766  0.083769  0.083773  0.083779  0.083787
   0.083797  0.083812  0.083835  0.083877  0.083960  0.084216  0.084896  0.087782  0.048864  0.088626
```

APPENDIX 2.

EXAMPLE 2. COMPUTER INPUTS AND OUTPUTS

–Generalized Underwood method

–Plate-by-plate method (ISHII)

```
'EXAMPLE 2'
'GENERALIZED UNDERWOOD'
'TOTAL CONDENSER'
'ALPHA'
'KCONSTANT'
'LB-MOLE/TIME', 'BTU/LB-MOLE', 'F'
6
'C3H8'
'n-C4'
'i-C5'
'n-C5'
'n-C6'
'n-C7'
2
100.0, 100.0
0.25, 0.20, 0.20, 0.20, 0.10, 0.05
0.05, 0.10, 0.20, 0.20, 0.20, 0.25
'[illegible]'
[illegible].11, [illegible]110.[illegible]
2, 5
0.[illegible]714, 0.[illegible]
11.04, [illegible], [illegible], 3.24, 1.77, 1.00
6
    5.[illegible]D-2, -50.70[illegible]D-5, 112.173[illegible]D-8,   -574.[illegible]D-12
0.0, [illegible].0
[illegible].0
[illegible].0
21[illegible].0
[illegible].0
[illegible].0
[illegible].0
[illegible].0
[illegible].0
[illegible]11.0
[illegible].0
[illegible].0
[illegible].0
```

```
MINIMUM REFLUX CALCULATION FOR MULTIPLE FEED COLUMN

METHOD: GENERALIZED UNDERWOOD
        TOTAL CONDENSER

MAXIMUM NUMBER OF COMPONENTS: 10
MAXIMUM NUMBER OF FEEDS: 5



******************************
SECTION 1: DATA
******************************
NDATA: EXAMPLE 2


SYSTEM:
NUMBER OF COMPONENTS:  6
NUMBER OF FEEDS: 2

RECOVERY OF LIGHT KEY AT THE TOP:    91.43714 %
RECOVERY OF HEAVY KEY AT THE BOTTOM: 86.53246 %

COMPONENTS: C3H8
            n-C4
            i-C5
            n-C5
            n-C6
            n-C7


PROPERTIES OF COMPONENTS:

COMP  KEYS  ALPHA      HL             HV             LAMBDA
                       BTU/LB-MOLE    BTU/LB-MOLE    BTU/LB-MOLE
----  ----  -------
 1          11.6400    10435.0000     16435.0000      6000.0000
 2     LK    5.0000    18872.0000     23535.0000      4663.0000
 3           3.0000    21703.0000     28011.0000      6308.0000
 4           2.3400    22375.0000     28716.0000      6341.0000
 5     HK    1.7700    25763.0000     34293.0000      8530.0000
 6           1.0000    28905.0000     40006.0000     11101.0000
```

```
DATA ON FEEDS:

FEED  FEED RATE   HFBP          HFDP          HF            DHF
      LB-MOLE/TIME BTU/TIME     BTU/TIME      BTU/TIME      BTU/TIME
----
  1    100.0000    2048780.00    2610625.00    2354430.11    305650.11
  2    100.0000    2386290.00    3140725.00    2655110.56    268820.56


TOTAL FEED:

COMP  T. FEED RATE  MOLE FRAC
      LB-MOLE/TIME
----                ---------
  1      30.0000    0.150000
  2      30.0000    0.150000
  3      40.0000    0.200000
  4      40.0000    0.200000
  5      30.0000    0.150000
  6      30.0000    0.150000
       ----------   --------
        200.0000    1.000000


FEED NO.1: FLASHED FEED

COMP  RATE          MOLE FRAC
      LB-MOLE/TIME
----                ---------
  1      25.0000    0.250000
  2      20.0000    0.200000
  3      20.0000    0.200000
  4      20.0000    0.200000
  5      10.0000    0.100000
  6       5.0000    0.050000
       ----------   --------
        100.0000    1.000000
```

```
FEED NO.2: FLASHED FEED

COMP   RATE             MOLE FRAC
       LB-MOLE/TIME
----                    ---------
 1         5.0000       0.050000
 2        10.0000       0.100000
 3        20.0000       0.200000
 4        20.0000       0.200000
 5        20.0000       0.200000
 6        25.0000       0.250000
       ----------       --------
         100.0000       1.000000
```

```
********************************
SECTION 2: RESULTS
********************************

DISTILLATE:

COMP  KEYS  RATE               MOLE FRAC  FRAC/FEED
            LB-MOLE/TIME
----  ----  ------------       ---------  ---------
  1             30.0000        0.272727   1.000000
  2   LK        27.4311        0.249374   0.914371
  3             25.7153        0.233776   0.642883
  4             22.8133        0.207394   0.570332
  5   HK         4.0403        0.036730   0.134676
  6              0.0           0.0        0.0
            ----------         ---------
               110.0000        1.000000

BOTTOM PRODUCT:

COMP  KEYS  RATE               MOLE FRAC  FRAC/FEED
            LB-MOLE/TIME
----  ----  ------------       ---------  ---------
  1              0.0           0.0        0.0
  2   LK         2.5689        0.028543   0.085629
  3             14.2847        0.158719   0.357117
  4             17.1867        0.190964   0.429668
  5   HK        25.9597        0.288442   0.865324
  6             30.0000        0.333333   1.000000
            ----------         ---------
                90.0000        1.000000

INTERMEDIATE SECTION NO.1: NET UPWARD FLOW

COMP  KEYS  RATE
            LB-MOLE/TIME
----  ----  ------------
  1                5.0000
  2   LK           7.4311
  3                5.7153
  4                2.8133
  5   HK          -5.9597
  6               -5.0000
            -------------
                  10.0000
```

```
LIQUID AND VAPOR FLOWRATES:

SECTION                     LIQUID         VAPOR
                            LB-MOLE/TIME   LB-MOLE/TIME

RECTIFYING      : TOP        80.5000       170.5000
                  PINCH      49.1133       139.1133
                  BOT        46.7013       136.7013

INTERMEDIATE(1): TOP         84.9600        94.9600
                  PINCH      80.9846        90.9846
                  BOT        74.8820        84.8820

STRIPPING       : TOP       133.7080        43.7080
                  PINCH     132.3307        42.3307
                  BOT       129.3329        39.3329


FLOWRATE CHANGES (FEED TRAYS):

FEED  DL             DV             TOTAL
      LB-MOLE/TIME   LB-MOLE/TIME   LB-MOLE/TIME
----
 1       38.2587        61.7413      100.0000
 2       58.8560        41.1440      100.0000


MINIMUM REFLUX:

EXTERNAL REFLUX RATIO (L/D):   0.880000473

INTERNAL REFLUX RATIO (L/V):   0.354630906
```

```
********************************
SECTION 3: ADDITIONAL RESULTS
********************************

FEED TRAYS COMPOSITION:

FEED TRAY NO.1

COMP  LQ MOLE FRAC  VP MOLE FRAC
  1    0.074601      0.213970
  2    0.141405      0.217829
  3    0.282867      0.240680
  4    0.272812      0.227646
  5    0.170555      0.077821
  6    0.057760      0.022054
       ---------     ---------
       1.000000      1.000000

FEED TRAY NO.2

COMP  LQ MOLE FRAC  VP MOLE FRAC
  1    0.098361      0.076715
  2    0.071435      0.158806
  3    0.104001      0.261380
  4    0.219880      0.262168
  5    0.247840      0.160406
  6    0.258481      0.080532
       ---------     ---------
       1.000000      1.000000
```

```
PINCH REGIONS COMPOSITION:

PINCH, RECTIFYING SECTION

COMP  LQ MOLE FRAC  VP MOLE FRAC
 1    [illegible]   0.21[illegible]
 2    0.148748      0.210822
 3    0.272841      0.348772
 4    0.[illegible] 0.234[illegible]
 5    0.[illegible] 0.088141
 6    0.0           0.0
      --------      --------
      1.000000      1.000000

PINCH, INTERMEDIATE SECTION NO.1

COMP  LQ MOLE FRAC  VP MOLE FRAC
 1    [illegible]   0.074881
 2    0.[illegible] 0.168816
 3    0.277341      0.3[illegible]
 4    0.[illegible] 0.388704
 5    0.1[illegible] 0.0[illegible]
 6    0.[illegible] 0.088421
      --------      --------
      1.000000      1.000000

PINCH, STRIPPING SECTION

COMP  LQ MOLE FRAC  VP MOLE FRAC
 1    0.0           0.0
 2    0.074888      0.171087
 3    0.1[illegible] 0.[illegible]
 4    0.217080      0.272849
 5    0.281818      0.172[illegible]
 6    0.[illegible] 0.1[illegible]
      --------      --------
      1.000000      1.000000
```

TEMPERATURE PROFILE:

DISTILLATE: 275.08 F
PINCH(1): 312.06 F
FEED TRAY(1): 317.36 F
PINCH(2): 334.06 F
FEED TRAY(2): 356.67 F
PINCH(3): 383.84 F
BOTTOM PRODUCT: 384.34 F

```
EXAMPLE 2
[illegible]  (PLATE-BY-PLATE ALGORITHM)

6,1,                              > NCP, JCASE
6-component, constant alpha, constant enthalpy model.
[illegible],3,2,0,0,0,110.0,1.0,0.[illegible],0,1,  > NPLT,TYPE,JF,JSL,JSV,JQ,D,ZM,REF,IVAL,JPRINT
0,1,1                        > NPRINT,NCALC,JCALC
2, 1.0E-[illegible], 45.0                > ISATHE, BATOL, BASLO
[illegible].0,0.0,270.0,[illegible].0,300.0,   > PP(1), PD, TT(1), TT(NPLT), PP(2)
[illegible],2,[illegible].0,310.0,0.4,310.0,    > NF(J),JFEED(J),PF(J),TF(J),ZLF(J),TFWV(J)
[illegible].0, 20.0, 20.0, 20.0, 10.0, 5.0   > ZF(I,J)
120, 2, [illegible].0, [illegible].0, 0.0, [illegible].0
5.0, 10.0, 20.0, 20.0, 30.0, 25.0
.1e-14,[illegible],                > TOL, LIMIT
1.,1.,1.,1.,1.,1.              > EFFI on tray 1
1.,1.,1.,1.,1.,1.              > EFFI on tray 2 to nplt-1
1.,1.,1.,1.,1.,1.              > EFFI on tray nplt

[illegible]
n-C4
i-C5
n-C5
n-C6
n-C7
   -14.[illegible]D-2,   [illegible].[illegible]D-5,   -5.305[illegible]D-8,  -173.[illegible]D-12
   -14.1017[illegible]D-2,   36.[illegible]D-5,   16.5214[illegible]D-8,  -240.[illegible]D-12
     -7.[illegible]D-2,    3.[illegible]D-5,  [illegible].5073[illegible]D-8,  -414.[illegible]D-12
     -7.[illegible]D-2,    2.0[illegible]D-5,  [illegible].1[illegible]D-8,  -413.124[illegible]D-12
      1.[illegible]D-2,  -30.[illegible]D-5,   97.7[illegible]D-8,  -[illegible].[illegible]D-12
      5.[illegible]D-2,  -50.7[illegible]D-5,  112.173[illegible]D-8,   -574.[illegible]D-12
 [illegible].,0.,0.,
 [illegible].,0.,0.,
 21[illegible].,0.,0.,
 [illegible].,0.,0.,
 [illegible].,0.,0.,
 [illegible].,0.,0.,
 [illegible].,0.,0.,
 [illegible].,0.,0.,
 [illegible]11.,0.,0.,
 [illegible].,0.,0.,
 [illegible].,0.,0.,
 [illegible].,0.,0.,
 .T.
 11.04, 5.[illegible], 3.[illegible], 3.24, 1.77, 1.00
```

```
***** EQUILIBRIUM AND ENTHALPY DATA *****
-0.[illegible]+000      0.[illegible]-008     -0.5505100-007      -0.1736833-008
-0.[illegible]+000      0.[illegible]-008      0.1662141-006      -0.2462384-008
-0.[illegible]-001      0.[illegible]-004      0.5650734-006      -0.4146232-008
-0.[illegible]-001      0.[illegible]-004      0.5012824-006      -0.4131341-008
 0.1[illegible]-001    -0.[illegible]-008      0.6776640-006      -0.5423684-008
 0.[illegible]-001     -0.[illegible]-008      0.1121734-005      -0.5746836-008
 0.[illegible]+000      0.0000000+000      0.0000000+000
 0.[illegible]+000      0.0000000+000      0.0000000+000
 0.[illegible]+000      0.0000000+000      0.0000000+000
 0.[illegible]+000      0.0000000+000      0.0000000+000
 0.[illegible]+000      0.0000000+000      0.0000000+000
 0.[illegible]+000      0.0000000+000      0.0000000+000
 0.[illegible]+000      0.0000000+000      0.0000000+000
 0.[illegible]+000      0.0000000+000      0.0000000+000
 0.[illegible]+000      0.0000000+000      0.0000000+000
 0.[illegible]+000      0.0000000+000      0.0000000+000
 0.[illegible]+000      0.0000000+000      0.0000000+000
 0.[illegible]+000      0.0000000+000      0.0000000+000
 0.11[illegible]+000    0.3[illegible]+001     0.3680000+001       0.3240000+001
 0.177[illegible]+001   0.1000000+001
```

```
6-COMPONENT, CONSTANT ALPHA, CONSTANT ENTHALPY MODEL.


TYPE OF COLUMN.................. 3
NO. OF PLATES...................**
PRESSURE AT TOP PLATE (PSIA)..    300.00
PRESSURE DROP PER PLATE (PSIA)    0.0000

NO. OF FEEDS.................... 2

   ENTERING PLATE OF FEED 1......60
   FEED QUANTITY.................. 0.10000+003
   PRESSURE OF FEED...............    300.00
   LIQUID RATIO OF FEED...........  0.4000

   ENTERING PLATE OF FEED 2......**
   FEED QUANTITY.................. 0.10000+003
   PRESSURE OF FEED...............    300.00
   LIQUID RATIO OF FEED...........  0.6000

REFLUX RATIO.................          0.980
LIQUID RATIO OF TOP PRODUCT...     1.0000
SPECIFIED TOP PRODUCT......... 0.11000+003

EFFICIENCIES

PLATE  1.....  1.00  1.00  1.00  1.00  1.00  1.00
PLATE 2 ON...  1.00  1.00  1.00  1.00  1.00  1.00
PLATE100.....  1.00  1.00  1.00 .1.00  1.00  1.00
```

```
*********************************************
*       CONVERGENCE OF ITERATION            *
*********************************************

  0   SUM OF SQUARES OF RESIDUALS  0.74687+001 (MAT. BAL.  0.74602+001   HEAT BAL.  0.48222-008)
 TEMPERATURE  (K)   [illegible] [illegible] 0.73101+000 0.73169+000 0.73236+000 0.73303+000 0.73369+000
 TEMPERATURE  (K)   0.73436+000 0.73503+000 0.73570+000 0.73637+000 0.73704+000 0.73771+000 0.73838+000
 TEMPERATURE  (K)   0.73906+000 0.73973+000 0.74040+000 0.74107+000 0.74174+000 0.74241+000 0.74308+000
 TEMPERATURE  (K)   0.74375+000 0.74442+000 0.74509+000 0.74576+000 0.74643+000 0.74710+000 0.74777+000
 TEMPERATURE  (K)   0.74844+000 0.74911+000 0.74978+000 0.75045+000 0.75112+000 0.75179+000 0.75246+000
 TEMPERATURE  (K)   0.75313+000 0.75380+000 0.75447+000 0.75514+000 0.75582+000 0.75649+000 0.75716+000
 TEMPERATURE  (K)   0.75783+000 0.75850+000 0.75917+000 0.75984+000 0.76051+000 0.76118+000 0.76185+000
 TEMPERATURE  (K)   0.76252+000 0.76319+000 0.76386+000 0.76453+000 0.76520+000 0.76587+000 0.76654+000
 TEMPERATURE  (K)   0.76721+000 0.76788+000 0.76855+000 0.76922+000 0.76989+000 0.77056+000 0.77123+000
 TEMPERATURE  (K)   0.77190+000 0.77257+000 0.77324+000 0.77391+000 0.77458+000 0.77525+000 0.77592+000
 TEMPERATURE  (K)   0.77660+000 0.77727+000 0.77794+000 0.77861+000 0.77928+000 0.77995+000 0.78062+000
 TEMPERATURE  (K)   0.78129+000 0.78196+000 0.78263+000 0.78330+000 0.78397+000 0.78464+000 0.78531+000
 TEMPERATURE  (K)   0.78598+000 0.78665+000 0.78732+000 0.78799+000 0.78866+000 0.78933+000 0.79001+000
 TEMPERATURE  (K)   0.79068+000 0.79135+000 0.79202+000 0.79269+000 0.79336+000 0.79403+000 0.79470+000
 TEMPERATURE  (K)   0.79537+000 0.79604+000 0.79671+000 0.79738+000 0.79805+000 0.79872+000 0.79939+000
 TEMPERATURE  (K)   0.80006+000 0.80073+000 0.80140+000 0.80207+000 0.80274+000 0.80341+000 0.80408+000
 TEMPERATURE  (K)   0.80475+000 0.80542+000 0.80609+000 0.80677+000 0.80744+000 0.80811+000 0.80878+000
 TEMPERATURE  (K)   0.80945+000 0.81012+000 0.81079+000 0.81146+000 0.81213+000 0.81280+000 0.81347+000
 TEMPERATURE  (K)   0.81414+000 0.81481+000 0.81548+000 0.81615+000 0.81682+000 0.81749+000 0.81816+000
 TEMPERATURE  (K)   0.81883+000 0.81950+000 0.82017+000 0.82084+000 0.82151+000 0.82218+000 0.82285+000
 TEMPERATURE  (K)   0.82352+000 0.82420+000 0.82487+000 0.82554+000 0.82621+000 0.82688+000 0.82755+000
 TEMPERATURE  (K)   0.82822+000 0.82889+000 0.82956+000 0.83023+000 0.83090+000 0.83157+000 0.83224+000
 TEMPERATURE  (K)   0.83291+000 0.83358+000 0.83425+000 0.83492+000 0.83559+000 0.83626+000 0.83693+000
 TEMPERATURE  (K)   0.83760+000 0.83827+000 0.83894+000 0.83961+000 0.84028+000 0.84095+000 0.84163+000
 TEMPERATURE  (K)   0.84230+000 0.84297+000 0.84364+000 0.84431+000 0.84498+000 0.84565+000 0.84632+000
 TEMPERATURE  (K)   0.84699+000 0.84766+000 0.84833+000 0.84900+000 0.84967+000
 VAPOR  FLOW  RATE  [illegible] 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003
 VAPOR  FLOW  RATE  0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003
 VAPOR  FLOW  RATE  0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003
 VAPOR  FLOW  RATE  0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003
 VAPOR  FLOW  RATE  0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003
 VAPOR  FLOW  RATE  0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003
 VAPOR  FLOW  RATE  0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003
 VAPOR  FLOW  RATE  0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.17050+003
 VAPOR  FLOW  RATE  0.17050+003 0.17050+003 0.17050+003 0.17050+003 0.11050+003 0.11050+003 0.11050+003
 VAPOR  FLOW  RATE  0.11050+003 0.11050+003 0.11050+003 0.11050+003 0.11050+003 0.11050+003 0.11050+003
 VAPOR  FLOW  RATE  0.11050+003 0.11050+003 0.11050+003 0.11050+003 0.11050+003 0.11050+003 0.11050+003
 VAPOR  FLOW  RATE  0.11050+003 0.11050+003 0.11050+003 0.11050+003 0.11050+003 0.11050+003 0.11050+003
 VAPOR  FLOW  RATE  0.11050+003 0.11050+003 0.11050+003 0.11050+003 0.11050+003 0.11050+003 0.11050+003
```

```
VAPOR FLOW RATE    0.11080+000 0.11080+000 0.11080+000 0.11080+000 0.11080+000 0.11080+000 0.11080+000
VAPOR FLOW RATE    0.11080+000 0.11080+000 0.11080+000 0.11080+000 0.11080+000 0.11080+000 0.11080+000
VAPOR FLOW RATE    0.11080+000 0.11080+000 0.11080+000 0.11080+000 0.11080+000 0.11080+000 0.11080+000
VAPOR FLOW RATE    0.11080+000 0.11080+000 0.11080+000 0.11080+000 0.11080+000 0.11080+000 0.11080+000
VAPOR FLOW RATE    0.11080+000 [illegible] 0.70800+002 0.70800+002 0.70800+002 0.70800+002 0.70800+002
VAPOR FLOW RATE    0.70800+002 [illegible] 0.70800+002 0.70800+002 0.70800+002 0.70800+002 0.70800+002
VAPOR FLOW RATE    0.70800+002 [illegible] 0.70800+002 0.70800+002 0.70800+002 0.70800+002 0.70800+002
VAPOR FLOW RATE    0.70800+002 [illegible] 0.70800+002 0.70800+002 0.70800+002 0.70800+002 0.70800+002
VAPOR FLOW RATE    0.70800+002 [illegible] 0.70800+002 0.70800+002 0.70800+002 0.70800+002 0.70800+002
VAPOR FLOW RATE    0.70800+002 [illegible] 0.70800+002 0.70800+002 0.70800+002 0.70800+002 0.70800+002
VAPOR FLOW RATE    0.70800+002 0.70800+002 0.70800+002 0.70800+002 0.70800+002 0.70800+002 0.70800+002
VAPOR FLOW RATE    0.70800+002 0.70800+002 0.70800+002 0.70800+002 0.70800+002 0.70800+002 0.70800+002
VAPOR FLOW RATE    0.70800+002 0.70800+002 0.70800+002 0.70800+002 0.70800+002

40    SUM OF SQUARES OF RESIDUALS  0.14881-012 (MAT. BAL.  0.47676-016   HEAT BAL.   0.14077-012)
TEMPERATURE (R)    0.75880+000 0.75880+000 0.75880+000 0.76812+000 0.77082+000 0.77081+000 0.77117+000
TEMPERATURE (R)    0.77150+000 0.77151+000 0.77158+000 0.77164+000 0.77167+000 0.77168+000 0.77170+000
TEMPERATURE (R)    0.77171+000 0.77171+000 0.77172+000 0.77172+000 0.77172+000 0.77172+000 0.77172+000
TEMPERATURE (R)    0.77172+000 0.77172+000 0.77172+000 0.77172+000 0.77172+000 0.77172+000 0.77173+000
TEMPERATURE (R)    0.77173+000 0.77173+000 0.77173+000 0.77173+000 0.77174+000 0.77174+000 0.77175+000
TEMPERATURE (R)    0.77176+000 0.77176+000 0.77177+000 0.77179+000 0.77180+000 0.77183+000 0.77188+000
TEMPERATURE (R)    0.77188+000 0.77188+000 0.77198+000 0.77205+000 0.77218+000 0.77234+000 0.77257+000
TEMPERATURE (R)    0.77288+000 0.77272+000 0.77299+000 0.77334+000 0.77388+000 0.77380+000 0.77440+000
TEMPERATURE (R)    0.77580+000 0.77588+000 0.77630+000 0.77700+000 0.78700+000 0.78115+000 0.78278+000
TEMPERATURE (R)    0.78349+000 0.78388+000 0.78401+000 0.78411+000 0.78417+000 0.78420+000 0.78423+000
TEMPERATURE (R)    0.78428+000 0.78428+000 0.78430+000 0.78430+000 0.78430+000 0.78430+000 0.78430+000
TEMPERATURE (R)    0.78431+000 0.78431+000 0.78432+000 0.78432+000 0.78432+000 0.78432+000 0.78432+000
TEMPERATURE (R)    0.78433+000 0.78433+000 0.78433+000 0.78433+000 0.78433+000 0.78433+000 0.78433+000
TEMPERATURE (R)    0.78433+000 0.78433+000 0.78433+000 0.78433+000 0.78434+000 0.78434+000 0.78434+000
TEMPERATURE (R)    0.78434+000 0.78435+000 0.78436+000 0.78436+000 0.78437+000 0.78439+000 0.78441+000
TEMPERATURE (R)    0.78445+000 0.78448+000 0.78458+000 0.78480+000 0.78470+000 0.78490+000 0.78530+000
TEMPERATURE (R)    0.78500+000 0.78500+000 0.78800+000 0.78816+000 0.79994+000 0.80081+000 0.80772+000
TEMPERATURE (R)    0.81084+000 0.81518+000 0.81840+000 0.82040+000 0.82127+000 0.82188+000 0.82230+000
TEMPERATURE (R)    0.82287+000 0.82289+000 0.82300+000 0.82316+000 0.82329+000 0.82330+000 0.82337+000
TEMPERATURE (R)    0.82341+000 0.82343+000 0.82346+000 0.82347+000 0.82348+000 0.82349+000 0.82349+000
TEMPERATURE (R)    0.82350+000 0.82350+000 0.82350+000 0.82350+000 0.82350+000 0.82350+000 0.82350+000
TEMPERATURE (R)    0.82351+000 0.82351+000 0.82351+000 0.82351+000 0.82351+000 0.82351+000 0.82351+000
TEMPERATURE (R)    0.82351+000 0.82351+000 0.82351+000 0.82351+000 0.82351+000 0.82351+000 0.82351+000
TEMPERATURE (R)    0.82352+000 0.82353+000 0.82355+000 0.82358+000 0.82358+000 0.82357+000 0.82360+000
TEMPERATURE (R)    0.82364+000 0.82368+000 0.82377+000 0.82390+000 0.82405+000 0.82431+000 0.82467+000
TEMPERATURE (R)    0.82582+000 0.82613+000 0.82700+000 0.83180+000 0.84481+000
VAPOR FLOW RATE    0.08800+000 0.17880+000 0.18274+000 0.18874+000 0.18881+000 0.18808+000 0.18844+000
VAPOR FLOW RATE    0.18861+000 0.18823+000 0.18818+000 0.18816+000 0.18814+000 0.18813+000 0.18812+000
VAPOR FLOW RATE    0.18812+000 0.18812+000 0.18812+000 0.18811+000 0.18811+000 0.18811+000 0.18811+000
```

```
VAPOR FLOW RATE    0.15811+000 0.15811+000 0.15811+000 0.15811+000 0.15811+000 0.15811+000 0.15811+000
VAPOR FLOW RATE    0.15811+000 0.15811+000 0.15811+000 0.15811+000 0.15810+000 0.15810+000 0.15810+000
VAPOR FLOW RATE    0.15810+000 [illegible] [illegible] [illegible] 0.15807+000 0.15806+000 0.15805+000
VAPOR FLOW RATE    [illegible] [illegible] [illegible] [illegible] [illegible] [illegible] 0.15802+000
VAPOR FLOW RATE    [illegible] [illegible] [illegible] [illegible] 0.15827+000 [illegible] 0.15787+000
VAPOR FLOW RATE    [illegible] 0.15734+000 [illegible] 0.15570+000 [illegible] [illegible] [illegible]
VAPOR FLOW RATE    [illegible] 0.91175+002 [illegible] [illegible] [illegible] [illegible] 0.91015+002
VAPOR FLOW RATE    [illegible] [illegible] [illegible] [illegible] [illegible] [illegible] [illegible]
VAPOR FLOW RATE    [illegible] [illegible] [illegible] [illegible] [illegible] [illegible] [illegible]
VAPOR FLOW RATE    [illegible] [illegible] [illegible] [illegible] [illegible] [illegible] [illegible]
VAPOR FLOW RATE    [illegible] [illegible] [illegible] [illegible] [illegible] [illegible] [illegible]
VAPOR FLOW RATE    [illegible] [illegible] [illegible] [illegible] [illegible] 0.90877+002 [illegible]
VAPOR FLOW RATE    [illegible] [illegible] [illegible] [illegible] [illegible] [illegible] 0.90701+002
VAPOR FLOW RATE    [illegible] [illegible] [illegible] [illegible] 0.88274+002 0.88440+002 0.87100+002
VAPOR FLOW RATE    [illegible] [illegible] [illegible] [illegible] 0.43791+002 0.42743+002 [illegible]
VAPOR FLOW RATE    [illegible] [illegible] [illegible] 0.43418+002 [illegible] 0.42377+002 [illegible]
VAPOR FLOW RATE    [illegible] [illegible] 0.42844+002 0.42840+002 [illegible] [illegible] [illegible]
VAPOR FLOW RATE    [illegible] [illegible] [illegible] [illegible] [illegible] [illegible] [illegible]
VAPOR FLOW RATE    [illegible] [illegible] [illegible] 0.42331+002 0.42331+002 0.42331+002 0.42331+002
VAPOR FLOW RATE    [illegible] [illegible] [illegible] [illegible] [illegible] 0.42330+002 [illegible]
VAPOR FLOW RATE    [illegible] [illegible] [illegible] [illegible] 0.42322+002 0.42318+002 0.42313+002
VAPOR FLOW RATE    [illegible] [illegible] 0.42277+002 0.42254+002 0.42230+002 0.42172+002 0.42101+002
VAPOR FLOW RATE    [illegible] [illegible] [illegible] 0.40840+002 [illegible]
```

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

NUMBER OF ITERATIONS  48

REFLUX RATIO         0.5800000000

PRESSUR , TEMPERATUR , ENTHALPY AND LIQUID FRACTION OF FEED

 0.30000+003 PSIA    0.30546+003 F    0.238443811+007 B.T.U.      0.40000

 0.30000+003 PSIA    0.36583+003 F    0.266811086+007 B.T.U.      0.60000

*** STAGE VARIABLES ***

  PLATE NO.     PRESSURE      TEMPERATURE     LIQ. F. R.     VAP. F. R.     FEED RATE      HEAT DUTY
                  PSIA             F          LB MOL/TIME    LB MOL/TIME    LB MOL/TIME     BTU/TIME
      1        0.30000+003    0.27042+003    0.60800+002    0.00000+000    0.00000+000   -0.88834+006
      2        0.30000+003    0.29826+003    0.52740+002    0.17080+003    0.00000+000    0.00000+000
      3        0.30000+003    0.30568+003    0.50745+002    0.16374+003    0.00000+000    0.00000+000
      4        0.30000+003    0.30846+003    0.50612+002    0.16074+003    0.00000+000    0.00000+000
      5        0.30000+003    0.31055+003    0.40647+002    0.16001+003    0.00000+000    0.00000+000
      6        0.30000+003    0.31114+003    0.40437+002    0.15986+003    0.00000+000    0.00000+000
      7        0.30000+003    0.31150+003    0.40311+002    0.15944+003    0.00000+000    0.00000+000
      8        0.30000+003    0.31171+003    0.40234+002    0.15881+003    0.00000+000    0.00000+000
      9        0.30000+003    0.31184+003    0.40187+002    0.15853+003    0.00000+000    0.00000+000
     10        0.30000+003    0.31192+003    0.40158+002    0.15819+003    0.00000+000    0.00000+000
     11        0.30000+003    0.31197+003    0.40141+002    0.15816+003    0.00000+000    0.00000+000
     12        0.30000+003    0.31200+003    0.40130+002    0.15814+003    0.00000+000    0.00000+000
     13        0.30000+003    0.31202+003    0.40123+002    0.15813+003    0.00000+000    0.00000+000
     14        0.30000+003    0.31203+003    0.40119+002    0.15812+003    0.00000+000    0.00000+000
     15        0.30000+003    0.31204+003    0.40117+002    0.15812+003    0.00000+000    0.00000+000
     16        0.30000+003    0.31204+003    0.40115+002    0.15812+003    0.00000+000    0.00000+000
     17        0.30000+003    0.31205+003    0.40114+002    0.15812+003    0.00000+000    0.00000+000
     18        0.30000+003    0.31205+003    0.40114+002    0.15811+003    0.00000+000    0.00000+000
     19        0.30000+003    0.31205+003    0.40113+002    0.15811+003    0.00000+000    0.00000+000
     20        0.30000+003    0.31205+003    0.40113+002    0.15811+003    0.00000+000    0.00000+000
     21        0.30000+003    0.31205+003    0.40113+002    0.15811+003    0.00000+000    0.00000+000
     22        0.30000+003    0.31205+003    0.40112+002    0.15811+003    0.00000+000    0.00000+000
     23        0.30000+003    0.31205+003    0.40112+002    0.15811+003    0.00000+000    0.00000+000
     24        0.30000+003    0.31205+003    0.40112+002    0.15811+003    0.00000+000    0.00000+000
     25        0.30000+003    0.31205+003    0.40111+002    0.15811+003    0.00000+000    0.00000+000
     26        0.30000+003    0.31205+003    0.40110+002    0.15811+003    0.00000+000    0.00000+000
```

27	0.30000+003	0.31205+003	0.49110+002	0.15911+003	0.00000+000	0.00000+000
28	0.30000+003	0.31206+003	0.49109+002	0.15911+003	0.00000+000	0.00000+000
29	0.30000+003	0.31206+003	0.49108+002	0.15911+003	0.00000+000	0.00000+000
30	0.30000+003	0.31206+003	0.49107+002	0.15911+003	0.00000+000	0.00000+000
31	0.30000+003	0.31206+003	0.49106+002	0.15911+003	0.00000+000	0.00000+000
32	0.30000+003	0.31206+003	0.49104+002	0.15911+003	0.00000+000	0.00000+000
33	0.30000+003	0.31207+003	0.49102+002	0.15910+003	0.00000+000	0.00000+000
34	0.30000+003	0.31207+003	0.49099+002	0.15910+003	0.00000+000	0.00000+000
35	0.30000+003	0.31208+003	0.49096+002	0.15910+003	0.00000+000	0.00000+000
36	0.30000+003	0.31209+003	0.49093+002	0.15910+003	0.00000+000	0.00000+000
37	0.30000+003	0.31209+003	0.49088+002	0.15909+003	0.00000+000	0.00000+000
38	0.30000+003	0.31210+003	0.49082+002	0.15909+003	0.00000+000	0.00000+000
39	0.30000+003	0.31212+003	0.49074+002	0.15908+003	0.00000+000	0.00000+000
40	0.30000+003	0.31213+003	0.49064+002	0.15907+003	0.00000+000	0.00000+000
41	0.30000+003	0.31216+003	0.49052+002	0.15906+003	0.00000+000	0.00000+000
42	0.30000+003	0.31219+003	0.49037+002	0.15905+003	0.00000+000	0.00000+000
43	0.30000+003	0.31222+003	0.49017+002	0.15904+003	0.00000+000	0.00000+000
44	0.30000+003	0.31226+003	0.48993+002	0.15902+003	0.00000+000	0.00000+000
45	0.30000+003	0.31231+003	0.48963+002	0.15900+003	0.00000+000	0.00000+000
46	0.30000+003	0.31238+003	0.48925+002	0.15896+003	0.00000+000	0.00000+000
47	0.30000+003	0.31246+003	0.48878+002	0.15893+003	0.00000+000	0.00000+000
48	0.30000+003	0.31257+003	0.48820+002	0.15888+003	0.00000+000	0.00000+000
49	0.30000+003	0.31270+003	0.48749+002	0.15882+003	0.00000+000	0.00000+000
50	0.30000+003	0.31285+003	0.48660+002	0.15875+003	0.00000+000	0.00000+000
51	0.30000+003	0.31305+003	0.48553+002	0.15866+003	0.00000+000	0.00000+000
52	0.30000+003	0.31329+003	0.48423+002	0.15855+003	0.00000+000	0.00000+000
53	0.30000+003	0.31357+003	0.48269+002	0.15842+003	0.00000+000	0.00000+000
54	0.30000+003	0.31391+003	0.48084+002	0.15827+003	0.00000+000	0.00000+000
55	0.30000+003	0.31432+003	0.47869+002	0.15808+003	0.00000+000	0.00000+000
56	0.30000+003	0.31479+003	0.47622+002	0.15787+003	0.00000+000	0.00000+000
57	0.30000+003	0.31533+003	0.47343+002	0.15762+003	0.00000+000	0.00000+000
58	0.30000+003	0.31596+003	0.47036+002	0.15734+003	0.00000+000	0.00000+000
59	0.30000+003	0.31663+003	0.46701+002	0.15703+003	0.00000+000	0.00000+000
60	0.30000+003	0.31736+003	0.94960+002	0.15670+003	0.10000+003	0.00000+000
61	0.30000+003	0.32742+003	0.92567+002	0.94960+002	0.00000+000	0.00000+000
62	0.30000+003	0.33148+003	0.91687+002	0.92567+002	0.00000+000	0.00000+000
63	0.30000+003	0.33312+003	0.91336+002	0.91687+002	0.00000+000	0.00000+000
64	0.30000+003	0.33382+003	0.91175+002	0.91336+002	0.00000+000	0.00000+000
65	0.30000+003	0.33416+003	0.91097+002	0.91175+002	0.00000+000	0.00000+000
66	0.30000+003	0.33434+003	0.91057+002	0.91097+002	0.00000+000	0.00000+000
67	0.30000+003	0.33444+003	0.91036+002	0.91057+002	0.00000+000	0.00000+000
68	0.30000+003	0.33450+003	0.91023+002	0.91036+002	0.00000+000	0.00000+000
69	0.30000+003	0.33453+003	0.91015+002	0.91023+002	0.00000+000	0.00000+000
70	0.30000+003	0.33456+003	0.91010+002	0.91015+002	0.00000+000	0.00000+000

```
 71   0.30000+003  0.33460+003  0.91007+002  0.91010+002  0.00000+000  0.00000+000
 72   0.30000+003  0.33460+003  0.91005+002  0.91007+002  0.00000+000  0.00000+000
 73   0.30000+003  0.33461+003  0.91003+002  0.91005+002  0.00000+000  0.00000+000
 74   0.30000+003  0.33462+003  0.91002+002  0.91003+002  0.00000+000  0.00000+000
 75   0.30000+003  0.33462+003  0.91000+002  0.91002+002  0.00000+000  0.00000+000
 76   0.30000+003  0.33463+003  0.90999+002  0.91000+002  0.00000+000  0.00000+000
 77   0.30000+003  0.33463+003  0.90999+002  0.90999+002  0.00000+000  0.00000+000
 78   0.30000+003  0.33464+003  0.90998+002  0.90999+002  0.00000+000  0.00000+000
 79   0.30000+003  0.33464+003  0.90998+002  0.90998+002  0.00000+000  0.00000+000
 80   0.30000+003  0.33465+003  0.90997+002  0.90998+002  0.00000+000  0.00000+000
 81   0.30000+003  0.33465+003  0.90997+002  0.90997+002  0.00000+000  0.00000+000
 82   0.30000+003  0.33466+003  0.90996+002  0.90997+002  0.00000+000  0.00000+000
 83   0.30000+003  0.33466+003  0.90996+002  0.90996+002  0.00000+000  0.00000+000
 84   0.30000+003  0.33466+003  0.90996+002  0.90996+002  0.00000+000  0.00000+000
 85   0.30000+003  0.33466+003  0.90996+002  0.90996+002  0.00000+000  0.00000+000
 86   0.30000+003  0.33466+003  0.90996+002  0.90996+002  0.00000+000  0.00000+000
 87   0.30000+003  0.33466+003  0.90995+002  0.90996+002  0.00000+000  0.00000+000
 88   0.30000+003  0.33466+003  0.90995+002  0.90995+002  0.00000+000  0.00000+000
 89   0.30000+003  0.33466+003  0.90995+002  0.90995+002  0.00000+000  0.00000+000
 90   0.30000+003  0.33466+003  0.90995+002  0.90995+002  0.00000+000  0.00000+000
 91   0.30000+003  0.33466+003  0.90995+002  0.90995+002  0.00000+000  0.00000+000
 92   0.30000+003  0.33466+003  0.90994+002  0.90995+002  0.00000+000  0.00000+000
 93   0.30000+003  0.33466+003  0.90994+002  0.90994+002  0.00000+000  0.00000+000
 94   0.30000+003  0.33466+003  0.90994+002  0.90994+002  0.00000+000  0.00000+000
 95   0.30000+003  0.33466+003  0.90993+002  0.90994+002  0.00000+000  0.00000+000
 96   0.30000+003  0.33467+003  0.90993+002  0.90993+002  0.00000+000  0.00000+000
 97   0.30000+003  0.33467+003  0.90992+002  0.90993+002  0.00000+000  0.00000+000
 98   0.30000+003  0.33467+003  0.90990+002  0.90992+002  0.00000+000  0.00000+000
 99   0.30000+003  0.33467+003  0.90989+002  0.90990+002  0.00000+000  0.00000+000
100   0.30000+003  0.33468+003  0.90986+002  0.90989+002  0.00000+000  0.00000+000
101   0.30000+003  0.33468+003  0.90982+002  0.90986+002  0.00000+000  0.00000+000
102   0.30000+003  0.33469+003  0.90977+002  0.90982+002  0.00000+000  0.00000+000
103   0.30000+003  0.33470+003  0.90969+002  0.90977+002  0.00000+000  0.00000+000
104   0.30000+003  0.33472+003  0.90959+002  0.90969+002  0.00000+000  0.00000+000
105   0.30000+003  0.33474+003  0.90943+002  0.90959+002  0.00000+000  0.00000+000
106   0.30000+003  0.33478+003  0.90922+002  0.90943+002  0.00000+000  0.00000+000
107   0.30000+003  0.33482+003  0.90891+002  0.90922+002  0.00000+000  0.00000+000
108   0.30000+003  0.33488+003  0.90848+002  0.90891+002  0.00000+000  0.00000+000
109   0.30000+003  0.33498+003  0.90787+002  0.90848+002  0.00000+000  0.00000+000
110   0.30000+003  0.33512+003  0.90701+002  0.90787+002  0.00000+000  0.00000+000
111   0.30000+003  0.33532+003  0.90579+002  0.90701+002  0.00000+000  0.00000+000
112   0.30000+003  0.33558+003  0.90407+002  0.90579+002  0.00000+000  0.00000+000
113   0.30000+003  0.33588+003  0.90161+002  0.90407+002  0.00000+000  0.00000+000
114   0.30000+003  0.33623+003  0.90161+002  0.90407+002  0.00000+000  0.00000+000
```

```
115    0.30000+003    0.33732+003    0.79808+002    0.80161+002    0.00000+000    0.00000+000
116    0.30000+003    0.33848+003    0.79274+002    0.80805+002    0.00000+000    0.00000+000
117    0.30000+003    0.34027+003    0.78448+002    0.82274+002    0.00000+000    0.00000+000
118    0.30000+003    0.34314+003    0.77100+002    0.85446+002    0.00000+000    0.00000+000
119    0.30000+003    0.34858+003    0.74862+002    0.87100+002    0.00000+000    0.00000+000
120    0.30000+003    0.35637+003    0.13371+003    0.84862+002    0.10000+000    0.00000+000
121    0.30000+003    0.35843+003    0.13336+003    0.43708+002    0.00000+000    0.00000+000
122    0.30000+003    0.35975+003    0.13303+003    0.43556+002    0.00000+000    0.00000+000
123    0.30000+003    0.36052+003    0.13289+003    0.43080+002    0.00000+000    0.00000+000
124    0.30000+003    0.36100+003    0.13274+003    0.42881+002    0.00000+000    0.00000+000
125    0.30000+003    0.36216+003    0.13263+003    0.42743+002    0.00000+000    0.00000+000
126    0.30000+003    0.36262+003    0.13255+003    0.42634+002    0.00000+000    0.00000+000
127    0.30000+003    0.36285+003    0.13249+003    0.42553+002    0.00000+000    0.00000+000
128    0.30000+003    0.36310+003    0.13245+003    0.42484+002    0.00000+000    0.00000+000
129    0.30000+003    0.36336+003    0.13242+003    0.42450+002    0.00000+000    0.00000+000
130    0.30000+003    0.36348+003    0.13239+003    0.42418+002    0.00000+000    0.00000+000
131    0.30000+003    0.36358+003    0.13238+003    0.42395+002    0.00000+000    0.00000+000
132    0.30000+003    0.36365+003    0.13236+003    0.42377+002    0.00000+000    0.00000+000
133    0.30000+003    0.36370+003    0.13236+003    0.42365+002    0.00000+000    0.00000+000
134    0.30000+003    0.36374+003    0.13235+003    0.42356+002    0.00000+000    0.00000+000
135    0.30000+003    0.36376+003    0.13234+003    0.42349+002    0.00000+000    0.00000+000
136    0.30000+003    0.36378+003    0.13234+003    0.42344+002    0.00000+000    0.00000+000
137    0.30000+003    0.36380+003    0.13234+003    0.42340+002    0.00000+000    0.00000+000
138    0.30000+003    0.36381+003    0.13234+003    0.42338+002    0.00000+000    0.00000+000
139    0.30000+003    0.36382+003    0.13233+003    0.42336+002    0.00000+000    0.00000+000
140    0.30000+003    0.36382+003    0.13233+003    0.42334+002    0.00000+000    0.00000+000
141    0.30000+003    0.36383+003    0.13233+003    0.42333+002    0.00000+000    0.00000+000
142    0.30000+003    0.36383+003    0.13233+003    0.42333+002    0.00000+000    0.00000+000
143    0.30000+003    0.36383+003    0.13233+003    0.42332+002    0.00000+000    0.00000+000
144    0.30000+003    0.36383+003    0.13233+003    0.42332+002    0.00000+000    0.00000+000
145    0.30000+003    0.36383+003    0.13233+003    0.42331+002    0.00000+000    0.00000+000
146    0.30000+003    0.36383+003    0.13233+003    0.42331+002    0.00000+000    0.00000+000
147    0.30000+003    0.36383+003    0.13233+003    0.42331+002    0.00000+000    0.00000+000
148    0.30000+003    0.36384+003    0.13233+003    0.42331+002    0.00000+000    0.00000+000
149    0.30000+003    0.36384+003    0.13233+003    0.42331+002    0.00000+000    0.00000+000
150    0.30000+003    0.36384+003    0.13233+003    0.42331+002    0.00000+000    0.00000+000
151    0.30000+003    0.36384+003    0.13233+003    0.42331+002    0.00000+000    0.00000+000
152    0.30000+003    0.36384+003    0.13233+003    0.42331+002    0.00000+000    0.00000+000
153    0.30000+003    0.36384+003    0.13233+003    0.42331+002    0.00000+000    0.00000+000
154    0.30000+003    0.36384+003    0.13233+003    0.42331+002    0.00000+000    0.00000+000
155    0.30000+003    0.36384+003    0.13233+003    0.42331+002    0.00000+000    0.00000+000
156    0.30000+003    0.36384+003    0.13233+003    0.42330+002    0.00000+000    0.00000+000
157    0.30000+003    0.36384+003    0.13233+003    0.42330+002    0.00000+000    0.00000+000
158    0.30000+003    0.36384+003    0.13233+003    0.42330+002    0.00000+000    0.00000+000
```

159	0.30000+000	0.38384+000	0.13233+000	0.42330+002	0.00000+000	0.00000+000
160	0.30000+000	0.38384+000	0.13233+000	0.42330+002	0.00000+000	0.00000+000
161	0.30000+000	0.38384+000	0.13233+000	0.42329+002	0.00000+000	0.00000+000
162	0.30000+000	0.38385+000	0.13233+000	0.42329+002	0.00000+000	0.00000+000
163	0.30000+000	0.38386+000	0.13233+000	0.42328+002	0.00000+000	0.00000+000
164	0.30000+000	0.38386+000	0.13232+000	0.42326+002	0.00000+000	0.00000+000
165	0.30000+000	0.38387+000	0.13232+000	0.42325+002	0.00000+000	0.00000+000
166	0.30000+000	0.38388+000	0.13232+000	0.42322+002	0.00000+000	0.00000+000
167	0.30000+000	0.38390+000	0.13231+000	0.42318+002	0.00000+000	0.00000+000
168	0.30000+000	0.38393+000	0.13230+000	0.42313+002	0.00000+000	0.00000+000
169	0.30000+000	0.38397+000	0.13228+000	0.42305+002	0.00000+000	0.00000+000
170	0.30000+000	0.38402+000	0.13226+000	0.42293+002	0.00000+000	0.00000+000
171	0.30000+000	0.38410+000	0.13225+000	0.42277+002	0.00000+000	0.00000+000
172	0.30000+000	0.38422+000	0.13222+000	0.42254+002	0.00000+000	0.00000+000
173	0.30000+000	0.38439+000	0.13217+000	0.42220+002	0.00000+000	0.00000+000
174	0.30000+000	0.38464+000	0.13210+000	0.42172+002	0.00000+000	0.00000+000
175	0.30000+000	0.38500+000	0.13200+000	0.42101+002	0.00000+000	0.00000+000
176	0.30000+000	0.38555+000	0.13183+000	0.41996+002	0.00000+000	0.00000+000
177	0.30000+000	0.38646+000	0.13154+000	0.41830+002	0.00000+000	0.00000+000
178	0.30000+000	0.38816+000	0.13094+000	0.41543+002	0.00000+000	0.00000+000
179	0.30000+000	0.37216+000	0.12993+000	0.40840+002	0.00000+000	0.00000+000
180	0.30000+000	0.38434+000	0.90000+000	0.38333+002	0.00000+000	0.29186+000

```
*************************
*    MATERIAL BALANCES  *
*************************

FEEDS

                    PLATE NO.  80               PLATE NO. 120
               LB MOL/TIME    MOL FRC.     LB MOL/TIME    MOL FRC.
C3H8           0.25000+002   0.25000+000   0.50000+001   0.50000-001
N-C4           0.20000+002   0.20000+000   0.10000+002   0.10000+000
I-C5           0.20000+002   0.20000+000   0.20000+002   0.20000+000
N-C5           0.20000+002   0.20000+000   0.20000+002   0.20000+000
N-C6           0.10000+002   0.10000+000   0.20000+002   0.20000+000
N-C7           0.50000+001   0.50000-001   0.25000+002   0.25000+000
TOTAL          0.10000+003                 0.10000+003

PRODUCTS

                  VAPOR DISTILLATE               LIQUID DISTILLATE               BOTTOM PRODUCT
               LB MOL/TIME     MOL FRC.       LB MOL/TIME     MOL FRC.       LB MOL/TIME     MOL FRC.
C3H8           0.00000000+000 0.27272727+000 0.30000000+002 0.27272727+000 0.38700565-008 0.43000627-010
N-C4           0.00000000+000 0.24937401+000 0.27431141+002 0.24937401+000 0.25688862+001 0.28541880-001
I-C5           0.00000000+000 0.23377547+000 0.25715302+002 0.23377547+000 0.14284888+002 0.15871887+000
N-C5           0.00000000+000 0.20738857+000 0.22813300+002 0.20738857+000 0.17186707+002 0.19096341+000
N-C6           0.00000000+000 0.36728862-001 0.40402628+001 0.36728862-001 0.25959737+002 0.28844152+000
N-C7           0.00000000+000 0.12823434-007 0.14105777-005 0.12823434-007 0.29999999+002 0.33333332+000
TOTAL          0.00000000+000                0.11000000+003                0.90000000+002
```

```
***** COMPOSITION PROFILE *****

*** LIQUID PHASE ***

C3H8
  0.272727  0.114000  0.086280  0.081170  0.079801  0.079380  0.079115  0.078954  0.078856  0.078796
  0.078730  0.078737  0.078723  0.078715  0.078710  0.078707  0.078705  0.078704  0.078703  0.078702
  0.078702  0.078702  0.078701  0.078701  0.078701  0.078700  0.078700  0.078699  0.078698  0.078697
  [illegible] 0.078694  0.078691  0.078688  0.078684  0.078680  0.078673  0.078666  0.078656  0.078644
  [illegible] [illegible] 0.078606  0.078585  0.078517  0.078470  0.078411  0.078338  0.078249  0.078138
  [illegible] 0.077080  0.077641  0.077405  0.077127  0.076805  0.076437  0.076025  0.075573  0.075089
  [illegible] 0.027055  0.022806  0.022641  0.022542  0.022440  0.022400  0.022361  0.022370  0.022364
  [illegible] 0.022355  0.022352  0.022350  0.022346  0.022346  0.022345  0.022344  0.022343  0.022342
  [illegible] 0.022341  0.022341  0.022340  0.022340  0.022340  0.022339  0.022339  0.022339  0.022339
  [illegible] [illegible] 0.022339  0.022338  0.022338  0.022338  0.022337  0.022337  0.022336  0.022336
  [illegible] [illegible] 0.022331  0.022328  0.022324  0.022318  0.022309  0.022297  0.022280  0.022255
  [illegible] 0.022173  0.022105  0.022088  0.021871  0.021672  0.021375  0.020913  0.020109  0.018861
  0.014105  0.010514  0.007772  0.005726  0.004212  0.003082  0.002267  0.001660  0.001215  0.000889
  [illegible] 0.000476  0.000346  0.000254  0.000186  0.000136  0.000099  0.000072  0.000053  0.000039
  [illegible] 0.000021  0.000015  0.000011  0.000008  0.000006  0.000004  0.000003  0.000002  0.000002
  0.000001  0.000001  0.000001  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000

N-C4
  0.349874  0.184702  0.167043  0.157040  0.153339  0.151719  0.150880  0.150438  0.150166  0.150002
  [illegible] 0.148941  0.149804  0.148761  0.148767  0.148756  0.148753  0.148750  0.148748  0.148746
  0.148745  0.148744  0.148743  0.148743  0.148742  0.148741  0.148739  0.148736  0.148736  0.148733
  0.148739  0.148735  0.148720  0.148713  0.148704  0.148683  0.148678  0.148661  0.148636  0.148610
  0.148575  0.148560  0.148474  0.148405  0.148316  0.148209  0.148074  0.146906  0.146890  0.148444
  0.148182  0.147792  0.147296  0.146751  0.146110  0.145386  0.144516  0.143565  0.142822  0.141405
  0.128872  0.107555  [illegible] 0.084415  0.081962  0.080839  0.080523  0.080532  0.080314  0.080155
  0.080113  [illegible] [illegible] 0.080012  0.080486  0.080083  0.080073  0.080005  0.080006  0.080052
  [illegible] [illegible] [illegible] [illegible] 0.080035  0.080053  0.080032  0.080030  0.080029  0.080026
  [illegible] [illegible] [illegible] [illegible] 0.080022  0.080021  0.080019  0.080017  0.080014  0.080010
  [illegible] [illegible] [illegible] [illegible] 0.080042  0.080008  0.079780  0.080002  0.080006  0.080496
  [illegible] 0.087555  0.057613  0.057074  0.080312  0.080216  0.083511  0.081169  0.077344  0.071406
  0.072140  0.062712  0.073184  0.073448  0.073888  0.072886  0.073883  0.074077  0.074146  0.074155
  [illegible] 0.074550  0.074270  0.074286  0.074304  0.074312  0.074317  0.074321  0.074324  0.074326
  [illegible] 0.074350  0.074350  0.074351  0.074331  0.074331  0.074352  0.074332  0.074332  0.074331
  0.074551  0.074351  0.074336  0.074359  0.074327  0.074325  0.074352  0.074317  0.074310  0.074301
  0.074557  0.074357  0.074236  0.074167  0.074138  0.074052  0.073830  0.073783  0.073500  0.073137
  0.072615  0.071065  0.070780  0.066686  0.067080  0.063812  0.069400  0.052966  0.043200  0.028843
```

```
I-05
 0.289778  0.285760  0.286434  0.285762  0.282808  0.278696  0.276301  0.274660  0.273888  0.273462
 0.273141  0.272946  0.272806  0.272764  0.272700  0.272662  0.272666  0.272656  0.272648  0.272644
 0.272641  0.272639  0.272636  0.272634  0.272632  0.272629  0.272626  0.272622  0.272616  0.272610
 0.272598  0.272591  0.272578  0.272562  0.272541  0.272514  0.272481  0.272439  0.272386  0.272320
 0.272236  0.272132  0.272001  0.271836  0.271631  0.271375  0.271056  0.270661  0.270172  0.269570
 [illegible] 0.267646  0.266902  0.265676  0.264086  0.262310  0.260306  0.258062  0.255602  0.252967
 0.274165  0.266271  0.264679  0.265483  0.265013  0.264236  0.263375  0.262542  0.261784  0.261114
 [illegible] [illegible] 0.276907  0.278844  0.278806  0.278675  0.278464  0.278267  0.278108  0.277974
 0.277851  0.277765  0.277684  0.277616  0.277567  0.277508  0.277466  0.277431  0.277401  0.277375
 0.277358  0.277334  0.277317  0.277301  0.277287  0.277272  0.277257  0.277238  0.277218  0.277191
 0.277155  0.277107  0.277040  0.276947  0.276816  0.276631  0.276370  0.276002  0.275490  0.274745
 0.273708  0.272260  0.270266  0.267384  0.263607  0.257623  0.248481  0.237610  0.219832  0.194001
 0.195144  0.195516  0.196860  0.197145  0.197505  0.197771  0.197967  0.198110  0.198216  0.198293
 0.198350  0.198392  0.198422  0.198444  0.198460  0.198472  0.198481  0.198487  0.198492  0.198495
 0.198498  0.198500  0.198501  0.198502  0.198503  0.198503  0.198504  0.198504  0.198504  0.198504
 0.198505  0.198505  0.198505  0.198506  0.198506  0.198507  0.198508  0.198510  0.198513  0.198516
 0.198521  0.198528  0.198540  0.198555  0.198577  0.198608  0.198655  0.198720  0.198814  0.198947
 0.199135  0.199401  0.199765  0.200251  0.200846  0.201441  0.201566  0.199686  0.190578  0.156719
II-05
 0.297884  0.297665  0.312807  0.311728  0.308808  0.305089  0.300840  0.298884  0.297441  0.296742
 [illegible] 0.296044  0.295930  0.295761  0.295710  0.295692  0.295680  0.295644  0.295635  0.295629
 [illegible] 0.295622  0.295619  0.295617  0.295614  0.295610  0.295606  0.295601  0.295596  0.295587
 0.295577  0.295565  0.295549  0.295530  0.295505  0.295473  0.295434  0.295384  0.295321  0.295242
 0.295140  0.295016  0.294868  0.294687  0.294423  0.294116  0.293739  0.293266  0.292686  0.291970
 0.291094  0.290030  0.288748  0.287220  0.285421  0.283331  0.280947  0.278276  0.275346  0.272212
 [illegible] 0.308916  0.315516  0.318616  0.322275  0.324177  0.325613  0.326740  0.327647  0.328391
 [illegible] [illegible] 0.330557  0.330582  0.330830  0.330860  0.331105  0.331293  0.331450  0.331582
 0.331694  0.331786  0.331865  0.331935  0.331996  0.332041  0.332082  0.332116  0.332144  0.332166
 0.332187  0.332205  0.332215  0.332224  0.332230  0.332229  0.332225  0.332214  0.332196  0.332167
 0.332132  0.332057  0.331983  0.331827  0.331659  0.331386  0.330963  0.330404  0.329614  0.328498
 [illegible] 0.324780  0.321669  0.317289  0.311164  0.303067  0.290823  0.273343  0.248272  0.212880
 0.215724  0.214534  0.215630  0.215711  0.216888  0.216532  0.216836  0.216868  0.216773  0.216880
 [illegible] 0.216946  0.216976  0.217000  0.217016  0.217028  0.217036  0.217043  0.217047  0.217051
 0.217053  0.217055  0.217056  0.217057  0.217058  0.217058  0.217059  0.217059  0.217059  0.217060
 0.217060  0.217060  0.217060  0.217061  0.217061  0.217062  0.217063  0.217064  0.217067  0.217070
 0.217074  0.217080  0.217089  0.217102  0.217121  0.217148  0.217186  0.217242  0.217323  0.217438
 [illegible] [illegible] 0.218212  0.218736  0.219480  0.220560  0.221825  0.222386  0.217769  0.190863
```

N=66

0.000730	0.000000	0.138275	0.161344	0.177188	0.187142	0.192344	0.197183	0.198647	0.200000
0.201657	0.208431	0.202764	0.208888	0.208080	0.208166	0.208211	0.208238	0.208298	0.208265
0.208270	0.208272	0.208272	0.208270	0.208867	0.208263	0.208257	0.208290	0.208341	0.208229
0.208215	0.208167	0.208174	0.208146	0.208111	0.208087	0.208012	0.208342	0.208886	0.202745
0.208207	0.208434	0.208217	0.201844	0.201804	0.201178	0.200640	0.188801	0.190178	0.196178
[illegible]	0.185488	0.186674	0.181888	0.188082	0.186102	0.182788	0.179006	0.174842	0.170888
0.170700	0.182110	0.188640	0.184382	0.184774	0.184888	0.185136	0.188224	0.188308	0.185331
[illegible]	[illegible]	0.188416	0.185434	0.185440	0.185482	0.188473	0.188482	0.188480	0.185446
[illegible]	[illegible]	0.188510	0.188513	0.188516	0.188519	0.188522	0.188524	0.188627	0.188829
[illegible]	0.188867	0.188542	0.188880	0.188880	0.188574	0.188888	0.188621	0.188880	0.185715
[illegible]	[illegible]	0.188082	0.188386	0.188804	0.187088	0.187684	0.188888	0.188676	0.191680
0.184211	0.187746	0.208888	0.208884	0.216188	0.229480	0.242716	0.250647	0.251486	0.247540
[illegible]	0.248838	0.240771	0.250178	0.250480	0.250702	0.250867	0.250867	0.251076	0.251141
0.251166	0.251228	0.251240	0.251267	0.251281	0.251291	0.251298	0.251306	0.251307	0.251310
0.251312	0.251314	0.251315	0.251316	0.251316	0.251317	0.251317	0.251317	0.251317	0.251318
0.251315	0.251316	0.251316	0.251316	0.251316	0.251318	0.251320	0.251321	0.251322	0.251323
[illegible]	0.251380	0.251355	0.251342	0.251380	0.251388	0.251380	0.251421	0.251467	0.251532
0.251627	0.251764	0.251667	0.252276	0.252778	0.253884	0.256615	0.260142	0.270761	0.288442

N=67

0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000001	0.000001	0.000001	0.000001
[illegible]	[illegible]	[illegible]	[illegible]	0.000004	0.000005	0.000007	0.000009	0.000011	0.000014
[illegible]	[illegible]	[illegible]	[illegible]	0.000045	0.000057	0.000072	0.000090	0.000114	0.000143
0.000161	[illegible]	0.000007	0.000051	0.000485	0.000573	0.000722	0.000909	0.001144	0.001430
0.001611	0.000277	0.000061	[illegible]	0.004808	0.005890	0.007071	0.009036	0.011016	0.013700
0.015804	0.000873	0.000776	0.051507	0.080254	0.048085	0.080025	0.080087	0.078014	0.067766
[illegible]	0.000445	0.008804	[illegible]	0.080434	0.088510	0.085554	0.082661	[illegible]	0.083612
[illegible]	[illegible]	0.080864	[illegible]	0.085642	0.088645	0.088640	0.083080	[illegible]	0.083863
[illegible]	[illegible]	0.085567	[illegible]	[illegible]	[illegible]	0.088880	0.083080	0.083861	0.083861
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.088867	[illegible]	0.083672	0.083876	0.083862
[illegible]	0.085704	0.085721	0.085746	0.085782	0.088882	0.088804	0.084007	0.084153	0.084363
[illegible]	0.085129	0.085845	0.087061	0.090167	0.106380	0.112184	0.131419	0.172826	0.256461
[illegible]	[illegible]	0.257488	0.257768	0.256000	0.256247	0.256301	0.256497	0.256574	0.256631
[illegible]	0.256766	0.256735	0.256741	0.256780	0.256782	0.256766	0.256773	0.256776	0.256779
0.256791	0.256782	0.256780	0.256784	0.256784	0.256785	0.256785	0.256785	0.256785	0.256786
[illegible]	0.256785	0.256785	0.256786	0.256786	0.256787	0.256787	0.256788	0.256789	0.256790
[illegible]	0.256784	0.256786	0.258804	0.256812	0.258823	0.258830	0.258863	0.258806	0.258845
[illegible]	0.260116	0.260863	0.258480	0.258817	0.260882	0.261582	0.264871	0.277088	0.333333

```
*** VAPOR PHASE ***

[illegible]
  0.[illegible]  0.272727  0.221000  0.213002  0.212886  0.212763  0.212779  0.212790  0.212814  0.212823
  [illegible]  [illegible]  0.212834  0.212835  0.212837  0.212837  0.212838  0.212838  0.212838  0.212839
  [illegible]  [illegible]  0.212839  0.212839  0.212839  0.212839  0.212840  0.212840  0.212840  0.212841
  [illegible]  [illegible]  0.212843  0.212844  0.212845  0.212847  0.212848  0.212850  0.212853  0.212857
  [illegible]  [illegible]  0.212874  0.212882  0.212884  0.212898  0.212925  0.212947  0.212974  0.213007
  [illegible]  [illegible]  0.213100  0.213351  0.213317  0.213417  0.213534  0.213665  0.213811  0.213970
  [illegible]  [illegible]  0.078841  0.075841  0.075175  0.074954  0.074898  0.074883  0.074864  0.074848
  [illegible]  [illegible]  0.074841  0.074838  0.074838  0.074837  0.074836  0.074835  0.074835  0.074834
  [illegible]  [illegible]  0.074833  0.074833  0.074833  0.074833  0.074832  0.074832  0.074832  0.074832
  [illegible]  [illegible]  0.074832  0.074832  0.074832  0.074832  0.074832  0.074832  0.074832  0.074832
  [illegible]  [illegible]  0.074834  0.074835  0.074837  0.074838  0.074843  0.074846  0.074855  0.074864
  [illegible]  [illegible]  0.074885  0.074905  0.075004  0.075112  0.075282  0.075486  0.075817  0.076718
  [illegible]  [illegible]  [illegible]  [illegible]  0.017706  0.013106  0.008831  0.007066  0.005181  0.003794
  [illegible]  [illegible]  0.001488  0.001086  0.000794  0.000661  0.000434  0.000310  0.000227  0.000166
  [illegible]  [illegible]  [illegible]  0.000047  0.000034  0.000025  0.000018  0.000013  0.000010  0.000007
  [illegible]  [illegible]  [illegible]  [illegible]  0.000001  0.000001  0.000001  0.000001  0.000000  0.000000
  [illegible]  [illegible]  [illegible]  [illegible]  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000
  [illegible]  [illegible]  [illegible]  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000  0.000000

[illegible]
  0.248874  0.248874  0.231678  [illegible]  0.220516  0.218807  0.218694  0.218663  0.218784  0.218730
  [illegible]  [illegible]  0.218844  [illegible]  0.218830  0.218827  0.218825  0.218824  0.218823  0.218822
  [illegible]  [illegible]  [illegible]  [illegible]  [illegible]  0.218822  0.218822  0.218821  0.218821  0.218821
  [illegible]  [illegible]  [illegible]  0.218816  0.218816  0.218816  0.218814  0.218812  0.218808  0.218806
  [illegible]  [illegible]  [illegible]  [illegible]  [illegible]  [illegible]  [illegible]  0.218617  0.218401  0.218430
  0.218418  [illegible]  0.218813  [illegible]  0.218180  0.218082  0.217880  0.217823  0.217682  0.217620
  [illegible]  [illegible]  0.170440  0.168484  0.165684  0.163440  0.162284  0.161678  0.161308  0.161148
  0.161840  [illegible]  [illegible]  [illegible]  0.160880  0.160877  0.160866  0.160856  0.160851  0.160845
  0.160841  [illegible]  [illegible]  0.160831  [illegible]  0.160826  0.160825  0.160823  0.160822  0.160821
  [illegible]  0.160816  0.160816  0.160816  0.160817  0.160817  0.160816  0.160815  0.160813  0.160812
  [illegible]  [illegible]  0.160801  [illegible]  [illegible]  0.160773  0.160755  0.160728  0.160682  0.160640
  [illegible]  [illegible]  [illegible]  0.159116  [illegible]  0.158440  0.158812  0.158175  0.157167  0.155806
  [illegible]  [illegible]  [illegible]  [illegible]  [illegible]  0.168874  [illegible]  0.170224  0.170614  0.170901
  0.171112  [illegible]  0.171370  0.171462  0.171582  0.171586  [illegible]  0.171622  0.171640  0.171652
  0.171651  [illegible]  0.171673  0.171677  0.171676  0.171681  0.171662  0.171663  0.171663  0.171663
  [illegible]  [illegible]  0.171681  0.171670  0.171675  0.171671  0.171664  0.171654  0.171640  0.171620
  [illegible]  0.171540  [illegible]  0.171402  0.171277  0.171087  0.170830  0.170466  [illegible]  [illegible]
  [illegible]  [illegible]  0.164217  [illegible]  [illegible]  [illegible]  0.140011  0.126246  [illegible]  0.076730
```

```
I-[illegible]
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.347701     0.[illegible]  0.246479     0.248301
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.245794     0.245766     0.245760     0.245776     0.245774
0.345770     0.345772     0.345771     0.345770     0.345770     0.245760     0.245766     0.245767     0.245705     0.245764
0.345751     0.345750     0.345755     0.345751     0.345746     0.245738     0.245729     0.245718     0.245704     0.245667
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.245436     0.245361     0.245245     0.245114     0.244962
0.344750     0.344811     0.344216     0.[illegible]  0.[illegible]  0.243890     0.242307     0.241796     0.241080     0.240390
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.316405     0.315767     0.315086     0.314281     0.313619
0.[illegible]  0.[illegible]  0.[illegible]  0.311[illegible]  0.311[illegible]  0.311056     0.310657     0.310880     0.310484     0.310383
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.309830     0.309769     0.309751     0.309725
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.309511     0.309607     0.[illegible]  0.[illegible]
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]17  0.[illegible]  0.[illegible]  0.[illegible]16  0.[illegible]
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]01  0.279847     0.381369
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.381086     0.381636     0.382019
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.382973     0.[illegible]  0.[illegible]  0.383046
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.383081     0.383082
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.383108     0.383106     0.383112     0.383121
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.383445     0.[illegible]  0.383830     0.384135
0.[illegible]  0.383101     0.383175     0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.384390     0.[illegible]  0.383482
0.[illegible]  0.[illegible]  0.[illegible]130  0.[illegible]  0.[illegible]  0.381139

II-[illegible]
0.[illegible]  0.[illegible]  0.[illegible]  0.241047     0.[illegible]  0.[illegible]  0.237098     0.236163     0.[illegible]  0.235217
0.[illegible]  0.[illegible]  0.[illegible]  0.234711     0.234670     0.[illegible]  0.234646     0.[illegible]  0.234634     0.234631
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.234622     0.234631     0.234619     0.234617
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.234673     0.[illegible]  0.234641     0.234619
0.[illegible]  0.[illegible]  0.234411     0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.233667     0.233781     0.[illegible]
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]
0.[illegible]  0.[illegible]  0.[illegible]  0.311[illegible]  0.315416     0.317760     0.319472     0.[illegible]  0.321751     0.[illegible]
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]12  0.325443     0.[illegible]  0.[illegible]  0.[illegible]
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.274350     0.353169
0.[illegible]  0.[illegible]  0.[illegible]  0.317140     0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.271167     0.271836
0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.272461     0.272403     0.272400
0.[illegible]  0.[illegible]  0.272140     0.[illegible]  0.[illegible]  0.[illegible]  0.273431     0.272540     0.272541     0.272543
0.[illegible]  0.[illegible]  0.[illegible]  0.272881     0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]  0.[illegible]
0.[illegible]  0.[illegible]  0.272544     0.272840     0.[illegible]  0.[illegible]  0.272551     0.[illegible]  0.[illegible]  0.[illegible]
0.[illegible]  0.[illegible]  0.272611     0.272841     0.[illegible]  0.272746     0.[illegible]  0.[illegible]  0.273146     0.273415
0.[illegible]  0.[illegible]  0.275173     0.[illegible]  0.[illegible]  0.[illegible]  0.384240     0.[illegible]  0.381401     0.275106
```

N-66

[illegible]	0.085730	0.086130	0.086185	0.078578	0.080400	0.083388	0.086206	0.086341	0.087088
[illegible]	0.087730	0.087680	0.087086	0.088046	0.088083	0.088105	0.088116	0.088126	0.088131
[illegible]	0.088105	0.088105	0.088108	0.088134	0.088128	0.088131	0.088128	0.088126	0.088123
[illegible]	0.088110	0.088105	0.088088	0.088057	0.088074	0.088088	0.088067	0.088011	0.087878
[illegible]	0.087867	0.087682	0.087741	0.087640	0.087513	0.087388	0.087180	0.086815	0.086614
[illegible]	[illegible]	[illegible]	0.084884	0.083817	0.082808	0.081680	0.080871	0.079888	0.077821
[illegible]	[illegible]	0.087284	[illegible]	[illegible]	[illegible]	0.088231	[illegible]	[illegible]	0.088447
[illegible]	0.088811	[illegible]	0.088851	[illegible]	0.088878	[illegible]	[illegible]	[illegible]	0.088612
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.088804	0.088837	[illegible]	0.088841	0.088843
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.088871	[illegible]	0.088700	0.088723	0.088757
[illegible]	0.088871	0.088887	0.100100	0.100204	0.100807	0.100884	0.101808	0.103275	0.108876
[illegible]	0.107801	0.110110	0.114807	0.118880	0.127884	0.138880	0.147883	0.157784	0.160408
[illegible]	[illegible]	0.167817	0.168867	0.169810	0.170848	0.170884	0.171288	0.171878	0.171788
[illegible]	0.172071	0.172108	0.172210	0.172264	0.172288	0.172282	0.172840	0.172288	0.172282
[illegible]	0.172076	0.172078	0.172881	0.172886	0.172894	0.172886	0.172886	0.172887	0.172888
[illegible]	[illegible]	[illegible]	[illegible]	0.172880	0.172891	0.172882	0.172888	0.172886	0.172880
[illegible]	0.172410	0.172480	0.172480	0.172483	0.172481	0.172882	0.172880	0.172884	0.172786
[illegible]	0.172816	0.172880	0.174126	0.174088	0.176382	0.178888	0.184408	0.187888	0.230808

N-67

[illegible]	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
[illegible]	0.000001	0.000001	0.000001	0.000001	0.000001	0.000002	0.000002	0.000003	0.000006
[illegible]	[illegible]	0.000007	0.000008	0.000011	0.000014	0.000018	0.000022	0.000030	0.000035
[illegible]	[illegible]	0.000070	[illegible]	0.000112	0.000140	0.000177	0.000223	0.000280	0.000353
[illegible]	[illegible]	0.000702	[illegible]	0.001107	0.001380	0.001730	0.002175	0.002716	0.003383
[illegible]	[illegible]	0.008411	[illegible]	0.008884	0.011030	0.013584	0.016887	0.019480	0.022854
[illegible]	[illegible]	[illegible]	0.088297	0.088224	[illegible]	[illegible]	[illegible]	[illegible]	0.088379
[illegible]	[illegible]	[illegible]	0.088401	0.088404	0.088407	0.088409	0.088411	0.088412	0.088414
0.088415	0.088416	0.088416	0.088417	0.088418	0.088418	0.088419	0.088419	0.088419	0.088420
[illegible]	0.088420	0.088421	0.088421	0.088422	0.088423	0.088424	0.088425	0.088427	0.088430
[illegible]	0.088440	0.088449	0.088461	0.088477	0.088501	0.088535	0.088594	0.088656	0.088752
[illegible]	0.088107	0.088427	0.088837	0.088913	0.088449	0.085778	0.043070	[illegible]	[illegible]
0.088175	0.088482	0.087430	0.088108	0.088722	0.089135	0.089440	[illegible]	[illegible]	[illegible]
[illegible]	0.100110	0.100155	0.100186	0.100210	0.100237	0.100251	0.100261	0.100268	0.100274
[illegible]	0.100281	0.100282	0.100284	0.100285	0.100286	0.100287	0.100288	0.100288	0.100289
[illegible]	0.100289	0.100289	0.100290	0.100290	0.100290	0.100290	0.100291	0.100292	0.100294
[illegible]	0.100300	0.100305	0.100312	0.100322	0.100337	0.100358	0.100389	0.100429	0.100486
[illegible]	0.100717	0.100907	0.101185	0.101602	0.102264	0.103436	0.105171	0.114685	0.150867