New Jersey Institute of Technology

Digital Commons @ NJIT

Theses

Electronic Theses and Dissertations

6-30-1973

Distillation design techniques

Ronald Michael Carlucci

New Jersey Institute of Technology

Follow this and additional works at: https://digitalcommons.njit.edu/theses

Part of the Chemical Engineering Commons

Recommended Citation

Carlucci, Ronald Michael, "Distillation design techniques" (1973). *Theses*. 2233.
https://digitalcommons.njit.edu/theses/2233

This Thesis is brought to you for free and open access by the Electronic Theses and Dissertations at Digital Commons @ NJIT. It has been accepted for inclusion in Theses by an authorized administrator of Digital Commons @ NJIT. For more information, please contact digitalcommons@njit.edu.

Copyright Warning & Restrictions

The copyright law of the United States (Title 17, United States Code) governs the making of photocopies or other reproductions of copyrighted material.

Under certain conditions specified in the law, libraries and archives are authorized to furnish a photocopy or other reproduction. One of these specified conditions is that the photocopy or reproduction is not to be "used for any purpose other than private study, scholarship, or research." If a, user makes a request for, or later uses, a photocopy or reproduction for purposes in excess of "fair use" that user may be liable for copyright infringement,

This institution reserves the right to refuse to accept a copying order if, in its judgment, fulfillment of the order would involve violation of copyright law.

Please Note: The author retains the copyright while the New Jersey Institute of Technology reserves the right to distribute this thesis or dissertation

Printing note: If you do not wish to print this page, then select "Pages from: first page # to: last page #" on the print dialog screen

The Van Houten library has removed some of the personal information and all signatures from the approval page and biographical sketches of theses and dissertations in order to protect the identity of NJIT graduates and faculty.

DISTILLATION DESIGN TECHNIQUES

BY

RONALD MICHAEL CARLUCCI

A THESIS
PRESENTED IN PARTIAL FULFILLMENT OF
THE REQUIREMENTS FOR THE DEGREE
OF
MASTER OF SCIENCE IN CHEMICAL ENGINEERING
AT
NEWARK COLLEGE OF ENGINEERING

This thesis is to be used only with due regard to the rights of the author(s). Bibliographical references may be noted, but passages must not be copied without permission of the College and without credit being given in subsequent written or published work.

Newark, New Jersey
1973

APPROVAL OF THESIS

DISTILLATION DESIGN TECHNIQUES

BY

RONALD MICHAEL CARLUCCI

FOR

DEPARTMENT OF CHEMICAL ENGINEERING

BY

FACULTY COMMITTEE

APPROVED:

NEWARK, NEW JERSEY

JUNE, 1973

TABLE OF CONTENTS

ABSTRACT

A design method for binary distillation systems is presented that minimizes the required rigorous calculations. A computer program is developed that finds the number of theoretical stages, and feed stage for a specified separation and reboiler vapor rate. Results for three binary systems are presented.

The design method and computer program are extended to the multicomponent case at the condition of total reflux. Results for one ternary system are presented. The possibility of using the method at other than total reflux is discussed. Usage of the method to search for multicomponent azeotropes and results are also presented.

Analytic equations are developed for a non-linear two stage system, and multicomponent distillation with constant KV/L values. The effect of small, linear change in the KV/L values are also investigated.

The computer programs used for the stage calculations are listed and their structure and usage are explained. Convergence methods for the rigorous calculation techniques are presented.

CHAPTER I

INTRODUCTION

The usual distillation design procedure involves the determination of how many theoretical stages are required to produce a stream of a desired purity or concentration. For a given set of parameters such as feed concentration, feed temperature, and heat input or reflux ratio, the number of theoretical stages is unique. Usually the heat input or reflux ratio is varied and the relationship between these quantities and the number of theoretical stages is found.

Solving for the number of stages is not a simple task especially for multicomponent systems, for which rigorous solutions are desired. The relationships are very non-linear and trial and error techniques, usually computer aided are required. Considerable difficulty is particularly encountered for the design case where the number of stages is not known, but the desired separation is known.

This is opposed to the rating method, where the number of stages is specified and the resulting separation is computed. The answer is compared to the desired separation and if they are not similar, then the calculations must be repeated for a new set of conditions. This results in a roundabout design method.

The goal of this thesis work is to develop a theoretical insight and a means of solution for the design problem wherein the required separation is maintained and the number of stages is determined. A fast and efficient method, based on computer computations is desired because the rigorous problems are so highly non-linear. The method of calculation is to be similar to the Lewis-Matheson procedure. Theoretical stage requirements and feed point location are the primary output information generated.

To avoid undue complexity, the main purpose of this work is directed at binary separations. A single feed distillation column with top and bottom products is simulated, and the feasibility of extending the method to the multicomponent case is investigated. Wherever possible analytical expressions are developed in order to gain insight into stagewise processes, simplify calculations, and to decrease dependence on the computer.

The actual computer based approach is developed in a manner that gives the required stages for a given separation and heat input. Calculation methods and the relationships utilized are rigorous. Both ideal and non-ideal liquid behavior is used, depending on the binary system. All of the calculations are confined to pressures of 1000mm Hg or less. Thus ideal vapor behavior for the vapor phase is assumed. Material and heat balances are rigorously calculated, except for heats of mixing. The calculation sequence begins at the base of the column, proceeds upward, brings in the feed at an appropriate stage, continues upward, and closes out the calculations without returning to any previous stages. This technique is designed to reduce the trial and error calculations to a minimum and aids convergence.

Calculations begin at the base of the column since the liquid phase activity coefficients are easily found from the liquid compositions which are specified for the bottoms product. This results in requiring only bubble point calculations instead of dew point calculations. Considerable simplification is thereby attained since dew point calculations are more difficult. The temperature, liquid phase compositions, and activity coefficients are unknowns for the dew point whereas temperature is the only unknown for the bubble point. Activity coefficients are also unknown, but approximate values are available for the bubble point calculations as they are stronger functions of the liquid phase composition than the temperature. Hence, the temperature convergence speed and stability is superior with this approach.

A Newton-Raphson convergence approach is used to solve the bubble point problem with the Antoine equation forming the basis of the technique. Energy balances are solved by the method of successive substitutions. Liquid compostions are straightforwardly determined from material balances. Vapor compositions are easily found from the bubble point calculations.

A special technique is required in order to finish the calculations on the last stage at the top of the column since the computational approach is "once through". The concept of a "parallel" and partial condenser is developed to satisfy the final heat and material balances. A partial condenser alone normally cannot be used to compute the final balances. Also, a total condenser is a special case of this concept.

Analytic expressions are derived in order to determine the stage value of the "parallel" and partial condenser concept from computer generated solutions. Further expressions are derived in an attempt to find a method of expanding the Edmister absorption and stripping factor technique.

The conclusion or result of this study is that a binary separation may be calculated rigorously with minimal effort by the computer design technique developed here. Results for three binary systems are presented.

Azeotropic separations are an exception. If the presence of an azeotrope is unsuspected, then the specified separation will be impossible to obtain under certain conditions and the computer solution will not converge. However, the unconverged output will display the presence of the azeotrope. Consequently, the separation specifications can be amended to reflect the azeotrope composition and converged solutions may be readily calculated by the simulation program.

Total reflux rigorous simulations can be made for binary and multicomponent systems. Results for one ternary system are presented. A ternary azeotrope is present and the computer program correctly predicts it from knowledge of the binary systems comprising the ternary system. Hence, the program can be used for total reflux calculations or for seeking multicomponent azeotropes which can be verified by experimental work.

Multicomponent systems can possibly be simulated by this computer technique at other than total reflux. However, this is only feasible if the two lowest boiling components comprise the overhead product and all other component concentrations present in this stream are very small.

All of the binary separations show that the stage value of the partial and "parallel" condenser is always equal to unity. A total condenser is a special case of this concept when the partial condenser duty becomes zero.

There is no simple analytic equation that represents most stage processes. The case of constant KV/L values in the stripping and rectifying sections can be described by reasonable expressions for the terminal conditions represented by a total condenser, partial condenser, or total condenser and decanter. For the case of the KV/L value changing linearly over each stage, the equations become too formidable to be used for design purposes.

After completing the overall component balance, the distillation stage to stage calculations can begin. The design method presented in Chapter II is briefly summarized below. Detailed explanations and discussions of the various steps are given in the text.

Specification of the streams is required before any calculations can begin followed by the solution of the overall and component material balances.

$$F = B+D \text{ (overall balance)}$$

$$X_fF = X_bB+X_dD \text{ (component balance)}$$

Manipulating these equations results in the following forms.

$$B/D = (X_d-X_f) \;/\; (X_f-X_b)$$

or $$D/F = (X_f-X_b) \;/\; (X_d-X_b)$$

where:
B = Bottoms flow
D = Distillate flow
F = Feed flow
X_b, X_d, X_f = Component mole fractions in B, D, and F.

Normally the feed flow and composition are known. For a binary or multicomponent separation, specification of the composition of a component in the B and D streams determines their values. In a binary system, both compositions in a stream are known once one composition is selected, while this is not the case with a multicomponent system. Specifications for a given component in each multicomponent (>2) stream only fixes the magnitude of the streams. For each other component, one of its compositions in B or D must be selected in order to determine its composition in the other stream. This can be seen from the above equations.

SUMMARY OF DESIGN METHOD

Step 1 - Determine the unspecified pressure or temperature and vapor composition for Stage 1 (bottom of the column).

Step 2 - Select a vapor flow from Stage 1. Find the liquid flow and liquid compositions from Stage 2 (material balances).

Step 3 - Introduce the temperature and vapor phase compositions on Stage 2 (bubble point calculation).

Step 4 - Find the reboiler duty (energy balance).

Step 5 - Select a vapor flow from Stage 2. Solve for the liquid flow and liquid compositions from Stage 3 (material balances).

Step 6 - Find the bubble point temperature and vapor compositions on Stage 3. Do an energy balance around Stage 2 and solve for the vapor flow from Stage 2.

Step 7 - Compare the selected and calculated vapor flows from Stage 2. If they are not equal, select a new vapor flow and repeat Steps 5, 6, and 7 till they are equal.

Step 8 - Compare the liquid composition on Stage 3 with the feed composition. If there is a match, introduce the feed onto Stage 3.

Step 9 - Continue the stage to stage calculations comprised of Steps 5, 6, 7, and 8. For example, in Step 5, a vapor flow would be selected from Stage 3. Then the liquid flow and liquid compositions from Stage 4 are solved for, etc.

Step 10 - When the vapor flow calculation is finished at the end of Step 7, the vapor compositions on the next stage are known from the bubble point calculation (Step 6). Compare these vapor compositions with the required distillate composition. The first time the light component's vapor composition exceeds the required distillate composition means that the stage to stage calculations are finished; the partial and parallel condenser calculations are done next.

SUMMARY OF DESIGN METHOD - continued

Step 11 - The stage where the vapor phase exceeds the distillate composition for the light component is replaced by the partial and parallel condensers. Solve the dew point calculation to find the liquid in equilibrium with the specified distillate. Next calculate the liquid flow from and vapor to the partial condenser. From a heat balance, find the partial condenser duty. An overall heat balance is then calculated to find the parallel condenser duty.

In the following chapter a subscripted variable is written in the Fortran language notation with the subscripts in parentheses. This is done to eliminate confusion between the text and simulation program listings. The first subscript represents the theoretical stage and is generally symbolized by "J". Component identification appear in the second subscript and are generally symbolized by "I". Single subscripted variables also appear and will refer to a stage or component depending on whether the subscript is a J or I. In all equations when there are summation signs (Σ), the sum is always over the components for which I varies from 1 to N, where N is the total number of components.

CHAPTER II

THEORETICAL STAGE DESIGN METHOD

Extensive work has been carried out to develop and test a design method for binary separations. A computer program was written only for binary separations, and is applicable for multicomponent systems with some modifications. A second computer program was created from the original program and can simulate multicomponent systems at total reflux or can be used to investigate vapor-liquid equilibrium and is particularly useful for determining azeotropes.

A. Calculation Sequences. Liquid compositions are specified in the base of the column comprised of theoretical stages. Stage 1 is the base of the column and the vapor leaving is assumed to be in equilibrium with the liquid, which is true when a kettle reboiler or once through thermosyphon is used. No attempt has been made to simulate the recirculating type reboiler design wherein the reboiler feed and the bottoms product have the same composition.

An option is available so either the reboiler temperature or pressure is specified. If the temperature is given, then the pressure is calculated by summing up the partial pressures found from the equilibrium equations.

This is a desireable selection when temperatures in the reboiler must be specified for heat sensitive materials or when heat transfer limitations exist. When the pressure is specified, then the temperature is calculated by a bubble point calculation. This is useful when analyzing equilibrium behavior which is normally available at a set pressure, i.e. 760mm Hg. Methods of determining the unspecified temperature or pressure are described in more detail when calculation convergence methods are discussed.

The determination of the reboiler or reboiler base pressure or temperature allows the vapor compositions to be straightforwardly calculated. Ideal vapor behavior is assumed, but vapor phase non-ideality could be incorporated without affecting the design method.

Instead of specifying a reflux ratio, a molar vapor rate from Stage 1 (base) is given, sometimes termed the "Boil-Up". Many shortcut methods are available for calculating minimum reflux ratios and these can be used with an energy balance to find a minimum "Boil-Up" so an intelligent choice can be made before using the design method. Having selected a base vapor rate, and since the bottoms flow is known from the material balance which defines the separation, the molar liquid rate from

Stage 2 is found from their sum.

$$L(2) = L(1) + V(1) \tag{1}$$

Compositions in L(2) are determined from the component material balances expressed in equation (2).

$$X(2,I) = (Y(1,I)*V(1) + X(1,I)*L(1))/L(2) \tag{2}$$

where: $Y(1,I)$ = component I's vapor composition from Stage 1

$V(1)$ = molar vapor flow specified from Stage 1

$X(1,I)$ = component I's liquid composition from Stage 1, specified by overall material balance

$L(1)$ = molar bottoms flow from Stage 1, specified by overall material balance

$L(2)$ = molar liquid flow from equation (1)

$X(2,I)$ = component I's liquid composition from Stage 2

The temperature on Stage 2, T(2), is needed to compute the reboiler duty. Pressure on Stage 2, SP(2), is found by subtracting from Stage 1's pressure, SP(1), a specified pressure drop.

$$SP(2) = SP(1) - DP \tag{3}$$

DP equals the pressure drop per stage, and is assumed the same for all stages. The temperature on Stage 2 is then calculated by a bubble point technique described later. Vapor phase compostions are found simultaneously.

An energy balance may now be made around Stage 1 to find the reboiler duty.

$$\begin{aligned} Q(\text{reboiler}) = {} & (Y(1,I)*HV(1,I)*V(1) \\ & + X(1,I)*HL(1,I)*L(1) \\ & - X(2,I)*HL(2,I)*L(2)) \end{aligned} \tag{4}$$

where: $HV(1,I)$ = molar vapor enthalpy of component I in $V(1)$
$HL(J,I)$ = molar liquid enthalpy of component I in $L(J)$

The calculations may now proceed to the next stage. Initially a vapor rate from Stage 2 is assumed equal to V(1). The L(3) is determined from equation (5).

$$L(J) = V(J-1) + L(J-1) - V(J-2) - NF*F \tag{5}$$

where: J = number of the stage being calculated
$NF = 0$ if the feed hasn't been introduced
$NF = 1$ if the feed has been introduced on Stage J-1
F = molar flow of feed

The criteria for introducing the feed are discussed later.

The liquid composition of L(3) may be found from the component material balance given in equation (6).

$$\begin{aligned} X(J,I) = {} & (Y(J-1)*V(J-1) - NF*FX(I)*F \\ & + X(J-1,I)*L(J-1) \\ & - Y(J-2,I)*V(J-2))/L(J) \end{aligned} \tag{6}$$

where: $FX(I)$ = mole fraction of component I in the feed

The pressure at Stage 3 is found from equation (7).

$$SP(J) = SP(J-1) - DP \tag{7}$$

A bubble point calculation is done next to determine the stage temperature, T(J). Equation (8) is then used to find V(2) by an energy balance to see if the value is the same as that originally assumed.

```
V(J-1) = (NF*FX(I)*F*HF(I) + Y(J-2,I)*
         V(J-2)*HV(J-2,I)
         + X(J,I)*L(J)*HL(J,I)
         - X(J-1)*L(J-1)*HL(J,I)/ (Y(J-1,I)*
         HV(J-1,I))                               (8)
```

for J greater than 3

If the two values of V(J-1) are not within a specified tolerance, then a new value of V(J-1) is used as described later. Equations (5), (6), and (8) and the bubble point calculation are repeated till the values of V(J-1) are sufficiently close.

Thus, in general:

1. the material balance equations are used to find the liquid flow and liquid compositions from Stage J; a vapor flow from Stage J-1 is assumed or calculated in order to begin,
2. vapor phase compositions and temperature on Stage J are found from the liquid compositions using a bubble point calculation with the stage pressure being obtained from equation (7); the bubble point calculation consists of the vapor-liquid equilibrium equations and the

vapor mole fractions sum equation equal to 1.0 within a specified tolerance,

3. vapor flow from Stage J-1 is found by an energy balance on Stage J-1; the equation involves flows from Stages J-2, J-1, and J; if the value assumed for the vapor flow doesn't match the calculated value within a given tolerance then a new vapor flow value is used and steps 1. through 3. are repeated.

B. Choice of Feed Location. In this work, the feed is always specified as a liquid before entering the column and a simple criteria is used to find the feed stage. Starting at Stage 2, the difference between the liquid composition and the feed composition of the light component is noted. If the difference is zero or positive, the feed is brought in on Stage J and the computer program variable NF is changed from zero to one. This causes the feed to be considered in the material and energy balances on the feed stage.

In some cases the feed temperature was less than that of the feed stage, while in other cases, it was higher. Interestingly enough, none of the binary cases studied suffered from use of this simple and loose criteria. None of the cases displayed the effect of an incorrect feed point whereby liquid compositions on the stages increased, then decreased, and then increased again.

If the feed is a vapor before entering the stage, the vapor phase composition could be compared with the feed. However, this variation wasn't studied and the computer program doesn't include it, but could be easily incorporated, as well as a two phase feed.

Once the feed is brought in on a stage, by whatever criteria the designer chooses, the stage calculations continue past the feed point in the same previous manner. The only difference is noted in the feed stage energy and material balances, which now include the feed contributions to them.

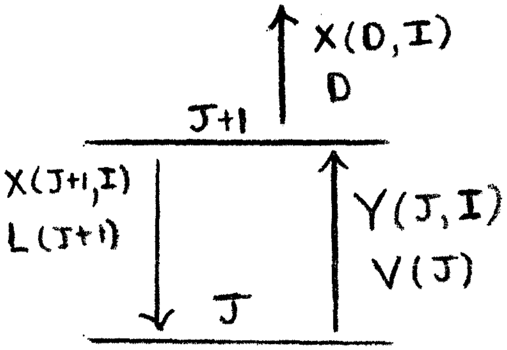
C. Calculations on Last Stage. At some point in the stage calculations, it is normally desired that the vapor composition from a stage equals the required distillate composition. This comes about because most distillation columns use total condensers. However, even for a binary system, this physical requirement causes difficulty in the calculations. This difficulty arises quite naturally from the discontinuous behavior of theoretical stage processes. For example, if the required distillate mole fraction for the light component is .99, as dictated by the specified overall material balance, and the vapor composition on two consecutive stages are .980 and .995, we cannot satisfy the material balance using either of these vapor flows.

To obtain an exact solution, one possible course of action would be to make adjustments in the vapor flow from Stage 1 and recalculate stages till some stage has the vapor composition required. This is inefficient and introduces a mathematical discontinuity, since only discrete vapor flows from Stage 1 would give exact solutions.

Another course of action is to define a "fraction" of a theoretical stage. In the previous example, the required vapor composition was between the vapor composition of two consecutive stages. If a suitable definition could be found, then it could be established that 18.3 theoretical stages, for example, are needed for the separation.

A mathematical definition of a stage, whether fractional or unity in value is one of the thesis objectives. Before the developed expression could be tested by using calculated values for the final theoretical stage, the design method had to include a way to properly terminate the problem.

It was decided that the stipulation requiring vapor compositions equal to distillate compositions was too restrictive and hence not required. Consider the material balance around the top of the column,



as given by equation (9a)

$$X(J+1,I) = Y(J,I)*\frac{V(J)}{L(J+1)} - X(D,I)\frac{*D}{L(J+1)} \qquad (9a)$$

If $Y(J,I) = X(D,I)$ and since $V(J) = L(J+1) + D$, then $X(J+1,I) = X(D,I) = Y(J,I)$

Suppose $Y(J,I) > X(D,I)$. Hence, $X(D,I)/Y(J,I) = a < 1.0$. The material balance, equation (9a), becomes

$$X(J+1,I) = Y(J,I)\ (V(J) - aD)/L(J+1) \qquad (9b)$$

Since $V(J)-D = L(J+1)$ then $V(J) - aD > L(J+1)$, whereby $X(J+1,I) > Y(V,I)$. Equation (10) summarizes these inequalities.

$$X(J+1,I) > Y(J,I) > X(D,I) \qquad (10)$$

Consider the case where a given stage has produced $Y(J,I) > X(D,I)$ for the light component, where $X(D,I)$ is specified by the overall material balance. Inequality (10) would provide a solution to the problem, and may be physically accomplished by putting flow $V(J)$ into a partial condenser, withdrawing the condensate and distillate, totally condensing the remaining vapor in another condenser, and returning it as reflux. In the partial condenser the light component concentrates in the vapor phase and $Y(J,I) > X(D,I)$. The light component's liquid dew point composition is always less than the initial vapor composition except when total condensation occurs, for then they are equal. This series of inequalities was not used since the usual commerical method produces a vapor distillate from the partial condenser with the generated liquid being returned to the cascade as reflux.

Consider $Y(J,I) < X(D,I)$ for the light component instead of the previous opposite case. Then $X(D,I)/Y(J,I) = b > 1.0$. Equation (9b) becomes

$$X(J+1,I) = Y(J,I)(V(J) - bD)/L(J+1) \qquad (11)$$

$$V(J) = L(J+1) + D \text{ and } V(J) - bD < L(J+1)$$
$$\text{Therefore } X(J+1,I) < Y(J,I) < X(D,I)$$

To obtain this inequality, vapor from the stage <u>before</u> the stage where $Y(J,I) > X(D,I)$, is sent to a partial condenser. A portion is condensed until the remaining vapor composition equals X(D,I). Condensate is returned as reflux and the vapor distillate can then enter a total condenser if desired or left in the vapor state. The inequality is satisfied by this arrangement as the light component's vapor composition in the partial condenser is always greater than the inlet vapor composition. Also the light component's liquid composition is always less than the inlet vapor composition to the partial condenser as previously discussed.

Based on these conditions, the design procedure, as outlined in equations (5) through (8), is used as before until the vapor flow is converged on Stage (J-1), whereby the bubble point calculation on Stage (J) has previously converged, and the light component's vapor composition on Stage (J) exceeds the required distillate composition. At this point, a dew point calculation is done to find the liquid compositions and temperature in equilibrium with the required vapor distillate at the known pressure in the partial condenser which takes the place of Stage (J).

When the dew point calculation is complete, the following are known. First, the vapor distillate composition and flow are specified by the original material balance giving the desired separation. Second, the composition and temperature of the liquid in equilibrium with the vapor distillate are known from the dew point solution. Third, the composition of the vapor to the partial condenser was previously calculated at the stage before the need for the partial condenser was determined. The only unknown flow quantities left are the vapor to and liquid from the partial condenser.

One method of calculating these flows is from a component material balance such as equation (12).

$$L(J) = D(XD(I) - Y(J-1,I))/(Y(J-1,I) - X(J,I)) \tag{12}$$

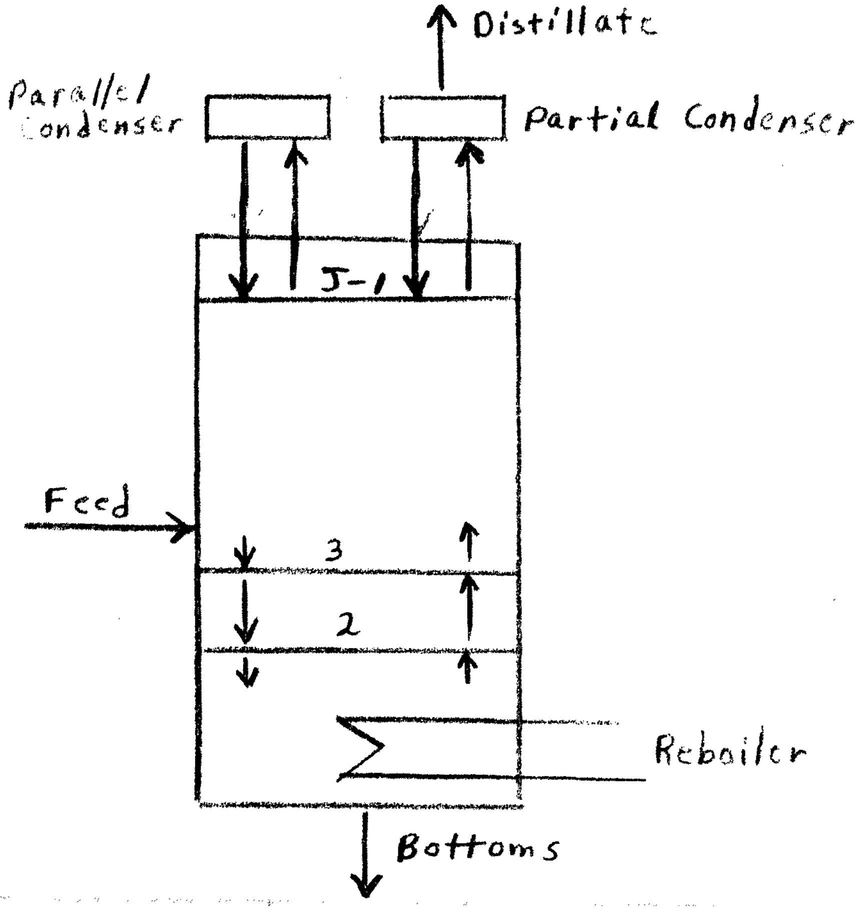
where: $L(J)$ = liquid flow from partial condenser
D = vapor distillate flow from partial condenser
$XD(I)$ = component I vapor distillate composition
$Y(J-1,I)$ = component I vapor composition to partial condenser
$X(J,I)$ = component I liquid composition from partial condenser

Having found $L(J)$, then $V(J-1)$, the flow to the partial condenser can be found from equation (13).

$$V(J-1) = L(J) + D \tag{13}$$

Only one problem remains to be solved. An enthalpy balance on the stage before the partial condenser must be satisfied. It turns out that equation (12) is a very sensitive function. The values calculated for the partial condenser flows can be drastically different from the flows on previous stages as illustrated by the computer solutions. As a result, the excess enthalpy is removed in a "parallel" condenser. The excess vapor from the stage below the partial condenser is condensed. This condensate is returned to the stage and, therefore, does not affect the stage material balance.

The excess enthalpy is calculated from an overall enthalpy balance. Temperatures, flows, and compositions of the feed, distillate, and bottoms are known, hence their enthalpies may be calculated. The reboiler and partial condenser may also be calculated. Therefore, the parallel condenser duty is the difference between the input and output quantities.



To further illustrate the need for a parallel condenser, consider the following development which solves for L(J), the liquid from the partial condenser, from an enthalpy balance on the last stage, whereas equation (12) solves for L(J) from a material balance.

Enthalpy leaving the top stage (J-1) is;

$$V(J-1)*\sum HV(J-1,I)*Y(J-1,I) + L(J-1)*\sum HL(J-1,I)*X(J-1,I)$$

Enthalpy entering the top stage is;

$$V(J-2)*\sum HV(J-2,I)*Y(J-2,I) + (V(J-1)-D)*\sum HL(J,I)*X(J,I)$$

where L(J) is substituted from equation (13). All quantities except V(J-1) are known at this point in the calculations and V(J-1) may be solved for directly. Then L(J) from the partial condenser may be found from equation (13). Therefore, two completely independent solutions for L(J) exist (the material balance of equation (12) or from the enthalpy balance on the top stage) and actual computer trials demonstrated that the answers are not equivalent. This is also illustrated by the values calculated in the final computer case study printouts for parallel condenser duties, which never approached zero. The computer program calculates the flows by equation (12) and does an overall heat balance to find the parallel condenser duty.

The concept of a partial and parallel condenser produces mathematical continuity between the bottom vapor rate and theoretical stage requirements. This allows the calculation sequence to require only one pass up the column and therefore considerably reduces the calculations needed for an exact solution.

D. Total Condenser Equivalence. If at some given "Boil-Up", the vapor composition exactly matches the required distillate composition, then equation (12) sets the partial condenser liquid flow to zero. Equation (13) then shows that the vapor flow to the partial condenser equals the required distillate flow. Hence, the partial condenser duty is zero. The parallel condenser produces a liquid condensate of exactly the same composition as the vapor distillate. If an external condenser is used to condense the vapor distillate, a total condenser equivalence is established since now the distillate and parallel condenser condensate are identical in composition and physical state.

These solutions, representing a total condenser, are only a series of discrete points on a continuous curve. It is easier to choose an arbitrary bottom vapor rate and use the partial and parallel condenser method than to insist on reaching a total condenser point on the curve.

Indeed, it may be deduced that the total condenser solution is in the neighborhood, as follows: if an arbitrary bottom vapor rate gave a vapor composition of .995 on a stage, when we need only .990, then the partial and parallel condensers yield a solution of 18 stages, for example; if the bottom vapor rate is somewhat reduced, the vapor composition which was .995 will decrease and .990 will be reached. The number of stages will then still be 18, but a total condenser situation is attained. This occurs because the former case required 17 stages (the 18th stage gave Y=.995), plus a partial condenser which is later shown to be a whole theoretical stage. In the latter case, the 18th stage requires a total condenser which is equal to zero theoretical stages. Therefore, over a range of vapor rates, the same number of stages are needed, but each solution has a different partial condenser duty.

CHAPTER III

CONVERGENCE METHODS

Three basic problem parts of the design method require solutions to non-linear relationships. These problems are the bubble point temperature, dew point temperature, and vapor flow from a stage.

Iterative calculations are required for the above, and therefore procedures have been worked out so that they are both simplistic and efficient. The procedures were inserted into the computer design method and yield reasonable computer time requirements. Minor convergence problems were noted only for the dew point temperature case, but the insertion of a damping factor produced stability.

A. Bubble Point Temperatures. In this design method, the stage liquid composition and pressure are always known for all but two exceptions.

Exception 1 - when the calculations begin in the first stage, the temperature instead of the pressure may be specified. In this case we merely solve for the sum of the partial pressures.

PP(I) = X(1,I)*ACT(I)*VP(I) (14)

where: X(J,I) = specified composition of component I in Stage 1.
ACT(I) = activity coefficient of component I at the specified compositions and temperature. The actual equation used for ACT(I) is incorporated in a computer subroutine.
VP(I) = vapor pressure of pure component I at the specified temperature.

By summing up the component partial pressures, the total pressure (Stage 1 pressure) is found. The vapor compositions are then calculated by dividing each component's partial pressure by the total pressure. No vapor phase non-ideality calculations were incorporated into the method. This total pressure calculation sets the various stage pressures since each stage pressure (except Stage 1) will equal the previous stage's pressure minus a specified and constant pressure drop.

> Exception 2 - in the partial condenser, the liquid composition isn't known and the dew point solution is required and is described later.

For all the other stages, the Antoine pure component vapor pressure equation forms the basis for the bubble point temperature convergence method.

$$\mathrm{LOG}_{10}\ \mathrm{VP(I)} = \mathrm{A(I)} - \mathrm{B(I)}/(\mathrm{T} + \mathrm{C(I)})$$

$$\text{or } \mathrm{LN\ VP(I)} = 2.303\ \mathrm{A(I)} - 2.303\mathrm{B(I)}/(\mathrm{T} + \mathrm{C(I)})$$

Differentiating this equation with respect to temperature gives

$$d(\mathrm{LN\ VP(I)})/d\mathrm{T} = 2.303\mathrm{B(I)}/(\mathrm{T} + \mathrm{C(I)})^2 \qquad (15)$$

$$\text{Since } \mathrm{Y(J,I)} = \mathrm{ACT(I)}*\mathrm{X(J,I)}*\mathrm{VP(I)}/\mathrm{SP(J)} \qquad (16)$$

The solution to the bubble point temperature occurs when the sum of the vapor compositions equals one.

$$SY = \sum ACT(I)*X(J,I)*VP(I)/SP(J) \tag{17}$$

If an arbitrary temperature is too high, then each component's vapor pressure will also be high, and SY will be greater than one. The opposite is true if the temperature is lower than the correct temperature. However, the difference (error) between SY and 1.0 can be used to correct the temperature, thereby converging on the correct temperature as follows.

Let SY = 1.0 - SY, which can be replaced by the differential d(SY).

Differentiating SY (equation (17)) with respect to temperature we obtain

$$d(SY)/dT = \sum ACT(I)*X(J,I)/SP(J)*d(VP(I))/dT \tag{18}$$

X(J,I) and SP(J) are constants. ACT(I) is usually a weak function of temperature, strongly affected by liquid composition, and therefore assumed constant at this point. However, at each new temperature trial, ACT(I) is recalculated before finding SY from equation (17).

Substituting from equation (15) into equation (18) for d(VP(I))/dT,

$$\begin{aligned} d(SY)/dT = \sum(&ACT(I)*X(J,I)*2.303B(I)*VP(I))/ \\ &(SP(J)/(T + C(I))^2 \end{aligned} \tag{19}$$

Solving for dT,

$$\begin{aligned} dT = \sum(&1.0 - SY)/(ACT(I)*X(J,I)*2.303B(I)* \\ &VP(I)/SP(J)/(T + C(I)^2) \end{aligned} \tag{20}$$

A temperature correction, dT or rather ΔT, can be estimated from the error and present temperature guess from equation (20).

$$T(\text{next guess}) = T(\text{present guess}) + \Delta T$$

All quantities in the denominator are positive. If the temperature guess is too high, then 1.0 - SY is negative. This produces a negative correction giving a lower temperature guess. Therefore, 1.0 - SY is the correct error definition.

The experience from the computer trials done with the work showed that this technique is satisfactory, with no convergence or stability problems. However, they might occur if the temperature guess is far from the solution. The largest range used in this work was about 31°C for a binary and 55°C for a ternary system.

It is noted that this method is suitable for multicomponent problems. A ternary system was calculated by this design method using the bubble point convergence technique. A criteria is used to determine how small the error should be to stop the calculations. Normally SY = 1.0 ± .001 was used in this work. This is a maximum error and the actual result is frequently smaller. In one example, it is seen that error in the sum of Y is often less than .001. However, it is a difficult separation in the upper stages and the temperatures and compositions vary very slightly. The effect of the error criteria of .001 is shown in the temperature's second decimal place. A decreasing temperature should be observed and isn't. The case was rerun using an error criteria of .0001 and the temperature no longer oscillates and always decreases. In general the tolerance of .001 is usually adequate. If inconsistencies in the temperature map are observed, these may be eliminated by decreasing the tolerance, and of course increasing the number of iterations required for the bubble point calculation.

Normalization of the sum of Y is felt to be beneficial in reducing the round off error accumulating during the stage calculations. The sum of Y is divided into each Y(J,I) when the bubble point problem is solved so that the final sum of Y exactly equals unity.

Initial temperature guesses as a new stage's calculation begins are arrived at in various ways. Temperature profiles are approximately linear and previous stage temperatures provide an estimate. The computer design program estimating method sets the temperature difference between Stages J-1 and J.

$$T(J-1) - T(J) = T(J-2) - T(J-1)$$

or

$$T(J) = 2T(J-1) - T(J-2) \qquad (21)$$

For Stage 1, a pure guess is used while the Stage 2 temperature guess is Stage 1's bubble point, the remaining stages using equation (21).

B. Dew Point Temperature. The only time a dew point temperature is required is when the partial condenser is reached. At this point the vapor compositions (specified distillate) and pressure are known while liquid composition and temperature are unknown.

Once again, the convergence technique is based on the Antoine equation.

$$X(J,I) = Y(J,I)*SP(J)/ACT(I)*VP(I)) \qquad (22)$$

$$\text{Sum of } X = SX = \sum X(J,I) \qquad (23)$$

Differentiating with respect to temperature and using equation (15) for the derivative,

$$\begin{aligned} d(SX)/dT &= \sum Y(J,I)*SP(J)/ACT(I)*d(1/VP(I))/dT \\ &= \sum \frac{-Y(J,I)*SP(J)}{ACT(I)*(VP(I))^2} * \frac{d(VP(I))}{dT} \\ &= \sum \frac{-Y(J,I)*SP(J)*2.303B(I)}{ACT(I)*VP(I)*(T + C(I))^2} \qquad (24) \end{aligned}$$

Therefore,

$$dT = \frac{-d(SX)}{\sum \frac{Y(J,I)*SP(J)*2.303B(I)}{ACT(I)*VP(I)*(T + C(I))^2}} \qquad (25)$$

and $d(SX) = 1.0 - SX$ (26)

If the temperature guess is too high, SX will be positive and less than 1.0 from equations (22) and (23). The temperature correction dT or rather ΔT should then be negative and will be since all quantities are positive in equation (25). Conversely, if the temperature is low, then dT is positive as required. Initial guesses for ACT(I) and T(I) in the partial condenser are the values from the earlier bubble point solution for the stage replaced by the partial condenser.

This derivation is simplistic and not as stable as desired, since ACT(I) was held constant and is a strong function of X(J,I). For a binary system, the values of ACT(I) change rapidly as X(J,I) approaches zero. Since most separations are done to produce a distillate with one of the compositions close to 1.0 and the other (the high boiler) close to 0.0, the technique is relatively stable for this case. The reason is that the denominator of equation (25) contains a summation, and that if X(J,I) is close to zero then so usually is Y(J,I), also ACT(I) is in the denominator. Even if ACT(I) is fluctuating widely, the high boiler's term may be small compared to the other term.

The above procedure was demonstrated and no convergence problems were encountered. These cases were typified by high purity products and an upper equilibrium pinch region.

Several cases though caused convergence problems. Original trials took excessive iterations and did not guarantee convergence. Rather than extend the convergence technique, a simple damping factor was used. The temperature correction was divided by two and then applied. This did not eliminate the tendency to increase the error in one direction, then the other direction, and suddenly converge several iterations after beginning the search. Nevertheless, it worked and note that these cases were typified by a desired distillate of only 75 mole% Ethanol in a Ethanol-Water binary. This region on the Y - X diagram for Ethanol-H_2O shows X changing rapidly for a small change in Y.

It is interesting to note the sensitivity of this binary system. An error criteria of SX = 1.0 ± .001 was used. Table I below illustrates the various dew point solutions to the same problem, all of which have the same actual solution when the pressure and vapor compositions are invariant.

TABLE I

Case	Pressure mmHg	Temperature °C	SX	Iterations
12	760	78.51	1.000669	9
13	760	78.44	1.000354	9
14	760	78.65	1.000329	1
15	760	78.57	1.000582	9
16	670	76.11	1.000596	9
17	670	75.31	1.000638	9

The iteration count and SX are taken from program monitored printout. For the other case outputs, the dew points converged within two iterations.

Table I shows that the lower SX values have the higher temperatures at constant pressure, except for a discrepancy between cases 13 and 15. The data illustrate the extreme sensitivity change of the temperature on a small SX change. This is why the temperature correction factor was reduced for these cases.

This experience showed why this design procedure starting from the base of a distillation column and thereby avoiding dew point calculations, has decided advantages. Dew point calculations are more difficult and unstable than bubble point calculations when the vapor phase behavior is ideal and liquid phase behavior is non-ideal.

C. Vapor Flow from a Stage.

Vapor and liquid flows from the first stage are always found by a material balance. Vapor flows from succeeding stages are to be found by an enthalpy balance, except for vapor flow to the partial condenser (see page 21).

The enthalpy balance is done for Stage J-1 after the temperature of Stage J is established. A vapor flow from Stage J-1 is estimated, whereby the material balances yield liquid composition and flow from Stage J. From this data and the pressure on Stage J, the bubble point calculation is done. Now all temperatures, flows, and compositions to and from Stage J-1 are known.

Equation (8) is then used to calculate the vapor flow from Stage J-1. If it is not the same as the original estimate, the value calculated from equation (8) is used as the next estimate. The material balances and bubble point calculations are repeated and equation (8) is again used to find the vapor flow. This sequence is repeated until the difference between two successive vapor flows is within a given tolerance. The computer output cases used a relative tolerance of .0001 which equals the difference in the vapor flows divided by the estimated flow. The tolerance was held at this level in the belief that round-off error accumulation would be minimized since an error in the vapor rate is propagated through the material balances.

This convergence method by successive substitution is simple but inefficient. Under the proper conditions, it should always converge and under the improper conditions it should always diverge. Without having investigated the mathematical properties of the equations, the method was used and never was unstable or failed to converge.

At one time, a programming oversight did not supply the design computer program with an initial estimate. Whatever value that happened to be in computer storage was used by the program as an initial vapor flow for each stage after Stage 1. The program still converged but required about twice the time actually used later when this situation was corrected.

To supply an initial vapor flow estimate from each stage, it is noted that vapor flow variations are usually small and approximately linear from stage to stage. The estimate is then provided by equation (27) for J greater than 2, the criteria being the same as for providing temperature estimates (equation (21)).

$$V(J) = 2*V(J-1) - V(J-2) \tag{27}$$

For Stage 2, the initial guess is equal to the vapor flow from Stage 1.

CHAPTER IV

EXTENSION TO MULTICOMPONENT SYSTEMS

Multicomponent separations by distillation constitute the majority of industrial problems. Binary separations by distillation form the scope of this thesis predominantly, but it is desireable to see if this theoretical stage design method can be extended to multicomponent systems. The answer is both yes and no, but for different reasons. Various applications of this design method to multicomponent systems and explanations are presented.

A. Total Reflux. The design method is especially well suited to binary and multicomponent total reflux calculations and no difficulties of any kind arise. However, one fundamental problem must be resolved. In binary separations, the specification of the Stage 1 liquid composition (bottoms product) is straightforward. There is no question as to the value for a component's composition when the other component's composition is given since they must add up to unity. Multicomponent separations give a distribution of components in both product streams. Because of the phase rule, and the number of variables that may be specified for a calculation, it is difficult to decide exactly what the bottom liquid compositions should be for the multicomponent case.

Once the designer decides on a representative bottom's composition for all components, it is a straightforward calculation. The design method is applied as done previously, but with the bottoms flow equal to zero, any arbitrary bottom vapor flow, no feed, and no partial condenser. When the overhead specification is reached, for the light key usually, the total reflux stage requirement is then known.

A separate computer program for multicomponent systems was generated from the original binary program for these calculations. It is easy to use and the results should be more accurate than various less rigorous short cut methods for calculating total reflux-stage requirements.

B. Azeotropes. Multicomponent minimum boiling azeotropes may be found by using this computer design method. The various binaries comprising the multicomponent system are fitted to a vapor-liquid equilibrium model such as the Wilson equation before using the design method. A total reflux problem is then calculated with the stage pressure drops set at zero. Depending on the starting bottoms composition, the design method will search for the nearest azeotrope whether it is binary or multicomponent.

An illustration of this is shown in one case of the computer outputs. The ternary azeotrope of Methanol, Acetone, and 2,3-Dimethylbutane reported by Willock and Van Winkle is being searched for by the computer program. Reported experimental values for this system's azeotrope at 760mm and 43.2°C are

Xmethanol = .254
Xacetone = .229
XDMB = .517

Using the Wilson parameters given by the authors, but not using a temperature polynomial for molar volumes, the program predicts an azeotrope at 44.2°C which is also the same temperature predicted by the authors. The results for the composition are

Xmethanol = .2522
Xacetone = .2181
XDMB = .5297

Slightly different values may have resulted if the program was allowed to continue. However, the results were changing so slowly that the calculation was terminated.

Only liquid mole fractions are shown since at total reflux the vapor composition leaving a stage equals the liquid composition on the stage above. Hence, the liquid on Stage 9 is in equilibrium with a vapor whose composition is the liquid on Stage 10.

The particular azeotrope search referenced above was started with the Stage 1 liquid compositions specified so the values were about equal. The reason for choosing values in this manner is to possibly avoid heading towards one of the binary azeotropes during the search. The results illustrate how binary data can be combined and used by the program to find multicomponent azeotropes which can later by experimentally verified, thereby possibly saving time and effort.

C. General Separations. Calculations for the separation of multicomponent systems into two product streams by this design method at other than total reflux are limited. Not all of the limitations and pitfalls or the means of eliminating them are known since only a theoretical feasibility investigation was done. Some useful conclusions can be drawn and are discussed below.

The main problem appears in the partial condenser. Except for this and perhaps finding a suitable feed stage, all the stage to stage calculations should present no difficulty.

To understand the problem arising in the partial condenser, consider the following. After solving the dew point problem, it is necessary that the component material balances (equation (27)) around the partial condenser are satisfied.

```
L(J) = D*(XD(I) - Y(J-1,I))/(Y(J-1,I)
       - X(J,I))                                  (27)
```

This is equivalent to saying that each component balance will predict the same liquid flow from the partial condenser since the distillate flow and composition are specified, the dew point calculation gives the liquid composition X(J,I), and the vapor composition to the partial condenser Y(J-1,I), results from the stage calculations. This vapor composition is very important and is the only variable that can be manipulated, but only indirectly. The values of the vapor composition result mainly from Stage 1's specified vapor flow and liquid compositions, and the number of stages, Equation (27) is a sensitive function of the vapor composition and the equation will not predict the same L(J) from each component unless exactly the right set of compositions are available. Since it is very difficult to predict the top stage vapor composition from the Stage 1 values controlling it, an iterative procedure would have to be developed. This would result in specification changes for the overall unit material balance. However, if a separation is being done where only the two lowest boiling components are to be in the distillate, and consequently all other component mole fractions are to be negligible, then equation (27) can be satisfied to a degree for the two main components. If the other mole fractions are negligible then,

$$\begin{aligned} Y(J-1,2) &= 1.0 - Y(J-1,1) - Ey \\ XD(2) &= 1.0 - XD(1) - Ed \\ X(J,2) &= 1.0 - X(J,1) - Ex \end{aligned}$$

where E is the sum of the other fractions.

For component 1,

$$L(J) = \frac{D(XD(1) - Y(J-1,1))}{(Y(J-1,1) - X(J,1))} \qquad (28a)$$

For component 2,

$$\begin{aligned} L(J) &= \frac{D(XD(2) - Y(J-1,2))}{(Y(J-1,2) - X(J,2))} \\ &= \frac{D((1.0 - XD(1) - Ed) - (1.0-Y(J-1,1) - Ey))}{((1.0 - Y(J-1,1) - Ey) - (1.0-X(J,1) - Ex))} \\ &= \frac{D(XD(1) - Y(J-1,1) + (Ed - Ey))}{(Y(J-1,1) - X(J,1) + (Ey - Ex))} \qquad (28b) \end{aligned}$$

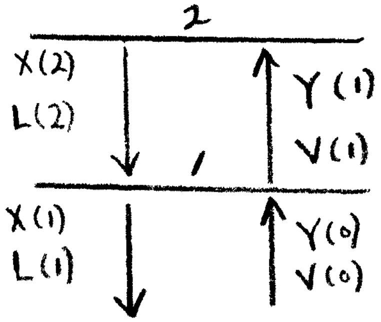
If the E values are negligible or cancel out, then the same L(J) values are predicted from equations (28) and (29) and a converged solution is obtained for the separation. The distillate has, therefore, been reduced to a binary system and this design method can be utilized. For binary separations the E values are exactly zero and the L(J) values from the component balance equations are identical.

CHAPTER V

ANALYTIC EQUATIONS

Countercurrent stagewise processes, such as the simple distillation columns studied in this work, are of an involved mathematical nature. To gain more insight into the phenomena, some analytic functions were derived. One of these is needed to find the stage value of the partial condenser. Other functions are rederivations of the Edmister equations and an extension thereof. In general, it is concluded that the stagewise process is usually too complex to be represented in useable analytic form.

A. Partial Condenser Evaluation. Consider a two stage system as shown in figure 1 below.



On Stage 1, the component material balance is,

$$X(2) = Y(1)V(1)/L(2) + X(1)L(1)/L(@) - Y(0)V(0)/L(2)$$

The vapor and liquid compositions are related by the form $Y=KX$. Substituting this in the balance, and adding and subtracting $Y(0)/K(1)$,

$$\begin{aligned}X(2) = {} & X(1)(L(1)/L(2)+ K(1)V(1)/L(2)) \\ & - Y(0)/K(1)(1 + K(1)V(0)/L(2))+ Y(0)/K(1)\end{aligned}$$

Let $L(1) = L(2) + dL$ or $L(1)/L(2) = 1 + dL/L(2)$

Let $V(0) = V(1) + dV$ or $V(0)/L(2) = V(1)/L(2)+ dV/L(2)$

Where "d" is either a differential or finite difference operator. Substituting the equations into the component balance, we obtain

$$\begin{aligned}X(2) = {} & X(1)(1 + K(1)V(1)/L(2)) - Y(0)/K(1)(1 + K(1)V(1)/L(2)) \\ & + Y(0)/K(1) + X(1)\,dL/L(2) - Y(0)dV/L(2)\end{aligned}$$

Rearranging the equation results in the form,

$$\frac{X(2)- Y(0)/K(1)+ Y(0)dV/L(2)- X(1)dL/L(2)}{X(1) - Y(0)/K(1)} = 1+K(1)V(1)/L(2)$$

The right hand side of the equation is the first two terms of a geometric series of the form $1 + a + a^2 + \cdots + a^{N-1}$ whose sum is $(a^N-1)/(a-1)$. Therefore, the right hand side may be replaced by

$$\frac{(K(1)V(1)/L(2))^N-1}{K(1)V(1)/L(2)-1} \quad \text{where } N = \text{number of stages}$$

The equation is not to be used for N greater than 2 because of the definitions assigned to dL and dV.
By solving for N, an equation is now available that can evaluate N for cases involving changing K, V, and L values for at least two stages.

The final equation is

$$N=\frac{\log\left[(K(1)V(1)/L(2)-1)\dfrac{X(2)-Y(0)/K(1)+Y(0)dV/L(2)-X(1)dL/L(2)}{X(1)-Y(0)/K(1)}+1\right]}{\log(K(1)V(1)/L(2))} \qquad (29)$$

Results from the computer cases were used in this equation to determine the stage value of the partial condenser. During the design calculation, a whole stage gave a vapor composition exceeding that needed to satisfy the overall unit material balance. The partial condenser was then used to produce the required distillate composition. It was believed initially that depending on the amount of condensing required of the partial condenser, various fractional stage values would be calculated. If this was true then a one to one mapping of heat input (or bottom vapor flow) to stages could be obtained.

The results from six randomly selected computer cases are shown in Table II.

TABLE II

Case	N	% difference from N=2
1	1.977	-1.15
2	2.107	5.38
3	1.945	-2.73
7	1.978	-1.06
9	1.866	-6.70
14	2.000	0.0

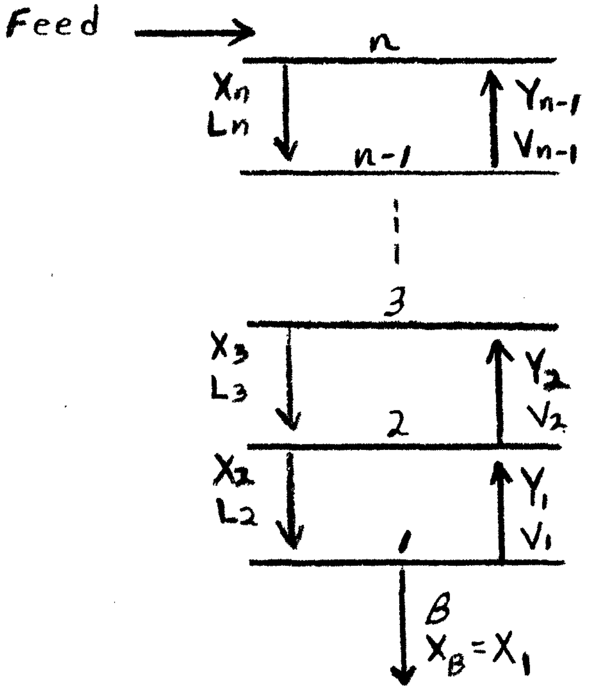
The last two stages shown in the output cases which represent the last stage and partial condenser are used to evaluate the stage value of the partial condenser. Since the last stage is a whole theoretical stage, then N-1 is the stage value for the partial condenser. The printout values are truncated and this is believed to cause the small deviations from N=2 shown in Table II. It appears that no fractional values result and the partial condenser is a whole theoretical stage for the binary systems studied.

The light component compositions were used to find the values in Table I. It makes no difference which component compositions are used even though this is not obvious from equation (29).

Only the flows around the partial condenser were used in the calculations. The parallel condenser flows were not considered since it only condenses and returns material to the stage and the terms would cancel out of the material balance equation at the start of the derivation.

B. General Equations. Analytic functions describing the countercurrent stage process are derived. Only simplistic solutions can be readily found because of the complexity of the phenomena. These are valuable, however, in providing insight into the behavior and effect of the important variables.

1. Stripping section equations begin their derivation on the bottom stage with a component material balance.



The Stage 1 component balance is

$$X_2L_2 = Y_1V_1 + X_1B \tag{30}$$

Equilibrium between Y and X is of the form Y = KX. Therefore, the component balance becomes

$$X_2 = X_1\ (K_1V_1/L_2 + B/L_2) \tag{31}$$

The Stage 2 component balance is

$$X_3L_3 = Y_2V_2 + X_1B$$

The equilibrium equation is $Y_2 = K_2X_2$

$$X_3L_3 = K_2X_2V_2 + X_1B$$

Substituting for X_2 from equation (31),

$$X_3 = (K_1V_1/L_2)(K_2V_2/L_3)X_1 + (X_1B/L_3)(1 + K_2V_2/L_2) \tag{32}$$

The Stage 3 component balance is

$$X_4L_4 = Y_3V_3 + X_1B$$

$Y_3 = K_3X_3$ from the equilibrium equation

$$X_4L_4 = K_3X_3V_3 + X_1B$$

Substituting for X_3 from equation (32), and rearranging terms,

$$X_4 = X_1\ \frac{K_1V_1}{L_2}\ \frac{K_2V_2}{L_3}\ \frac{K_3V_3}{L_4} + \frac{X_1B}{L_4}\left[\frac{K_3V_3}{L_3} + \frac{K_2V_2}{L_2}\ \frac{K_3V_3}{L_3}\right] + \frac{X_1B}{L_4}$$

$$= X_1\ \frac{K_1V_1}{L_2}\ \frac{K_2V_2}{L_3}\ \frac{K_3V_3}{L_4} + \frac{X_1B}{L_4}\left[1 + \frac{K_3V_3}{L_3} + \frac{K_2V_2}{L_2}\ \frac{K_3V_3}{L_3}\right] \tag{33}$$

Multiplying the first term by L_1/L_1,

$$X_4 = \frac{K_1V_1}{L_1}\frac{K_2V_2}{L_2}\frac{K_3V_3}{L_3}\frac{L_1}{L_4}x_1 + \frac{X_1B}{L_4}\left[1 + \frac{K_3V_3}{L_3} + \frac{K_2V_2}{L_2}\frac{K_3V_3}{L_3}\right] \tag{34}$$

The general series expansion can be deduced to yield

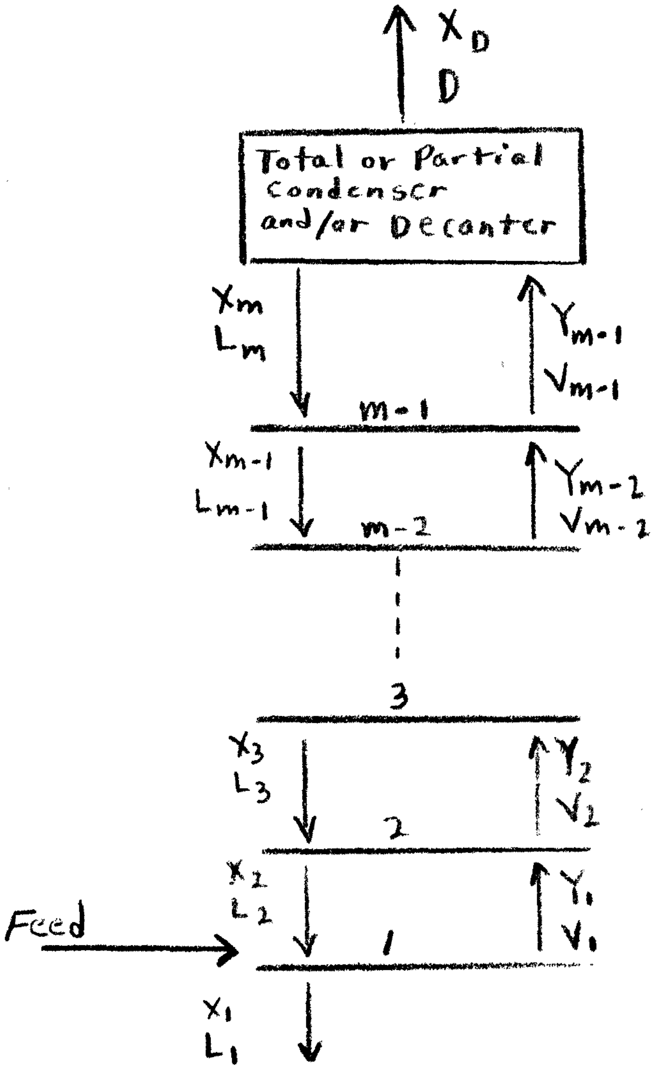
$$X_n = \frac{K_1V_1}{L_1}\frac{K_2V_2}{L_2}\cdots\frac{K_{n-1}V_{n-1}}{L_{n-1}}\frac{L_1}{L_n}X_1$$
$$+ \frac{X_1B}{L_n}\left[1 + \frac{K_{n-1}V_{n-1}}{L_{n-1}} + \cdots + \frac{K_2V_2}{L_2}\frac{K_3V_3}{L_3}\cdots\frac{K_{n-1}V_{n-1}}{L_{n-1}}\right] \tag{35}$$

If the KV/L values are constant, and $L_1 = L_n$, then the geometric series sum formula $(a^n-1)/(a-1)$ equal to $1 + a + a^2 + \cdots + a^{n-1}$ can be used for the second term. With this result and since $X_1 = X_B$,

$$X_n = X_B\left\{\left(\frac{KV}{L}\right)^{n-1} + \frac{B}{L_n}\left[\frac{(KV/L)^{n-1} - 1}{(KV/L) - 1}\right]\right\} \tag{36}$$

This equation gives the liquid composition from the feed stage as a function of B, L_n, KV/L, X_1 and n for a multicomponent system. The condition of KV/L being a constant is usually unrealistic. The V/L ratio is frequently relatively constant, but the K values are not. An "average" KV/L ratio is difficult to define because of the sensitivity of the series sum. Equation (36) will be subsequently used with a similar equation for the rectifying section to yield an overall expression which gives insight into stagewise processes.

2. The derivation in the rectifying section consisting of m-1 stages also utilizes component balances and the equilibrium relationship expressed as Y = KX.



The Stage 2 component balance (feed is on Stage 1) is

$X_2 = Y_1V_1/L_2 - X_DD/L_2$.

$Y_1 = K_1X_1$, and

$$X_2 = X_1K_1V_1/L_2 - X_DD/L_2. \qquad (37)$$

The Stage 3 component balance is

$X_3 = Y_2V_2/L_3 - X_DD/L_3$.

$Y_2 = K_2X_2$, and

$X_3 = X_2K_2V_2/L_3 - X_DD/L_3$.

Substituting for X_2 from equation (37),

$$X_3 = \frac{K_2V_2}{L_3}\left[\frac{K_1V_1X_1}{L_2} - \frac{X_DD}{L_2}\right] - \frac{X_DD}{L_3},$$

or

$$X_3 = \frac{K_1V_1}{L_2}\,\frac{K_2V_2}{L_3}\,X_1 - \frac{X_DD}{L_3}\left[1 + \frac{K_2V_2}{L_2}\right], \qquad (38)$$

The Stage 4 component balance is

$X_4 = Y_3V_3/L_4 - X_DD/L_4$,

$Y_3 = K_3X_3$, and

$X_4 = X_3K_3V_3/L_4 - X_DD/L_4$.

Substituting for X_3 from equation (38) and rearranging terms,

$$X_4 = \frac{K_1V_1}{L_2}\,\frac{K_2V_2}{L_3}\,\frac{K_3V_3}{L_4}\,X_1 - \frac{X_DD}{L_4}\left[1 + \frac{K_3V_3}{L_3} + \frac{K_2V_2}{L_2}\,\frac{K_3V_3}{L_3}\right].$$

Multiplying the first term by L_1/L_1,

$$X_4 = \frac{K_1V_1}{L_1}\frac{K_2V_2}{L_2}\frac{K_3V_3}{L_3}\frac{L_1}{L_4}X_1 - \frac{X_DD}{L_4}\left[1 + \frac{K_3V_3}{L_3} + \frac{K_2V_2}{L_2}\frac{K_3V_3}{L_3}\right]. \qquad (39)$$

The general form can be deduced to be

$$X_m = \frac{K_1V_1}{L_1}\frac{K_2V_2}{L_2} \cdots \frac{K_{m-1}V_{m-1}}{L_{m-1}}\frac{L_1}{L_m}X_1 - \frac{X_DD}{L_m}\left[1 + \frac{K_{m-1}V_{m-1}}{L_{m-1}} + \frac{K_{m-1}V_{m-1}}{L_{m-1}}\frac{K_{m-2}V_{m-2}}{L_{m-2}} + \cdots + \frac{K_2V_2}{L_2}\cdots\frac{K_{m-1}V_{m-1}}{L_{m-1}}\right]. \qquad (40)$$

Once again the second series term can be represented by a geometric series if the KV/L values are a constant.

If $L_1 = L_m$ and KV/L is constant,

$$X_m = \left(\frac{KV}{L}\right)^{m-1}X_1 - \frac{X_DD}{L_m}\left[\frac{(KV/L)^{m-1} - 1}{(KV/L) - 1}\right] \qquad (41)$$

3. Coupling the stripping and rectifying sections can be done easily since X_n in equation (36) is the feed stage liquid composition and so is X_1 from equation (41). Substituting for X_1 in equation (41) with X_n from equation (36),

$$X_m = (KV/L)_R^{m-1}\left\{(KV/L)_S^{n-1} + \frac{B}{L_n}\left[\frac{(KV/L)_S^{n-1} - 1}{(KV/L)_S - 1}\right]\right\}X_B - \frac{X_DD}{L_m}\left[\frac{(KV/L)_R^{m-1} - 1}{(KV/L)_R - 1}\right] \qquad (42)$$

In equation (42), the subscripts R and S are used to identify the KV/L terms for the rectification and stripping section, respectively.

For a total condenser, $X_M = X_D$ and equation (42) becomes

$$X_D = \frac{(KV/L)_R^{m-1}\left\{(KV/L)_S^{n-1} + \frac{B}{L_n}\left[\frac{(KV/L)_S^{n-1} - 1}{(KV/L)_S - 1}\right]\right\} X_B}{1 + \frac{D}{L_m}\left[\frac{(KV/L)_R^{m-1} - 1}{(KV/L)_R - 1}\right]} \tag{43}$$

For a partial (all vapor distillate) condenser, $X_M = X_D/K_M$ ($X_D = Y_M$) and equation (42) becomes

$$X_D = \frac{(KV/L)_R^{m-1}\left\{(KV/L)_S^{n-1} + \frac{B}{L_n}\left[\frac{(KV/L)_S^{n-1} - 1}{(KV/L)_S - 1}\right]\right\} X_B}{\frac{1}{K_m} + \frac{D}{L_m}\left[\frac{(KV/L)_R^{m-1} - 1}{(KV/L)_R - 1}\right]} \tag{44}$$

Equation (44) also results for the case of a total condenser and a decanter. In the decanter $X_M = X_D/K_D$ where K_D is the liquid-liquid equilibrium constant.

For a multicomponent separation, the specification of X_B and X_D for a component will determine B and D. Then if the KV/L values in each section are known and constant, equation (43) for example, may be solved to give the stage requirements for given values of either norm. For a given solution, the X_D/X_B ratios for the other components may be determined from equation (43). The values of X_D and and X_B are then found from the ratio and overall column component material balance.

4. The principal difficulty in employing the preceding equations is in the assumption of constant KV/L values in a section. An analysis of the series sum appearing in the previous derivations is presented here for the case where the KV/L values change linearly from stage to stage.

$$(KV/L)_{n-2} = (KV/L)_{n-1} + \Delta$$

For brevity, let $(KV/L)_i = S_i$

The series sum being investigated is of the form shown in equation (35) or

$$\text{Sum} = 1 + S_{n-1} + S_{n-1}S_{n-2} + \cdots + S_2S_3S_4 \cdots S_{n-1}$$

The last term contains n-2 factors. For linear changes in these factors, the series becomes

$$Sum = 1 + S_{n-1} + S_{n-1}(S_{n-1} + \Delta) + --- + S_{n-1}(S_{n-1} + \Delta) \cdots (S_{n-1} + n'\Delta)$$

The last term still contains n-2 factors. However, the coefficient of Δ in the last factor is n' and equals n-3.

The third term expansion is

$$S_{n-1}(S_{n-1} + \Delta) = S_{n-1}^2 + S_{n-1}(\Delta)$$

Similarly, the fourth term's expansion is

$$S_{n-1}(S_{n-1} + \Delta)(S_{n-1} + 2\Delta) = S_{n-1}^3 + 3S_{n-1}^2(\Delta) + 2S_{n-1}(\Delta^2)$$

and the fifth term is

$$S_{n-1}^4 + 6S_{n-1}^3(\Delta) + 11S_{n-1}^2(\Delta^2) + 6S_{n-1}(\Delta^3)$$

If Δ is close to zero, then the higher order Δ terms can be neglected. The series can then be written as

$$Sum = 1 + S_{n-1} + \left[S_{n-1}^2 + S_{n-1}(\Delta)\right] + \left[S_{n-1}^3 + 3S_{n-1}^2(\Delta)\right]$$
$$+ \left[S_{n-1}^4 + 6S_{n-1}^3(\Delta)\right] + --- + \left[S_{n-1}^{n-2} + \frac{(n-3)(n-2)}{2} S^{n-3}(\Delta)\right]$$

Separating the terms into two series gives

$$\text{Sum} = 1 + S_{n-1} + S_{n-1}^{2} + --- + S_{n-1}^{n-2}$$

$$+ \Delta\left[S_{n-1} + 3S_{n-1}^{2} + 6S_{n-1}^{3} + --- + \frac{(n-3)(n-2)}{2}S_{n-1}^{n-3}\right] \qquad (45)$$

Each term in the Δ series has a coefficient equal to m(m+1)/2 where m is the number of the term. For example, the second term is $3S_{n-1}^{2}$, and 2(2+1)/2 = 3.

The first series is a simple geometric series whose sum is $(S_{n-1}^{n-1} - 1)/(S_{n-1}-1)$. Developing a closed analytic expression for the second (Δ) series is more difficult. Writing this Δ series again with $S_{n-1} = a$,

$$a + 3a^{2} + 6a^{3} + --- + \frac{m(m+1)}{2}a^{m}$$

It is noted that this is really a summation of the following series.

$$\begin{array}{ll}
1) & a + a^{2} + a^{3} + a^{4} + --- + a^{m} \\
2) & \quad 2a^{2} + 2a^{3} + 2a^{4} + ---- + 2a^{m} \\
3) & \qquad 3a^{3} + 3a^{4} + ---- + 3a^{m} \\
\vdots & \qquad\qquad\qquad\qquad \vdots \\
m) & \qquad\qquad\qquad\qquad ma^{m} \\
\hline
\end{array}$$

$$\text{Sum} = a + 3a^{2} + 6a^{3} + -------- + \frac{m(m+1)}{2}a^{m}$$

Each of these has a convenient formula for its sum.

Series	Sum Formula
1)	$(a^{m+1}-a)/(a-1)$
2)	$2(a^{m+1}-a^2)/(a-1)$
$\vdots$	
m)	$m(a^{m+1}-a^m)/(a-1) = ma^m$

Each formula is derived by multiplying a series by the common term, subtracting the two and solving for the sum.

$$Sum = a + a^2 + a^3 + \cdots + a^m$$

$$a \times Sum = a^2 + a^3 + \cdots + a^m + a^{m+1}$$

Subtracting the two equations results in

$$Sum\,(a-1) = a^{m+1} - a$$

or

$$Sum = (a^{m+1}-a)/(a-1) \quad \text{for Series 1) above}$$

If all of the sum formulas are added together,

$$Sum = (a^{m+1}-a)/(a-1) + 2(a^{m+1}-a^2)/(a-1) + \cdots$$
$$\cdots + m(a^{m+1}-a^m)/(a-1)$$

or,

$$Sum = \frac{a^{m+1}(1+2+3+\cdots+m) - (a+2a^2+3a^3+\cdots+ma^m)}{(a-1)} \qquad (46)$$

The sum of an arithmetic series such as $1+2+3+\text{--}+m=m(m+1)/2$. Finding a sum formula for the series $a+2a^2+3a^3+\text{---}+ma^m$ requires use of the previous technique.

$$\begin{array}{ll}
1) & a+a^2+a^3+\text{---}+a^m \\
2) & \phantom{a+{}}a^2+a^3+\text{---}+a^m \\
\vdots & \\
m) & \phantom{a+a^2+a^3+\text{---}+{}}a^m \\
\hline
\text{Sum} = & a+2a^2+3a^3+\text{---}+ma^m
\end{array}$$

The formula sums are:

$$\begin{array}{ll}
1) & (a^{m+1}-a)/(a-1) \\
2) & (a^{m+1}-a^2)/(a-1) \\
\vdots & \\
m) & (a^{m+1}-a^m)/(a-1)
\end{array}$$

Adding these sum formulas gives

$$\left[m a^{m+1}-(a+a^2+\text{---}+a^m)\right]/(a-1)$$

$$=\frac{m a^{m+1}-(a^{m+1}-a)/(a-1)}{(a-1)}$$

Therefore, the series in equation (46) has the overall formula sum of

$$\text{Sum}=\frac{1}{(a-1)}\left\{\frac{m(m+1)}{2}a^{m+1}-\frac{1}{(a-1)}\left[m a^{m+1}-\frac{(a^{m+1}-a)}{(a-1)}\right]\right\} \tag{47}$$

and is the final form for the Δ series in equation (45).

Equation (45) then becomes

$$Sum = (S_{n-1}^{n-1} - 1)/(S_{n-1} - 1) + \frac{\Delta}{S_{n-1} - 1}\left\{\frac{m(m+1)S_{n-1}^{m+1}}{2} - \frac{1}{S_{n-1} - 1}\left[mS_{n-1}^{m+1} - \frac{(S_{n-1}^{m+1} - S_{n-1})}{(S_{n-1} - 1)}\right]\right\} \qquad (48)$$

(Note: m = n-3 as in the last term of equation (45).

The above equation is much more complex than that portion of equation (36), $\frac{(KV/L)^{n-1} - 1}{(KV/L) - 1}$ which represents the series in equation (35) that has just been investigated. Equation (48) reduces to the form $(S_{n-1}^{n-1} - 1)/(S_{n-1} - 1)$ $= [(KV/L)^{n-1} - 1]/[(KV/L - 1]$ when $\Delta = 0.0$, and illustrates the huge mathematical complexity that results when Δ is only slightly greater than zero and constant. It is concluded that it is extremely difficult to find a simple analytic form to represent a stagewise process when the KV/L values are not constant.

CHAPTER VI

COMPUTER PROGRAMS

Programs for binary distillation and multicomponent total reflux distillation were written in Fortran on a timesharing Honeywell G430 computer. The structure and usage is directed towards this particular system and the program would require some slight modifications in order to run on batch machines.

A. Program Structure and Usage.

A straightforward structure was used in designing the programs and only two subroutines are used. The programs are relatively short and this is the main reason they were not segmented into more subroutines. Each major calculation is in a discrete block and the program can be followed without difficulty when the logic is understood.

The program main logic was previously explained in Chapter I. Various other minor logical statements are used to control the calculation sequences and are obvious.

The major logic and calculation sequence is as follows for the binary distillation program RMC001.

1. Input Data
2. Stage 1 Calculations
3. General Stage Calculations (material balances)

4. Bubble Point Calculation
   a) For Stage 2, find the reboiler duty before proceeding to the next stage.
5. Component Enthalpy Calculations
6. Vapor Rate Calculation
   a) If unconverged, go to 3.
   b) If converged, go to 7 for the feed entrance test. For stages above the feed stage, go to 8.
7. Feed Entrance Test
8. Vapor Composition and Specified Distillate Comparison
   a) If the light component vapor composition is less than the requirement, go to 3.
   b) If the requirement is exceeded, go to 9.
9. Dew Point Calculation
10. Partial and Parallel Condenser Calculations
11. Printout

The multicomponent total reflux program (RMCTR) consists of steps 1 through 6, and 11. Step 8 could be included but the present version is programmed to run with a fixed number of stages as opposed to the binary program which determines the required stages. Running with a fixed number of stages creates an inconvenience for the total reflux design and azeotrope search cases since too few or too many calculations can result, depending on whether the desired result is reached with the specified number of stages.

Subroutines are used only for the liquid phase activity coefficient models. One is for the Wilson model and the other is for the ideal case.

Two fundamental data files are used to supply basic system properties. RC007 is a free field file containing each component's Antoine constants, liquid and vapor enthalpy temperature polynominal constants, and molecular weight. The equation forms are:

Antoine Equation: $\mathrm{Log}_{10}\mathrm{PmmHg} = A - B/(T + C)$

Liquid Enthalpy: $HL = AL + BL * T + CL*T^2 + DL * T^3$

Vapor Enthalpy: $HV = AV + BV * T + CV*T^2 + DV * T^3$

Where T is in degrees centigrade and the enthalpy is expressed as BTU/lb, data for a component is entered in the form A,B,C,AL,BL,CL,DL,AV,BV,CV,DV, molecular weight, followed by the constants for the next component, etc. For a binary system file, the light component's data is entered first. The multicomponent file data is arranged without distinctions. However, the order of the component data must be maintained once it is established since the other data file and program use this format.

A separate file (RC008) contains the Wilson parameters and component molar volumes if this model is to be used by the program. The parameters are expressed as cal/g mole while the volumes can be in any units as long as they are the same for each component. Parameters are read from the Wilson matrix in row order, such as g(1,1), g(1,2), g(2,1), g(2,2) for a binary system. Molar volumes are read next in component order, i.e., VM(1), VM(2). The main diagonal Wilson parameters do not have to be set to zero as is often done for convenience.

Once the files have been set up, the programs may be run. Input information for the binary program is:

1. Number of components
2. Temperature on Stage 1
3. Pressure on Stage 1
4. Total moles of bottoms product
5. Stage pressure drop
6. Equilibrium model code
7. Moles of component number one in bottoms product
8. Total moles of feed
9. Feed temperature
10. Moles of component number one in the feed

11. Moles of open steam
12. Mole fractions of components one and two in the open stream
13. Enthalpy (BTU/mole) of the open steam
14. Moles of vapor from Stage 1 (boilup)

If the temperature on Stage 1 is fixed, then item 3 should be zero. The program will calculate the pressure in this case. Should the Stage 1 pressure be fixed, its value should be given as item 3 and item 2 should contain a reasonable temperature estimate. The actual temperature will be calculated by the program and will converge faster if the estimate is given.

In items 4, 7, 8, and 10 the input is given in moles rather than mole fractions to reduce roundoff error. The distillate compositions and quantity are calculated from an overall material balance by the program.

The equilibrium model code is the integer 1 if the liquid phase is ideal. If the Wilson model is to be used, the integer 2 is required so the program will read file RC008 as previously explained.

Variables exist in the program that allow calculations involving open steam to the bottom of the column. Items 11, 12, and 13 are available for specifying the required input. This open steam option can also be used for a liquid or vapor feed to the base. No tests were run using this feature in either fashion.

The moles of vapor (boilup) from the base of the column is given as item 4. Its value will be primarily responsible for the magnitude of the stage requirements. Normally it is preferable to give large values when beginning to avoid being less than the minimum value for the system being studied. The program may not converge if this occurs. A maximum of one hundred stages is provided for in the program structure and is another reason for selecting a high boilup. No harm can be done with a high boilup since the calculations will approach a total reflux case with minimum stages.

The multicomponent program input data is shown below.

1. Number of components
2. Temperature on Stage 1
3. Pressure on Stage 1
4. Stage pressure drop
5. Equilibrium model code
6. Mole fractions of the liquid on Stage 1
7. Number of stages

Items 1 through 5 are treated in the same manner here as in the binary design program. The number of stages is specified and the reboiler is included as a whole stage.

After the numerical data is read into either program, a set of alphanumeric data is requested. The binary program has 24 spaces for the problem title followed by 6 spaces each for the names of two components. Presently, the multicomponent program also has 24 title spaces and 6 spaces each for three component names. Each program's printing and calculating capabilities are limited to the component quantities that can be read in as described above.

RMC001

```
100C  BINARY DISTILLATION PROGRAM BY R.M.CARLUCCI
110 DIMENSION A(3),B(3),C(3),VP(3),SP(100),X(100,3),Y(100,3),
120&T(100),SY(100),XL(100),V(100),HL(100,3),HV(100,3),AL(3),
130&AV(3),BL(3),BV(3),CL(3),CV(3),DL(3),DV(3),XMW(3),PP(3),G(3,3),
140&VM(3),K(100),M(100),FX(3),HF(3),XNAM(3),YNAM(3)
150 DIMENSION XF(3),FS(3),HS(3),HFL(3),HFV(3)
160 DIMENSION ACT(5),XD(3)
180 REAL TITLE(4),COM1,COM2
190 READ , N,T(1),SP(1),XL(1),DP,IEQ,X(1,1),F,TF,FX(1),FS(1),
200&XF(1),XF(2),HS,V(1)
210 READ 300, (TITLE(I),I=1,4),COM1,COM2
230 X(1,1)=X(1,1)/XL(1)
240 FX(1)=FX(1)/F
250 X(1,2)=1.0-X(1,1)
260 CALL OPENF (1,"RC007")
270 READ (1,) (A(I),B(I),C(I),AL(I),BL(I),CL(I),DL(I),AV(I),BV(I),
280&CV(I),DV(I),XMW(I),I=1,N)
290 NF=0
300 N1=2
310 NH=2
320 THB=0.
330 THD=0.
340 THF=0.
350 NA=0
360 GO TO (76,3),IEQ
370 3 CALL OPENF (2,"RC008")
380 READ (2,) ((G(I,J),J=1,N),I=1,N),(VM(I),I=1,N)
390C  START STAGE 1 CALCULATIONS
400 76 CONTINUE
410 J=1
415 IF (SP(1)) 99,99,12
420 99 GO TO (1,2),IEQ
430 1 CALL XIDEAL (N,ACT)
440 GO TO 74
450 2 CALL WILSON (N,T,G,X,VM,ACT,J)
460 74 DO 10 I=1,N
470 ANTEQ=A(I)-B(I)/(T(1)+C(I))
480 VP(I)=EXP10(ANTEQ)
490 PP(I)=X(1,I)*ACT(I)*VP(I)
500 SP(1)=SP(1)+PP(I)
510 10 CONTINUE
520 SY(1)=1.000
530 DO 11 I=1,N
540 Y(1,I)=PP(I)/SP(1)
550 11 CONTINUE
560C  END OF STAGE 1 CALCULATIONS
570 XD(1)=(F*FX(1)+FS(1)*XF(1)-XL(1)*X(1,1))/(F+FS(1)-XL(1))
580 DIS=F-XL(1)
590 XD(2)=1.-XD(1)
600 FX(2)=1.-FX(1)
```

RMC001 CONTINUED

```
620 DO 4 I=1,N
630 HFL(I)=AL(I)+BL(I)*TF+CL(I)*TF**2+DL(I)*TF**3
640 HFL(I)=HFL(I)*XMW(I)
650 4 HF(I)=HFL(I)
660 DELT=0.
670 53 CONTINUE
675C  START STAGE CALCULATIONS
680 DO 20 J=2,100
690 M(J-1)=0
700 IF (J.EQ.2) GO TO 19
710 32 XL(J)=V(J-1)+XL(J-1)-V(J-2)-NF*F
720 DO 21 I=1,N
730 X(J,I)=(Y(J-1,I)*V(J-1)-NF*FX(I)*F+X(J-1,I)*XL(J-1)-Y(J-2,I)
740&*V(J-2))/XL(J)
750 21 CONTINUE
760 GO TO 36
770 19 XL(2)=V(1)+XL(1)-FS(1)
780 DO 35 I=1,N
790 X(2,I)=(Y(1,I)*V(1)+X(1,I)*XL(1)-XF(I)*FS(1))/XL(2)
800 35 CONTINUE
810 36 IF (M(J-1).GT.0) GO TO 12
820 SP(J)=SP(J-1)-DP
830 IF(J.EQ.2) T(2)=T(1)
840 IF(J.GT.2) T(J)=2.*T(J-1)-T(J-2)
850 12 CONTINUE
855C BEGINNING OF BUBBLE POINT CALCULATION
860 K(J)=1
870 GO TO (6,7),IEQ
880 6 GO TO 22
890 7 CALL WILSON (N,T,G,X,VM,ACT,J)
900 22 SY(J)=0.
910 DO 23 I=1,N
920 ANTEQ=A(I)-B(I)/(T(J)+C(I))
930 VP(I)=EXP10(ANTEQ)
940 Y(J,I)=X(J,I)*ACT(I)*VP(I)/SP(J)
950 SY(J)=SY(J)+Y(J,I)
960 23 CONTINUE
970 DELY=1.-SY(J)
980 ADELY=ABS(DELY)
990 AB=0.
1000 IF(ADELY-.001) 25,25,24
1010 24 DO 26 I=1,N
1020 AX=X(J,I)*ACT(I)*B(I)*VP(I)/((T(J)+C(I))**2)
1030 AB=AB+AX
1040 26 CONTINUE
1050 DELT=SP(J)*DELY/AB/2.303
1060 T(J)=T(J)+DELT
1070 K(J)=K(J)+1
1080 GO TO (6,7),IEQ
1090 25 CONTINUE
```

RMC001 CONTINUED

```
1100C  END OF BUBBLE POINT CALCULATION,NORMALIZE Y VALUES
1110 DO 37 I=1,N
1120 Y(J,I)=Y(J,I)/SY(J)
1130 37 CONTINUE
1140C  Y NORMALIZATION COMPLETE
1145 IF(J.EQ.1)GOTO 11
1150 IF(J.EQ.2) GOTO27
1160 GO TO 28
1170 27 CONTINUE
1180C  FIND REBOILER DUTY (QR)
1190 DO 29 L=1,2
1200 DO 30 I=1,N
1210 HL(L,I)=AL(I)+BL(I)*T(L)+CL(I)*T(L)**2+DL(I)*T(L)**3
1220 HL(L,I)=HL(L,I)*XMW(I)
1230 HV(1,I)=AV(I)+BV(I)*T(1)+CV(I)*T(1)**2+DV(I)*T(1)**3
1240 HV(1,I)=HV(1,I)*XMW(I)
1250 30 CONTINUE
1260 29 CONTINUE
1270 QR=0.
1280 DO 31 I=1,N
1290 QRP=Y(1,I)*HV(1,I)*V(1)+XL(1)*X(1,I)*HL(1,I)-XL(2)*X(2,I)
1300&*HL(2,I)-FX(I)*NF*F*HF(I)
1310 QR=QR+QRP
1320 31 CONTINUE
1330 QR=QR-FS(1)*HS
1340C  END OF REBOILER DUTY CALCULATION
1350 PRINT, " Q REBOILER= ",QR
1360 V(2)=V(1)
1370C  PROCEED TO STATEMENT 33
1380 GO TO 33
1390 28 CONTINUE
1400C  COMPONENT ENTHALPY CALCULATIONS
1410 DO 40 I=1,N
1420 HL(J,I)=AL(I)+BL(I)*T(J)+CL(I)*T(J)**2+DL(I)*T(J)**3
1430 HL(J,I)=HL(J,I)*XMW(I)
1440 HV(J-1,I)=AV(I)+BV(I)*T(J-1)+CV(I)*T(J-1)**2+DV(I)*T(J-1)**3
1450 HV(J-1,I)=HV(J-1,I)*XMW(I)
1460 40 CONTINUE
1470 IF(NA.EQ.1) GOTO63
1480 IF (NH.EQ.1) GO TO 59
1490 VC=0.
1500C  FIND VAPOR RATE FROM PREVIOUS STAGE BY HEAT BALANCE
1510 YSIDE=0.
1520 DO 45 I=1,N
1530 RHS=FX(I)*NF*F*HF(I)+Y(J-2,I)*V(J-2)*HV(J-2,I)+
1540&XL(J)*X(J,I)*HL(J,I)-XL(J-1)*X(J-1,I)*HL(J-1,I)
1550 VC=VC+RHS
1560 45 CONTINUE
1570 DO 47 I=1,N
1580 PPHV=Y(J-1,I)*HV(J-1,I)
```

RMC001 CONTINUED

```
1590 YSIDE=YSIDE+PPHV
1600 47 CONTINUE
1610 VC=VC/YSIDE
1620C  COMPARE CALCULATED AND ASSUMED VAPOR RATE FROM STAGE J-1
1630 DELV=V(J-1)-VC
1640 RDELV=DELV/V(J-1)
1650 ADELV=ABS(RDELV)
1660 IF (ADELV-.0001) 33,33,34
1670 34 V(J-1)=VC
1680C  ERROR IN VAPOR RATE,GOBACK TO STAGE CALCULATIONS
1690 M(J-1)=M(J-1)+1
1700 GO TO 32
1705C  FEED ENTRANCE TEST
1710 33 IF (N1.EQ.1) GO TO 43
1720 IF (X(J,1)-FX(1)) 39,38,38
1730 39 GO TO 20
1740 38 NF=1
1750 N1=1
1760 PRINT , "FEED ON STAGE= ",J
1770 FDS=J
1780 IF (NF.EQ.1) GO TO 44
1790 43 NF=0
1800 44 CONTINUE
1805C  CHECK VAPOR COMPOSITION TO SEE IF STAGE CALCULATIONS SHOULD STOP
1810 IF (Y(J,2)-XD(2)) 51,51,20
1820C START DEW POINT FOR DISTILLATE
1830 41 GO TO 51
1840 42 CALL WILSON (N,T,G,X,VM,ACT,J)
1850 51 SUMX=0.
1860 DO 50 I=1,N
1870 ANTEQ=A(I)-B(I)/(T(J)+C(I))
1880 VP(I)=EXP10(ANTEQ)
1890 X(J,I)=XD(I)*SP(J)/(ACT(I)*VP(I))
1900 SUMX=SUMX+X(J,I)
1910 50 CONTINUE
1920 PRINT , "SX= ",SUMX
1930 DSX=1.-SUMX
1940 ADSX=ABS(DSX)
1950 IF (ADSX-.001) 57,57,55
1960 55 AB=0.
1970 DO 56 I=1,N
1980 AX=XD(I)*B(I)/ACT(I)/VP(I)/((T(J)+C(I))**2)
1990 AB=AB+AX
2000 56 CONTINUE
2010 DELT=-DSX/(2.303*SP(J)*AB)
2015 DELT=DELT/2.
2020 T(J)=T(J)+DELT
2030 GO TO (41,42),IEQ
2040 57 CONTINUE
2050C NORMALIZE X DEW POINT
```

RMC001 CONTINUED

```
2060 DO 58 I=1,N
2070 X(J,I)=X(J,I)/SUMX
2080 Y(J,I)=XD(I)
2090 58 CONTINUE
2100C END OF DISTILLATE DEW POINT CALCULATION
2110C FIND PARTIAL COND DUTY
2120 XL(J)=DIS*(XD(1)-Y(J-1,1))/(Y(J-1,1)-X(J,1))
2130 V(J-1)=XL(J)+DIS
2140 V(J)=DIS
2150 NH=1
2160 GO TO 28
2170 59 QPC=0.
2180 T(J+1)=T(J)
2190 J=J+1
2200 NA=1
2210 GO TO 28
2220 63 NS=J-1
2230 J=J-1
2240 DO 60 I=1,N
2250 QPC=QPC+V(J-1)*Y(J-1,I)*HV(J-1,I)-XL(J)*HL(J,I)*X(J,I)
2260&-DIS*HV(J,I)*Y(J,I)
2270 60 CONTINUE
2280C  FIND PARALLEL CONDENSER DUTY (QPC)
2290 V(J)=DIS
2300 QRC=0.
2310 DO 79 I=1,N
2320 QRC=QRC+F*FX(I)*HF(I)-DIS*XD(I)*HV(J,I)-XL(1)*X(1,I)*HL(1,I)
2330 79 CONTINUE
2340 QRC=QRC+QR-QPC+F*HS
2345C  PARALLEL CONDENSER DUTY KNOWN
2350 GOTO78
2360 20 IF(J.GT.2) V(J)=2.*V(J-1)-V(J-2)
2370 78 CONTINUE
2380 DO 80 I=1,N
2390 TB=XL(1)*X(1,I)*HL(1,I)
2400 TH=F*FX(I)*HF(I)
2410 TD=DIS*XD(I)*HV(J,I)
2420 THD=THD+TD
2430 THF=THF+TH
2440 80 THB=THB+TB
2450 QIN=QR+THF
2460 QOUT=QPC+QRC+THB+THD
2470 PRINT , "Q IN= ",QIN,"QOUT= ",QOUT
2480 PRINT , "NS= ",NS
2500 IF(NS.GT.21)GOTO209
2510 13 FORMAT (5X,I3,3(7X,F7.2),3X,F7.2)
2520 14 FORMAT (5X,I3,7X,F6.4,3X,F6.4,7X,F6.4,3X,F6.4,3X,F6.4)
2530 PRINT 201, (TITLE(I),I=1,4)
2540 201 FORMAT(//,24X,4A6,////)
2550 PRINT 202,
```

```
2560 202 FORMAT (43X,"FLOW LEAVING STAGE(MOLS)")
2570 PRINT 203,
2580 203 FORMAT(5X,"STAGE",5X,"PRESSURE",5X,"TEMPERATURE",5X,
2590&"LIQUID",5X,"VAPOR",/)
2600 PRINT 13,(J,SP(J),T(J),XL(J),V(J),J=1,NS)
2630 PRINT 204,
2640 204 FORMAT(5X,"STAGE  LIQUID MOL FRACTIONS  VAPOR MOL FRAC"
2650&"TIONS   SUM Y",/)
2655 PRINT 207, COM1,COM2,COM1,COM2
2660 PRINT 14,(J,(X(J,I),I=1,N),(Y(J,I),I=1,N),SY(J),J=1,NS)
2680 207 FORMAT (15X,A6,3X,A6,7X,A6,3X,A6,/)
2690 M1=2*NS
2695 DO 208 I=M1,50
2700 208 PRINT,
2710 GOTO215
2720 209 IF(NS.GT.51) GOTO211
2730 PRINT 201, (TITLE(I),I=1,4)
2740 PRINT 202,
2750 PRINT 203,
2760 PRINT 13,(J,SP(J),T(J),XL(J),V(J),J=1,NS)
2770 DO 210 I=NS,50
2780 210 PRINT ,'
2790 PRINT 201, (TITLE(I),I=1,4)
2800 PRINT 204,
2810 PRINT 207,COM1,COM2,COM1,COM2
2820 PRINT 14,(J,(X(J,I),I=1,N),(Y(J,I),I=1,N),SY(J),J=1,NS)
2830 DO 212 I=NS,50
2840 212 PRINT ,'
2850  GOTO215
2860 211 PRINT 201, (TITLE(I),I=1,4)
2870 PRINT 202,
2880 PRINT 203,
2890 PRINT 13, (J,SP(J),T(J),XL(J),V(J),J=1,50)
2900 PRINT 201, (TITLE(I),I=1,4)
2910 PRINT 202,
2920 PRINT 203,
2930 PRINT 13, (J,SP(J),T(J),XL(J),V(J),J=51,NS)
2940 DO 213 I=NS,100
2950 213 PRINT ,'
2960 PRINT 201, (TITLE(I),I=1,4)
2970 PRINT 204,
2980 PRINT 207, COM1,COM2,COM1,COM2
2990 PRINT 14, (J,(X(J,I),I=1,N),(Y(J,I),I=1,N),SY(J),J=1,50)
3000 PRINT 201, (TITLE(I),I=1,4)
3010 PRINT 204,
3020 PRINT 207, COM1,COM2,COM1,COM2
3030 PRINT 14, (J,(X(J,I),I=1,N),(Y(J,I),I=1,N),SY(J),J=51,NS)
3040 DO 214 I=NS,100
3050 214 PRINT ,'
3060 215 PRINT 201, (TITLE(I),I=1,4)
```

RMC001 CONTINUED

```
3070 PRINT 216,F,TF,FDS
3080 216 FORMAT (5X,"FEED STREAM ",F6.3," MOLS",2X,F6.2,
3090&" DEG C",2X,"FEED STAGE ",I3,/)
3100 PRINT 217, COM1,FX(1),COM2,FX(2)
3110 217 FORMAT (5X,A6," MOL FRACTION ",F6.4,3X,A6," MOL FRACTION ",
3120&F6.4,/)
3130 PRINT 218, DIS,T(NS)
3140 218 FORMAT (5X,"DISTILLATE ",F6.3," MOLS  ",F6.2," DEG C ",/)
3150 PRINT 217, COM1,XD(1),COM2,XD(2)
3160 PRINT 219, XL(1),T(1)
3170 219 FORMAT (5X,"BOTTOMS",5X,F6.3," MOLS  ",F6.2," DEG C",/)
3180 PRINT 217 , COM1,X(1,1),COM2,X(1,2)
3181 PRINT,"     HEAT BALANCE"
3182 PRINT 220,QR,THD
3183 220 FORMAT (5X,"REBOILER",6X,F10.0,"  DISTILLATE ENTHALPY ",
3184&F10.0/)
3185 PRINT 221,THF,THB
3186 221 FORMAT (5X,"FEED ENTHALPY ",F10.0,"  BOTTOMS",4X,"ENTHALPY ",
3187&F10.0/)
3188 PRINT 222,QPC
3190 300 FORMAT(6A6)
3191 222 FORMAT (33X,"PARTIAL CONDENSER ",F10.0/)
3192 PRINT 223,QRC
3193 223 FORMAT (32X,"PARALLEL CONDENSER ",F10.0/)
3194 PRINT 224,QIN,QOUT
3195 224 FORMAT (5X,"HEAT INPUT",4X,F10.0,"  HEAT OUTPUT",9X,F10.0/)
3196 DO 225 I=1,30
3197 225 PRINT ,
3200 81 END
3210 SUBROUTINE XIDEAL(N,ACT)
3220 DIMENSION ACT(5)
3230 DO 1 I=1,N
3240 ACT(I)=1.
3250 1 CONTINUE
3260 RETURN
3270 END
3280 SUBROUTINE WILSON (N,T,G,X,VM,ACT,J)
3290 DIMENSION SLAM(5,5),VM(3),G(3,3),X(100,3),ACT(5),T(100)
3300 DO 100 J1=1,N
3310 DO 101 I1=1,N
3320 GIJ=G(I1,J1)
3330 GII=G(I1,I1)
3340 SLAM(I1,J1)=VM(J1)/VM(I1)*EXP(-(GIJ-GII)/(1.987*(T(J)+273.)))
3350 101 CONTINUE
3360 100 CONTINUE
3370 DO 102 I1=1,N
3380 S=0.
3390 DO 103 K1=1,N
3400 S2=0.
3410 DO 104 J1=1,N
```

RMC001 CONTINUED

```
3420 S2=X(J,J1)*SLAM(K1,J1)+S2
3430 104 CONTINUE
3440 XXLAM=X(J,K1)*SLAM(K1,I1)/S2
3450 S=XXLAM+S
3460 103 CONTINUE
3470 S1=0.
3480 DO 105 J1=1,N
3490 XLXLAM=X(J,J1)*SLAM(I1,J1)
3500 S1=XLXLAM+S1
3510 105 CONTINUE
3520 S3=ALOG(S1)
3530 S4=1.-S3-S
3540 ACT(I1)=EXP(S4)
3550 102 CONTINUE
3560 RETURN
3570 END
```

RMCTR

```
100C  MULTICOMPONENT TOTAL REFLUX DISTILLATION PROGRAM BY R.M.CARLUCCI
110 DIMENSION A(3),B(3),C(3),VP(3),SP(100),X(100,3),Y(100,3),
120&T(100),SY(100),XL(100),V(100),HL(100,3),HV(100,3),AL(3),
130&AV(3),BL(3),BV(3),CL(3),CV(3),DL(3),DV(3),XMW(3),PP(3),G(3,3),
140&VM(3),K(100),M(100),FX(3),HF(3),XNAM(3),YNAM(3)
150 DIMENSION HFL(3),HFV(3)
160 DIMENSION ACT(5),XD(3)
180 REAL TITLE(4),COM1,COM2,COM3
190 READ , N,T(1),SP(1),DP,IEQ,(X(1,I),I=1,N),NS
210 READ 300, (TITLE(I),I=1,4),COM1,COM2,COM3
230 F=0.
250 XL(1)=0.
260 CALL OPENF (1,"RC007")
270 READ (1,) (A(I),B(I),C(I),AL(I),BL(I),CL(I),DL(I),AV(I),BV(I),
280&CV(I),DV(I),XMW(I),I=1,N)
290 NF=0
300 N1=2
310 NH=2
320 THB=0.
330 THD=0.
340 THF=0.
350 NA=0
360 GO TO (76,3),IEQ
370 3 CALL OPENF (2,"RC008")
380 READ (2,) ((G(I,J),J=1,N),I=1,N),(VM(I),I=1,N)
390C  START STAGE 1 CALCULATIONS
400 76 J=1
415 IF (SP(1)) 99,99,12
420 99 GO TO (1,2),IEQ
430 1 CALL XIDEAL (N,ACT)
440 GO TO 74
450 2 CALL WILSON (N,T,G,X,VM,ACT,J)
460 74 DO 10 I=1,N
470 ANTEQ=A(I)-B(I)/(T(1)+C(I))
480 VP(I)=EXP10(ANTEQ)
490 PP(I)=X(1,I)*ACT(I)*VP(I)
500 SP(1)=SP(1)+PP(I)
510 10 CONTINUE
520 SY(1)=1.000
530 DO 11 I=1,N
540 Y(1,I)=PP(I)/SP(1)
550 11 CONTINUE
560C  END OF STAGE 1 CALCULATIONS
610 V(1)=70.
660 DELT=0.
670 53 CONTINUE
675C  START STAGE CALCULATIONS
680 DO 20 J=2,NS
690 M(J-1)=0
700 IF (J.EQ.2) GO TO 19
```

RMCTR CONTINUED

```
710 32 XL(J)=V(J-1)+XL(J-1)-V(J-2)-NF*F
720 DO 21 I=1,N
730 X(J,I)=(Y(J-1,I)*V(J-1)-NF*FX(I)*F+X(J-1,I)*XL(J-1)-Y(J-2,I)
740&*V(J-2))/XL(J)
750 21 CONTINUE
760 GO TO 36
770 19 XL(2)=V(1)+XL(1)
780 DO 35 I=1,N
790 X(2,I)=(Y(1,I)*V(1)+X(1,I)*XL(1))/XL(2)
800 35 CONTINUE
810 36 IF (M(J-1).GT.0) GO TO 12
820 SP(J)=SP(J-1)-DP
830 IF(J.EQ.2) T(2)=T(1)
840 IF(J.GT.2) T(J)=2.*T(J-1)-T(J-2)
850 12 CONTINUE
855C BEGINNING OF BUBBLE POINT CALCULATION
860 K(J)=1
870 GO TO (6,7),IEQ
880 6 GO TO 22
890 7 CALL WILSON (N,T,G,X,VM,ACT,J)
900 22 SY(J)=0.
910 DO 23 I=1,N
920 ANTEQ=A(I)-B(I)/(T(J)+C(I))
930 VP(I)=EXP10(ANTEQ)
940 Y(J,I)=X(J,I)*ACT(I)*VP(I)/SP(J)
950 SY(J)=SY(J)+Y(J,I)
960 23 CONTINUE
970 DELY=1.-SY(J)
980 ADELY=ABS(DELY)
990 AB=0.
1000 IF(ADELY-.001) 25,25,24
1010 24 DO 26 I=1,N
1020 AX=X(J,I)*ACT(I)*B(I)*VP(I)/((T(J)+C(I))**2)
1030 AB=AB+AX
1040 26 CONTINUE
1050 DELT=SP(J)*DELY/AB/2.303
1060 T(J)=T(J)+DELT
1070 K(J)=K(J)+1
1080 GO TO (6,7),IEQ
1090 25 CONTINUE
1100C  END OF BUBBLE POINT CALCULATION,NORMALIZE Y VALUES
1110 DO 37 I=1,N
1120 Y(J,I)=Y(J,I)/SY(J)
1130 37 CONTINUE
1140C  Y NORMALIZATION COMPLETE
1145 IF(J.EQ.1)GOTO 11
1150 IF(J.EQ.2) GOTO27
1160 GO TO 28
1170 27 CONTINUE
1180C  FIND REBOILER DUTY (QR)
```

```
1190 DO 29 L=1,2
1200 DO 30 I=1,N
1210 HL(L,I)=AL(I)+BL(I)*T(L)+CL(I)*T(L)**2+DL(I)*T(L)**3
1220 HL(L,I)=HL(L,I)*XMW(I)
1230 HV(1,I)=AV(I)+BV(I)*T(1)+CV(I)*T(1)**2+DV(I)*T(1)**3
1240 HV(1,I)=HV(1,I)*XMW(I)
1250 30 CONTINUE
1260 29 CONTINUE
1270 QR=0.
1280 DO 31 I=1,N
1290 QRP=Y(1,I)*HV(1,I)*V(1)+XL(1)*X(1,I)*HL(1,I)-XL(2)*X(2,I)
1300&*HL(2,I)-FX(I)*NF*F*HF(I)
1310 QR=QR+QRP
1320 31 CONTINUE
1340C  END OF REBOILER DUTY CALCULATION
1350 PRINT, " Q REBOILER= ",QR
1360 V(2)=V(1)
1370C  PROCEED TO STATEMENT 33
1380 GO TO 33
1390 28 CONTINUE
1400C  COMPONENT ENTHALPY CALCULATIONS
1410 DO 40 I=1,N
1420 HL(J,I)=AL(I)+BL(I)*T(J)+CL(I)*T(J)**2+DL(I)*T(J)**3
1430 HL(J,I)=HL(J,I)*XMW(I)
1440 HV(J-1,I)=AV(I)+BV(I)*T(J-1)+CV(I)*T(J-1)**2+DV(I)*T(J-1)**3
1450 HV(J-1,I)=HV(J-1,I)*XMW(I)
1460 40 CONTINUE
1490 VC=0.
1500C  FIND VAPOR RATE FROM PREVIOUS STAGE BY HEAT BALANCE
1510 YSIDE=0.
1520 DO 45 I=1,N
1530 RHS=FX(I)*NF*F*HF(I)+Y(J-2,I)*V(J-2)*HV(J-2,I)+
1540&XL(J)*X(J,I)*HL(J,I)-XL(J-1)*X(J-1,I)*HL(J-1,I)
1550 VC=VC+RHS
1560 45 CONTINUE
1570 DO 47 I=1,N
1580 PPHV=Y(J-1,I)*HV(J-1,I)
1590 YSIDE=YSIDE+PPHV
1600 47 CONTINUE
1610 VC=VC/YSIDE
1620C  COMPARE CALCULATED AND ASSUMED VAPOR RATE FROM STAGE J-1
1630 DELV=V(J-1)-VC
1640 RDELV=DELV/V(J-1)
1650 ADELV=ABS(RDELV)
1660 IF (ADELV-.0001) 33,33,34
1670 34 V(J-1)=VC
1680C  ERROR IN VAPOR RATE,GOBACK TO STAGE CALCULATIONS
1690 M(J-1)=M(J-1)+1
1700 GO TO 32
1710 33 CONTINUE
```

RMCTR CONTINUED

```
1730 39 GO TO 20
2360 20 IF(J.GT.2) V(J)=2.*V(J-1)-V(J-2)
2370 78 NS=J-1
2500 IF(NS.GT.21)GOTO209
2510 13 FORMAT (5X,I3,3(7X,F7.2),3X,F7.2)
2520 14 FORMAT (5X,I3,13X,F6.4,4X,F6.4,4X,F6.4,7X,F6.4)
2530 PRINT 201, (TITLE(I),I=1,4)
2540 201 FORMAT(//,24X,4A6,////)
2550 PRINT 202,
2560 202 FORMAT (43X,"FLOW LEAVING STAGE(MOLS)")
2570 PRINT 203,
2580 203 FORMAT(5X,"STAGE",5X,"PRESSURE",5X,"TEMPERATURE",5X,
2590&"LIQUID",5X,"VAPOR",/)
2600 PRINT 13,(J,SP(J),T(J),XL(J),V(J),J=1,NS)
2630 PRINT 204,
2640 204 FORMAT (//,5X,"STAGE",14X,"LIQUID MOL FRACTIONS",12X,"SUM Y",/)
2655 PRINT 207, COM1,COM2,COM3
2660 PRINT 14,(J,(X(J,I),I=1,N),SY(J),J=1,NS)
2680 207 FORMAT (21X,A6,4X,A6,4X,A6,/)
2690 M1=2*NS
2695 DO 208 I=M1,50
2700 208 PRINT,
2710 GOTO215
2720 209 IF(NS.GT.51) GOTO211
2730 PRINT 201, (TITLE(I),I=1,4)
2740 PRINT 202,
2750 PRINT 203,
2760 PRINT 13,(J,SP(J),T(J),XL(J),V(J),J=1,NS)
2770 DO 210 I=NS,50
2780 210 PRINT ,'
2790 PRINT 201, (TITLE(I),I=1,4)
2800 PRINT 204,
2810 PRINT 207 , COM1,COM2,COM3
2820 PRINT 14,(J,(X(J,I),I=1,N),(Y(J,I),I=1,N),SY(J),J=1,NS)
2830 DO 212 I=NS,50
2840 212 PRINT ,'
2850  GOTO215
2860 211 PRINT 201, (TITLE(I),I=1,4)
2870 PRINT 202,
2880 PRINT 203,
2890 PRINT 13, (J,SP(J),T(J),XL(J),V(J),J=1,50)
2900 PRINT 201, (TITLE(I),I=1,4)
2910 PRINT 202,
2920 PRINT 203,
2930 PRINT 13, (J,SP(J),T(J),XL(J),V(J),J=51,NS)
2940 DO 213 I=NS,100
2950 213 PRINT ,'
2960 PRINT 201, (TITLE(I),I=1,4)
2970 PRINT 204,
2980 PRINT 207, COM1,COM2,COM3
```

RMCTR CONTINUED

```
2990 PRINT 14 , (J,(X(J,I),I=1,N),SY(J),J=1,50)
3000 PRINT 201, (TITLE(I),I=1,4)
3010 PRINT 204,
3020 PRINT 207, COM1,COM2,COM3
3030 PRINT 14, (J,(X(J,I),I=1,N),SY(J),J=51,NS)
3040 DO 214 I=NS,100
3050 214 PRINT ,'
3060 215 GO TO 81
3070 PRINT 216,F,TF,FDS
3080 216 FORMAT (//,5X,"FEED STREAM ",F6.3," MOLS",2X,F6.2,
3090&" DEG C",2X,"FEED STAGE ",I3,/)
3100 PRINT 217, COM1,FX(1),COM2,FX(2)
3110 217 FORMAT (//,5X,A6," MOL FRACTION ",F6.4,3X,A6," MOL FRACTION ",
3120&F6.4,/)
3130 PRINT 218, DIS,T(NS)
3140 218 FORMAT (//,5X,"DISTILLATE ",F6.3," MOLS  ",F6.2," DEG C ",/)
3150 PRINT 217, COM1,XD(1),COM2,XD(2)
3160 PRINT 219, XL(1),T(1)
3170 219 FORMAT (//,5X,"BOTTOMS",//,5X,F6.3," MOLS  ",F6.2," DEG C",/)
3180 PRINT 217 , COM1,X(1,1),COM2,X(1,2)
3181 PRINT,"     HEAT BALANCE"
3182 PRINT 220,QR,THD
3183 220 FORMAT (//,5X,"REBOILER",6X,F10.0,"  DISTILLATE ENTHALPY ",
3184&F10.0/)
3185 PRINT 221,THF,THB
3186 221 FORMAT (//,5X,"FEED ENTHALPY ",F10.0,"  BOTTOMS",4X,"ENTHALPY ",
3187&F10.0/)
3188 PRINT 222,QPC
3190 300 FORMAT (7A6)
3191 222 FORMAT (33X,"PARTIAL CONDENSER ",F10.0/)
3192 PRINT 223,QRC
3193 223 FORMAT (32X,"PARALLEL CONDENSER ",F10.0/)
3194 PRINT 224,QIN,QOUT
3195 224 FORMAT (//,5X,"HEAT INPUT",4X,F10.0,"  HEAT OUTPUT",9X,F10.0/)
3196 DO 225 I=1,30
3197 225 PRINT ,
3200 81 END
3210 SUBROUTINE XIDEAL(N,ACT)
3220 DIMENSION ACT(5)
3230 DO 1 I=1,N
3240 ACT(I)=1.
3250 1 CONTINUE
3260 RETURN
3270 END
3280 SUBROUTINE WILSON (N,T,G,X,VM,ACT,J)
3290 DIMENSION SLAM(5,5),VM(3),G(3,3),X(100,3),ACT(5),T(100)
3300 DO 100 J1=1,N
3310 DO 101 I1=1,N
3320 GIJ=G(I1,J1)
3330 GII=G(I1,I1)
```

RMCTR CONTINUED

```
3340 SLAM(I1,J1)=VM(J1)/VM(I1)*EXP(-(GIJ-GII)/(1.987*(T(J)+273.)))
3350 101 CONTINUE
3360 100 CONTINUE
3370 DO 102 I1=1,N
3380 S=0.
3390 DO 103 K1=1,N
3400 S2=0.
3410 DO 104 J1=1,N
3420 S2=X(J,J1)*SLAM(K1,J1)+S2
3430 104 CONTINUE
3440 XXLAM=X(J,K1)*SLAM(K1,I1)/S2
3450 S=XXLAM+S
3460 103 CONTINUE
3470 S1=0.
3480 DO 105 J1=1,N
3490 XLXLAM=X(J,J1)*SLAM(I1,J1)
3500 S1=XLXLAM+S1
3510 105 CONTINUE
3520 S3=ALOG(S1)
3530 S4=1.-S3-S
3540 ACT(I1)=EXP(S4)
3550 102 CONTINUE
3560 RETURN
3570 END
```

CHAPTER VII

COMPUTER CASE STUDIES

A. Discussion. Three binary systems and one ternary system were simulated by distillation calculations. The binary systems were (1) Benzene-Toluene, (2) Benzene-n-Butanol, and (3) Ethanol-Water. A ternary comprised of Methanol-Acetone-2,3,-Dimethylbutane was investigated. These systems were selected since the physical properties and vapor-liquid equilibria were readily available.

Each set of binary output consists of a section displaying the stage pressure, temperature, and flows. The last stage (top of the column) is the partial condenser and consequently the flows are usually quite different from the other stages. Vapor flow to the partial condenser from the previous stage is displayed. The vapor from this stage to the parallel condenser is not shown. A second section gives the stage compositions and the sum of vapor phase compositions on the stage. The third section summarizes the material and energy balances and feed stage. This format is followed for all of the binary cases.

Benzene and Toluene were treated as having ideal vapor-liquid equilibrium. Case studies 1 through 6 were run with varying boilup to determine the stage requirements to separate a feed of 75mole% Benzene into a 99.9mole% Benzene distillate stream and 99.9mole% Toluene bottoms stream.

Benzene and n-Butanol were studied in cases 7 through 11. The vapor-liquid is non-ideal and the Wilson model was used. The separation is difficult at 760mmHg as shown by cases 8 through 11. However, at 300mmHg, and for the same boilup as case 8, the results in case 7 show only 14 stages are required versus 36 stages at the higher pressure. Case 8 and case 8a were also run with different tolerances for the sum of the vapor phase compositions. The tolerance for case 8 is .001 and this allows the temperature to oscillate in the second decimal place for the difficult separation occuring in the upper stages. Case 8a with a tolerance of .0001 eliminates the temperature oscillation, but had no other outstanding effect. The stage requirements, compositions, and flows remain unchanged.

The Ethanol and Water separation is shown in cases 12 through 17. Again the Wilson model is used to describe the non-ideal equilibrium. Since an azeotrope is present, the overhead composition was set at 75mole% Ethanol to avoid any interference with the program's convergence towards a material balance.

The multicomponent program output is different than that from the binary program. The first section is the same and the third section is deleted since there is no feed or partial and parallel condensers. The second section displays only the stage liquid compositions and sum of the vapor compositions. At total reflux, the vapor leaving a stage is identical to the liquid from the stage above. The vapor in equilibrium with a liquid is the liquid on the next stage.

Case 18 shows the system Methanol-Acetone-2,3-Dimethylbutane in a ten stage column at total reflux. The presence of the ternary azeotrope is displayed since the compositions on stages 9 and 10 are almost equal. The program was used to search for the azeotrope and was easily found by starting the stage calculations close to the center of the ternary diagram and thereby avoiding the binary azeotropes.

The actual composition of the azeotrope at 760mmHg and 43.2 degrees C is Xmethanol = .254, Xacetone = .229, and XDMB = .517. From case 18, the predicted compositions are Xmethanol = .2522, Xacetone = .2181, and XDMB = .5297 which are quite close to the above values. Some of the difference can be attributed to the use of fixed molar volumes in the Wilson model subroutine used in the program. A polynomial expressing the molar volumes as functions of temperature could improve the accuracy. The use of constant values did not deleteriously affect the calculations and should be suitable for most problems.

Cases 19 and 20 illustrate the search results for 10 and 20 stages and the azeotropic compositions are slightly different from case 18. This occurs because the searches originated from different starting compositions. The amount of stages required to reach the neighborhood of the azeotrope is less for case 18 and demonstrates how the choice of starting compositions affects the calculation requirements.

B. Case studies. The computer printout results are presented here. Not all of the input data are printed out, and are listed below.

ANTOINE CONSTANTS

$\text{Log}_{10} P = A - B/(T+C)$; where P = mmHg, T = degrees C

	A	B	C
Acetone	7.0245	1161.0	224.00
Benzene	6.9050	1211.0	220.79
n-Butanol	8.2749	1873.9	230.00
2,3-Dimethylbutane	6.8098	1127.2	228.90
Ethanol	8.0449	1554.3	222.65
Methanol	7.8786	1473.1	230.00
Toluene	6.9530	1343.9	219.37
Water	7.9668	1668.2	228.00

LIQUID ENTHALPY CONSTANTS

$$HL(BTU/lb) = A + B*T + C*T^2 + D*T^3; \quad T = \text{degrees C}$$

	A	B	C	D
Acetone	0.0	0.7	0.0	0.0
Benzene	0.0	.722	$.4x10^{-3}$	$.3x10^{-5}$
n-Butanol	0.0	.9033	.00247	0.0
2,3-Dimethylbutane	0.0	0.6	0.0	0.0
Ethanol	0.0	.9574	$.158x10^{-4}$	$.116x10^{-6}$
Methanol	0.0	0.7	0.0	0.0
Toluene	0.0	.619	.00084	0.0
Water	0.0	1.7973	$-.9249x10^{-4}$	$.1308x10^{-5}$

(The Acetone, Methanol, and 2,3Dimethylbutane values are fictitious since the ternary azeotrope was being calculated and energy balances were not required but were always done by the program.)

VAPOR ENTHALPY CONSTANTS

$$HV(BTU/lb) = A + B*T + C*T^2 + D*T^3$$

	A	B	C	D
Acetone	275.0	.4	0.0	0.0
Benzene	194.8	.3683	.001125	$-.2083\text{x}10^{-5}$
n-Butanol	318.0	.5353	-.00083	$.167\text{x}10^{-4}$
2,3-Dimethylbutane	250.0	.4	0.0	0.0
Ethanol	410.9	.4925	$.825\text{x}10^{-4}$	$.2396\text{x}10^{-6}$
Methanol	300.0	.4	0.0	0.0
Toluene	191.0	.3984	.00031	$.29\text{x}10^{-4}$
Water	1075.0	.7795	.000243	$-.503\text{x}10^{-5}$

MOLAR VOLUMES (cc/mol)

Acetone	76.826
Benzene	92.260
n-Butanol	97.800
2,3-Dimethylbutane	132.060
Ethanol	64.370
Methanol	44.875
Water	18.844

WILSON MATRICES (g = cal/gmol)

Benzene = 1

g_{11} = 0.0
g_{21} = 817.67

Butanol = 2

g_{12} = 160.12
g_{22} = 0.0

Ethanol = 1

g_{11} = 0.0
g_{22} = 955.45

Water = 2

g_{12} = 382.3
g_{22} = 0.0

Methanol = 1

g_{11} = 0.0
g_{21} = 214.95
9_{31} = 449.08

Acetone = 2

g_{12} = 664.08
g_{22} = 0.0
g_{32} = 234.96

2,3-Dimethylbutane = 3

g_{13} = 2771.85
g_{23} = 948.29
g_{33} = 0.0

NOMENCLATURE

A(I)	constant in the Antoine equation
ACT(I)	activity coefficient of component I
B	bottom molar rate or flow
B(I)	constant in the Antoine equation
C(I)	constant in the Antoine equation
D	molar rate or moles of distillate
DP	pressure drop on a stage
Ed	distillate mole fraction sum of high boiling components
Ex	partial condenser liquid mole fraction sum of high boiling components
Ey	partial condenser inlet vapor mole fraction sum of high boiling components
F	molar rate or moles of feed
FX(I)	mole fraction of component I in feed
HF(I)	molar enthalpy of component I in feed
HL(J,I)	molar liquid enthalpy of component I on Stage J
HV(J,I)	molar vapor enthalpy of component I on Stage J
I	component designation
J	stage designation
K	ratio of a component's vapor and liquid compositions on a stage
L(J)	molar liquid rate or moles of liquid from Stage J
NF	logical variable equal to 1.0 on feed stage, zero elsewhere

PP(I)	partial pressure of component I
SP(J)	pressure on Stage J
SX(J)	sum of the liquid mole fractions on Stage J
SY(J)	sum of the vapor mole fractions on Stage J
T(J)	temperature on Stage J
V(J)	molar vapor rate or moles of vapor from Stage J
VP(I)	vapor pressure of component I
XD(I)	mole fraction of component I in vapor distillate
X(D,I)	mole fraction of component I in distillate
X(J,I)	mole fraction of component I in liquid on Stage J
Y(J,I)	mole fraction of component I in vapor from Stage J

BIBLIOGRAPHY

1. Edmister, W.C., Ind. Eng. Chem., 35, 837 (1943)
2. Edmister, W.C., Trans. A.I.Ch.E., 42, 15 (1946)
3. Edmister, W.C., Chem. Eng. Progr., 44, 615 (1948)
4. Edmister, W.C., A.I.Ch.E.J., 3, No. 2, 171 (1957)
5. Holms, M.J., Van Winkle, Matthew, Ind. Eng. Chem., 62, No. 1, 21 (1970)
6. Willock, J.M., Van Winkle, Matthew, J. Chem. Eng. Data, 15, No. 2, 281 (1970)

```
                    CASE 1 10/31/72 R M C



                                                  FLOW LEAVING STAGE(MOLS)
STAGE       PRESSURE        TEMPERATURE          LIQUID       VAPOR

  1           768.6            111.0               2.5        12.0
  2           768.6            110.9              14.5        12.0
  3           768.6            110.8              14.5        12.0
  4           768.6            110.7              14.5        12.1
  5           768.6            110.3              14.6        12.1
  6           768.6            109.6              14.6        12.2
  7           768.6            108.4              14.7        12.5
  8           768.6            106.3              15.0        12.8
  9           768.6            103.1              15.3        13.4
 10           768.6             98.9              15.9        14.1
 11           768.6             94.5              16.6        14.8
 12           768.6             90.8              17.3        15.3
 13           768.6             88.3              17.8        15.7
 14           768.6             86.8              18.2        15.9
 15           768.6             86.0              18.4        16.0
 16           768.6             85.6              18.5        15.2
 17           768.6             85.1               7.7        15.3
 18           768.6             84.5               7.8        15.4
 19           768.6             83.9               7.9        15.4
 20           768.6             83.3               7.9        15.5
 21           768.6             82.8               8.0        15.6
 22           768.6             82.3               8.1        15.6
 23           768.6             81.9               8.1        15.7
 24           768.6             81.5               8.2        15.7
 25           768.6             81.3               8.2        15.7
 26           768.6             81.1               8.2        15.8
 27           768.6             80.9               8.3        15.8
 28           768.6             80.8               8.3        15.8
 29           768.6             80.7               8.3        15.8
 30           768.6             80.6               8.3        15.8
 31           768.6             80.6               8.3         9.9
 32           768.6             80.6               2.4         7.5
```

```
                         CASE 1 10/31/72 R M C


STAGE  LIQUID MOL FRACTIONS  VAPOR MOL FRACTIONS   SUM Y

          BENZEN    TOLUOL        BENZEN    TOLUOL

  1       0.0010    0.9990        0.0023    0.9977    1.0000
  2       0.0021    0.9979        0.0049    0.9951    1.0000
  3       0.0043    0.9957        0.0099    0.9901    1.0000
  4       0.0084    0.9916        0.0195    0.9805    1.0000
  5       0.0163    0.9837        0.0375    0.9625    1.0000
  6       0.0313    0.9687        0.0707    0.9293    1.0001
  7       0.0589    0.9411        0.1289    0.8711    1.0002
  8       0.1075    0.8925        0.2227    0.7773    1.0004
  9       0.1867    0.8133        0.3554    0.6446    1.0008
 10       0.2997    0.7003        0.5103    0.4897    1.0010
 11       0.4337    0.5663        0.6542    0.3458    1.0006
 12       0.5599    0.4401        0.7609    0.2391    1.0001
 13       0.6545    0.3455        0.8270    0.1730    0.9998
 14       0.7136    0.2864        0.8634    0.1366    0.9995
 15       0.7462    0.2538        0.8821    0.1179    0.9995
 16       0.7630    0.2370        0.8913    0.1087    0.9996
 17       0.7870    0.2130        0.9041    0.0959    0.9994
 18       0.8129    0.1871        0.9175    0.0825    1.0005
 19       0.8397    0.1603        0.9307    0.0693    1.0000
 20       0.8662    0.1338        0.9433    0.0567    1.0000
 21       0.8911    0.1089        0.9547    0.0453    1.0000
 22       0.9135    0.0865        0.9646    0.0354    1.0000
 23       0.9328    0.0672        0.9728    0.0272    1.0000
 24       0.9488    0.0512        0.9796    0.0204    1.0000
 25       0.9618    0.0382        0.9849    0.0151    1.0000
 26       0.9720    0.0280        0.9890    0.0110    1.0000
 27       0.9800    0.0200        0.9922    0.0078    1.0000
 28       0.9860    0.0140        0.9945    0.0055    1.0000
 29       0.9905    0.0095        0.9963    0.0037    0.9991
 30       0.9939    0.0061        0.9976    0.0024    1.0000
 31       0.9964    0.0036        0.9986    0.0014    1.0004
 32       0.9974    0.0026        0.9990    0.0010    1.0004
```

```
                        CASE 1 10/31/72 R M C


   FEED STREAM  10.00 MOLS   70.00 DEG C  FEED STAGE  16

   BENZEN MOL FRACTION 0.7500   TOLUOL MOL FRACTION 0.2500

   DISTILLATE   7.50 MOLS   80.6 DEG C

   BENZEN MOL FRACTION 0.9990   TOLUOL MOL FRACTION 0.0010

   BOTTOMS       2.49 MOLS  111.0 DEG C

   BENZEN MOL FRACTION 0.0010   TOLUOL MOL FRACTION 0.9990

   HEAT BALANCE
   REBOILER         220628.  DISTILLATE ENTHALPY    135259.

   FEED ENTHALPY     42288.  BOTTOMS    ENTHALPY     18174.

                             PARTIAL CONDENSER     31486.

                             PARALLEL CONDENSER     77997.

   HEAT INPUT       262916.  HEAT OUTPUT           262916.

CPU:   20.7

READY
```

```
                              CASE 2 11/5/76  R M C



                                                    FLOW LEAVING STAGE(MOLS)
 STAGE        PRESSURE        TEMPERATURE          LIQUID        VAPOR

   1           768.64           111.00               2.49        15.00
   2           768.64           110.95              17.49        15.01
   3           768.64           110.84              17.51        15.03
   4           768.64           110.62              17.53        15.08
   5           768.64           110.20              17.57        15.17
   6           768.64           109.38              17.67        15.35
   7           768.64           107.88              17.85        15.68
   8           768.64           105.33              18.18        16.25
   9           768.64           101.48              18.75        17.09
  10           768.64            96.79              19.58        18.06
  11           768.64            92.20              20.56        18.94
  12           768.64            88.72              21.44        19.55
  13           768.64            86.57              22.05        19.91
  14           768.64            85.40              22.40        19.31
  15           768.64            84.04              11.81        19.52
  16           768.64            82.99              12.01        19.68
  17           768.64            82.14              12.17        19.80
  18           768.64            81.56              12.29        19.88
  19           768.64            81.16              12.37        19.93
  20           768.64            80.91              12.43        19.97
  21           768.64            80.75              12.47        19.99
  22           768.64            80.64              12.49        20.01
  23           768.64            80.58              12.51         9.95
  24           768.64            80.56               2.44         7.50
```

```
                    CASE 2 11/5/72  R M C


STAGE  LIQUID MOL FRACTIONS  VAPOR MOL FRACTIONS   SUM Y

          BENZEN    TOLUOL       BENZEN   TOLUOL

  1       0.0010    0.9990       0.0023   0.9977   1.0000
  2       0.0022    0.9978       0.0050   0.9950   1.0000
  3       0.0045    0.9955       0.0104   0.9896   1.0000
  4       0.0091    0.9909       0.0210   0.9790   1.0000
  5       0.0182    0.9818       0.0417   0.9583   1.0000
  6       0.0359    0.9641       0.0807   0.9193   1.0001
  7       0.0695    0.9305       0.1503   0.8497   1.0002
  8       0.1298    0.8702       0.2624   0.7376   1.0006
  9       0.2276    0.7724       0.4158   0.5842   1.0000
 10       0.3629    0.6371       0.5828   0.4172   1.0009
 11       0.5122    0.4878       0.7233   0.2767   1.0004
 12       0.6392    0.3608       0.8170   0.1830   1.0001
 13       0.7247    0.2753       0.8698   0.1302   0.9998
 14       0.7731    0.2269       0.8968   0.1032   0.9996
 15       0.8318    0.1682       0.9268   0.0732   0.9991
 16       0.8818    0.1182       0.9505   0.0495   1.0005
 17       0.9205    0.0795       0.9676   0.0324   0.9999
 18       0.9484    0.0516       0.9794   0.0206   1.0000
 19       0.9675    0.0325       0.9872   0.0128   1.0000
 20       0.9801    0.0199       0.9922   0.0078   1.0000
 21       0.9881    0.0119       0.9954   0.0046   1.0000
 22       0.9932    0.0068       0.9974   0.0026   1.0000
 23       0.9964    0.0036       0.9986   0.0014   1.0000
 24       0.9974    0.0026       0.9990   0.0010   0.9993
```

```
                          CASE 2 11/5/72  R M C


FEED STREAM  10.00 MOLS   70.00 DEG C  FEED STAGE  14

 BENZENMOL FRACTION 0.7500    TOLUOLMOL FRACTION 0.2500

DISTILLATE   7.50 MOLS   80.6 DEG C

 BENZENMOL FRACTION 0.9990    TOLUOLMOL FRACTION 0.0010

BOTTOMS        2.49 MOLS  111.0 DEG C

 BENZENMOL FRACTION 0.0010    TOLUOLMOL FRACTION 0.9990

HEAT BALANCE
REBOILER          275785.  DISTILLATE ENTHALPY     135260.

FEED ENTHALPY      42288.  BOTTOMS     ENTHALPY     18174.

                             PARTIAL CONDENSER      32175.

                            PARALLEL CONDENSER     132464.

HEAT INPUT        318073.  HEAT OUTPUT             318073.
```

```
CPU:    21.2
```

```
                         CASE  3 11/ 5/72 R M C



                                                FLOW LEAVING STAGE(MOLS)
STAGE      PRESSURE      TEMPERATURE        LIQUID      VAPOR

  1         768.64         111.00             2.49      50.00
  2         768.64         110.94            52.49      50.04
  3         768.64         110.81            52.54      50.13
  4         768.64         110.51            52.63      50.35
  5         768.64         109.87            52.84      50.82
  6         768.64         108.54            53.31      51.81
  7         768.64         105.96            54.30      53.74
  8         768.64         101.57            56.23      56.96
  9         768.64          95.71            59.46      61.05
 10         768.64          89.96            63.55      64.70
 11         768.64          85.85            67.19      66.25
 12         768.64          83.17            58.75      67.64
 13         768.64          81.75            60.13      68.34
 14         768.64          81.06            60.83      68.67
 15         768.64          80.75            61.17      68.82
 16         768.64          80.61            61.32      18.31
 17         768.64          80.55            10.81       7.50
STAGE   LIQUID MOL  FRACTIONS   VAPOR MOL  FRACTIONS     SUM Y

  1       0.0010     0.9990        0.0023     0.9977    1.0000
  2       0.0023     0.9977        0.0053     0.9947    1.0000
  3       0.0051     0.9949        0.0119     0.9881    1.0000
  4       0.0114     0.9886        0.0264     0.9736    1.0000
  5       0.0252     0.9748        0.0573     0.9427    1.0000
  6       0.0547     0.9453        0.1203     0.8797    1.0002
  7       0.1148     0.8852        0.2359     0.7641    1.0006
  8       0.2254     0.7746        0.4126     0.5874    1.0002
  9       0.3954     0.6046        0.6167     0.3833    1.0000
 10       0.5925     0.4075        0.7849     0.2151    1.0003
 11       0.7558     0.2442        0.8874     0.1126    1.0008
 12       0.8731     0.1269        0.9465     0.0535    1.0004
 13       0.9399     0.0601        0.9759     0.0241    1.0006
 14       0.9730     0.0270        0.9894     0.0106    1.0002
 15       0.9882     0.0118        0.9954     0.0046    1.0000
 16       0.9950     0.0050        0.9981     0.0019    1.0000
 17       0.9974     0.0026        0.9990     0.0010    1.0000
          BENZEN     TOLOUL        BENZEN     TOLOUL
```

```
                    CASE  3 11/ 5/72 R M C


FEED STREAM 10.000 MOLS  70.000 DEG C  FEED STAGE  11

BENZEN MOL FRACTION 0.7500   TOLOUL MOL FRACTION 0.2500

DISTILLATE  7.505 MOLS   80.5 DEG C

BENZEN MOL FRACTION 0.9990   TOLOUL MOL FRACTION 0.0010

BOTTOMS      2.495 MOLS  111.0 DEG C

BENZEN MOL FRACTION 0.0010   TOLOUL MOL FRACTION 0.9990

HEAT BALANCE
REBOILER         919284.  DISTILLATE ENTHALPY    135257.

FEED ENTHALPY     42288.  BOTTOMS    ENTHALPY     18174.

                            PARTIAL CONDENSER    142307.

                           PARALLEL CONDENSER    665833.

HEAT INPUT       961572.  HEAT OUTPUT            961572.
```

```
CPU:   18.8

READY
```

```
                         CASE  4 11/ 5/72 R M C



                                                  FLOW LEAVING STAGE(MOLS)
STAGE      PRESSURE       TEMPERATURE        LIQUID       VAPOR

  1         768.64          111.00              2.49       20.00
  2         768.64          110.94             22.49       20.02
  3         768.64          110.83             22.51       20.05
  4         768.64          110.59             22.54       20.12
  5         768.64          110.10             22.61       20.26
  6         768.64          109.13             22.76       20.55
  7         768.64          107.31             23.04       21.09
  8         768.64          104.22             23.58       22.00
  9         768.64           99.67             24.50       23.31
 10         768.64           94.46             25.80       24.71
 11         768.64           89.85             27.21       25.84
 12         768.64           86.73             28.34       26.54
 13         768.64           84.98             29.04       26.14
 14         768.64           83.22             18.63       26.49
 15         768.64           82.10             18.98       26.71
 16         768.64           81.38             19.20       26.85
 17         768.64           80.98             19.34       26.92
 18         768.64           80.75             19.42       26.97
 19         768.64           80.63             19.46       26.99
 20         768.64           80.57             19.48        8.21
 21         768.64           80.56              0.70        7.50
 STAGE   LIQUID MOL  FRACTIONS   VAPOR MOL  FRACTIONS     SUM Y

            BENZEN    TOLUOL         BENZEN    TOLUOL

   1        0.0010    0.9990         0.0023    0.9977    1.0000
   2        0.0022    0.9978         0.0051    0.9949    1.0000
   3        0.0047    0.9953         0.0109    0.9891    1.0000
   4        0.0098    0.9902         0.0227    0.9773    1.0000
   5        0.0203    0.9797         0.0465    0.9535    1.0000
   6        0.0415    0.9585         0.0926    0.9074    1.0001
   7        0.0827    0.9173         0.1760    0.8240    1.0003
   8        0.1575    0.8425         0.3092    0.6908    1.0008
   9        0.2778    0.7222         0.4830    0.5170    1.0001
  10        0.4364    0.5636         0.6567    0.3433    1.0008
  11        0.5966    0.4034         0.7878    0.2122    1.0003
  12        0.7185    0.2815         0.8663    0.1337    1.0003
  13        0.7919    0.2081         0.9067    0.0933    0.9999
  14        0.8695    0.1305         0.9448    0.0552    0.9995
  15        0.9234    0.0766         0.9689    0.0311    1.0007
  16        0.9571    0.0429         0.9830    0.0170    1.0000
  17        0.9767    0.0233         0.9909    0.0091    1.0000
  18        0.9878    0.0122         0.9952    0.0048    1.0000
  19        0.9938    0.0062         0.9976    0.0024    1.0000
  20        0.9971    0.0029         0.9989    0.0011    1.0000
  21        0.9974    0.0026         0.9990    0.0010    0.9991
```

```
                         CASE  4 11/ 5/72 R M C


          FEED STREAM 10.000 MOLS  70.000 DEG C  FEED STAGE  13

          BENZEN MOL FRACTION 0.7500   TOLUOL MOL FRACTION 0.2500

          DISTILLATE  7.505 MOLS   80.6 DEG C

          BENZEN MOL FRACTION 0.9990   TOLUOL MOL FRACTION 0.0010

          BOTTOMS      2.495 MOLS  111.0 DEG C

          BENZEN MOL FRACTION 0.0010   TOLUOL MOL FRACTION 0.9990

          HEAT BALANCE
          REBOILER         367714.  DISTILLATE ENTHALPY    135260.

          FEED ENTHALPY     42288.  BOTTOMS    ENTHALPY     18174.

                                      PARTIAL CONDENSER      9262.

                                     PARALLEL CONDENSER    247305.

          HEAT INPUT       410001.  HEAT OUTPUT            410001.




























      CPU:   19.8

      READY
```

```
                         CASE 5  11/ 5/72 R M C



                                                     FLOW LEAVING STAGE(MOLS)
STAGE       PRESSURE        TEMPERATURE          LIQUID        VAPOR

  1          768.64           111.00               2.49         30.00
  2          768.64           110.94              32.49         30.02
  3          768.64           110.82              32.52         30.08
  4          768.64           110.55              32.57         30.19
  5          768.64           109.98              32.69         30.44
  6          768.64           108.83              32.94         30.96
  7          768.64           106.62              33.45         31.94
  8          768.64           102.84              34.43         33.61
  9          768.64            97.57              36.11         35.86
 10          768.64            91.98              38.35         38.05
 11          768.64            87.57              40.54         39.60
 12          768.64            84.87              42.09         39.69
 13          768.64            82.83              32.19         40.31
 14          768.64            81.69              32.81         40.65
 15          768.64            81.08              33.14         40.82
 16          768.64            80.77              33.32         40.91
 17          768.64            80.63              33.40         40.95
 18          768.64            80.56              33.45          7.63
 19          768.64            80.53               0.12          7.50
STAGE   LIQUID MOL  FRACTIONS   VAPOR MOL  FRACTIONS      SUM Y

           BENZEN     TOLUOL          BENZEN     TOLUOL

  1        0.0010     0.9990          0.0023     0.9977     1.0000
  2        0.0022     0.9978          0.0052     0.9948     1.0000
  3        0.0049     0.9951          0.0115     0.9885     1.0000
  4        0.0107     0.9893          0.0247     0.9753     1.0000
  5        0.0228     0.9772          0.0521     0.9479     1.0000
  6        0.0482     0.9518          0.1068     0.8932     1.0001
  7        0.0989     0.9011          0.2069     0.7931     1.0004
  8        0.1920     0.8080          0.3635     0.6365     1.0000
  9        0.3385     0.6615          0.5558     0.4442     1.0001
 10        0.5197     0.4803          0.7294     0.2706     1.0005
 11        0.6846     0.3154          0.8460     0.1540     1.0004
 12        0.7959     0.2041          0.9088     0.0912     0.9995
 13        0.8877     0.1123          0.9532     0.0468     0.9996
 14        0.9427     0.0573          0.9770     0.0230     1.0004
 15        0.9720     0.0280          0.9890     0.0110     1.0001
 16        0.9868     0.0132          0.9949     0.0051     1.0000
 17        0.9939     0.0061          0.9976     0.0024     1.0000
 18        0.9973     0.0027          0.9990     0.0010     1.0000
 19        0.9974     0.0026          0.9990     0.0010     1.0000
```

```
                         CASE 5  11/ 5/72 R M C


      FEED STREAM 10.000 MOLS  70.000 DEG C  FEED STAGE  12

      BENZEN MOL FRACTION 0.7500   TOLUOL MOL FRACTION 0.2500

      DISTILLATE  7.505 MOLS   80.5 DEG C

      BENZEN MOL FRACTION 0.9990   TOLUOL MOL FRACTION 0.0010

      BOTTOMS      2.495 MOLS  111.0 DEG C

      BENZEN MOL FRACTION 0.0010   TOLUOL MOL FRACTION 0.9990

      HEAT BALANCE
      REBOILER          551570.  DISTILLATE ENTHALPY    135251.

      FEED ENTHALPY      42288.  BOTTOMS    ENTHALPY     18174.

                                   PARTIAL CONDENSER      1642.

                                  PARALLEL CONDENSER    438791.

      HEAT INPUT        593858.  HEAT OUTPUT            593858.




















  CPU:   19.0

  READY
  610 V(1)=40.
  [illegible]
```

```
                     CASE 6  11/ 5/72 R M C



                                                 FLOW LEAVING STAGE(MOLS)
STAGE      PRESSURE      TEMPERATURE      LIQUID      VAPOR

  1         768.64          111.00           2.49      40.00
  2         768.64          110.94          42.49      40.03
  3         768.64          110.81          42.53      40.11
  4         768.64          110.52          42.60      40.27
  5         768.64          109.91          42.77      40.63
  6         768.64          108.65          43.12      41.38
  7         768.64          106.22          43.87      42.83
  8         768.64          102.07          45.32      45.28
  9         768.64           96.43          47.77      48.45
 10         768.64           90.72          50.94      51.38
 11         768.64           86.49          53.87      53.31
 12         768.64           84.02          55.81      53.58
 13         768.64           82.23          46.07      54.29
 14         768.64           81.32          46.79      54.65
 15         768.64           80.87          47.15      54.82
 16         768.64           80.67          47.32      54.91
 17         768.64           80.58          47.40       9.44
 18         768.64           80.54           1.94       7.50
 STAGE   LIQUID MOL  FRACTIONS   VAPOR MOL  FRACTIONS    SUM Y

            BENZEN    TOLUOL        BENZEN    TOLUOL

  1         0.0010    0.9990        0.0023    0.9977    1.0000
  2         0.0023    0.9977        0.0053    0.9947    1.0000
  3         0.0050    0.9950        0.0118    0.9882    1.0000
  4         0.0111    0.9889        0.0257    0.9743    1.0000
  5         0.0243    0.9757        0.0553    0.9447    1.0000
  6         0.0522    0.9478        0.1150    0.8850    1.0002
  7         0.1085    0.8915        0.2245    0.7755    1.0005
  8         0.2122    0.7878        0.3936    0.6064    1.0001
  9         0.3731    0.6269        0.5937    0.4063    1.0001
 10         0.5647    0.4353        0.7645    0.2355    1.0003
 11         0.7291    0.2709        0.8724    0.1276    1.0006
 12         0.8334    0.1666        0.9276    0.0724    0.9995
 13         0.9160    0.0840        0.9657    0.0343    0.9999
 14         0.9603    0.0397        0.9843    0.0157    1.0003
 15         0.9819    0.0181        0.9930    0.0070    1.0001
 16         0.9920    0.0080        0.9969    0.0031    1.0000
 17         0.9966    0.0034        0.9987    0.0013    1.0000
 18         0.9974    0.0026        0.9990    0.0010    1.0000
```

```
                        CASE 6  11/ 5/72 R M C


    FEED STREAM 10.000 MOLS  70.000 DEG C  FEED STAGE  12

    BENZEN MOL FRACTION 0.7500   TOLUOL MOL FRACTION 0.2500

    DISTILLATE  7.505 MOLS   80.5 DEG C

    BENZEN MOL FRACTION 0.9990   TOLUOL MOL FRACTION 0.0010

    BOTTOMS      2.495 MOLS  111.0 DEG C

    BENZEN MOL FRACTION 0.0010   TOLUOL MOL FRACTION 0.9990

    HEAT BALANCE
    REBOILER          735427.  DISTILLATE ENTHALPY    135253.

    FEED ENTHALPY      42288.  BOTTOMS    ENTHALPY     18174.

                                 PARTIAL CONDENSER     25541.

                                PARALLEL CONDENSER    598747.

    HEAT INPUT        777715.  HEAT OUTPUT            777715.
















CPU:   18.8

READY
```

```
                         CASE  7 11/28/72 R M C



                                                        FLOW LEAVING STAGE(MOLS)
STAGE      PRESSURE      TEMPERATURE      LIQUID      VAPOR

  1         300.00          93.03            2.49      200.00
  2         300.00          91.63          202.49      196.19
  3         300.00          82.20          198.68      209.55
  4         300.00          61.08          212.04      261.31
  5         300.00          54.39          263.80      278.94
  6         300.00          53.32          271.43      283.81
  7         300.00          53.01          276.31      285.90
  8         300.00          52.88          278.39      287.03
  9         300.00          52.81          279.52      287.68
 10         300.00          52.77          280.18      288.06
 11         300.00          52.73          280.56      288.36
 12         300.00          52.73          280.85      288.54
 13         300.00          52.73          281.04       15.46
 14         300.00          52.73            7.95        7.50
STAGE   LIQUID MOL  FRACTIONS   VAPOR MOL  FRACTIONS    SUM Y

           BENZEN    N-BUOH        BENZEN    N-BUOH

  1        0.0010    0.9990        0.0087    0.9913    1.0004
  2        0.0086    0.9914        0.0716    0.9284    1.0000
  3        0.0708    0.9292        0.4178    0.5822    0.9999
  4        0.4129    0.5871        0.8459    0.1541    1.0005
  5        0.8379    0.1621        0.9408    0.0592    1.0006
  6        0.9392    0.0608        0.9697    0.0303    1.0001
  7        0.9689    0.0311        0.9824    0.0176    1.0003
  8        0.9820    0.0180        0.9892    0.0108    1.0000
  9        0.9889    0.0111        0.9931    0.0069    1.0000
 10        0.9930    0.0070        0.9955    0.0045    1.0000
 11        0.9954    0.0046        0.9971    0.0029    0.9994
 12        0.9970    0.0030        0.9981    0.0019    1.0000
 13        0.9980    0.0020        0.9987    0.0013    1.0004
 14        0.9985    0.0015        0.9990    0.0010    1.0006
```

```
                              CASE  7 11/28/72 R M C



    FEED STREAM 10.000 MOLS   70.00 DEG C  FEED STAGE   5

    BENZEN MOL FRACTION 0.7500   N-BUOH MOL FRACTION 0.2500

    DISTILLATE  7.505 MOLS   52.73 DEG C

    BENZEN MOL FRACTION 0.9990   N-BUOH MOL FRACTION 0.0010

    BOTTOMS      2.495 MOLS   93.03 DEG C

    BENZEN MOL FRACTION 0.0010   N-BUOH MOL FRACTION 0.9990

    HEAT BALANCE
    REBOILER        3998686.  DISTILLATE ENTHALPY    127300.

    FEED ENTHALPY     45318.  BOTTOMS    ENTHALPY     19489.

                                PARTIAL CONDENSER    110319.

                               PARALLEL CONDENSER   3786896.

    HEAT INPUT      4044004.  HEAT OUTPUT           4044004.
```

```
CPU:    18.8
```

```
                        CASE  8 11/28/72 R M C



                                                    FLOW LEAVING STAGE(MOLS)
STAGE      PRESSURE        TEMPERATURE        LIQUID       VAPOR

  1         760.00          117.25              2.49       200.00
  2         760.00          116.50            202.49       198.10
  3         760.00          112.26            200.59       197.90
  4         760.00           97.72            200.40       230.25
  5         760.00           84.43            232.74       265.07
  6         760.00           81.40            267.56       275.40
  7         760.00           80.71            267.90       279.85
  8         760.00           80.47            272.34       282.14
  9         760.00           80.36            274.64       283.56
 10         760.00           80.30            276.05       284.50
 11         760.00           80.23            276.99       285.23
 12         760.00           80.23            277.73       285.76
 13         760.00           80.23            278.25       286.18
 14         760.00           80.23            278.68       286.45
 15         760.00           80.19            278.95       286.70
 16         760.00           80.15            279.19       286.94
 17         760.00           80.18            279.44       287.14
 18         760.00           80.20            279.64       287.26
 19         760.00           80.17            279.75       287.37
 20         760.00           80.14            279.87       287.53
 21         760.00           80.16            280.02       287.65
 22         760.00           80.19            280.15       287.70
 23         760.00           80.16            280.19       287.74
 24         760.00           80.13            280.24       287.85
 25         760.00           80.15            280.34       287.95
 26         760.00           80.18            280.45       287.97
 27         760.00           80.15            280.47       287.99
 28         760.00           80.12            280.48       288.07
 29         760.00           80.15            280.57       288.15
 30         760.00           80.18            280.65       288.15
 31         760.00           80.15            280.64       288.15
 32         760.00           80.12            280.64       288.21
 33         760.00           80.15            280.71       288.28
 34         760.00           80.17            280.77       288.27
 35         760.00           80.14            280.76         8.11
 36         760.00           80.12              0.60         7.50
```

```
                    CASE  8 11/28/72 R M C



STAGE  LIQUID MOL FRACTIONS  VAPOR MOL FRACTIONS    SUM Y

          BENZEN    N-BUOH      BENZEN    N-BUOH

  1       0.0010    0.9990      0.0063    0.9937    1.0001
  2       0.0062    0.9938      0.0380    0.9620    1.0004
  3       0.0376    0.9624      0.2006    0.7994    1.0001
  4       0.1981    0.8019      0.6094    0.3906    1.0001
  5       0.6029    0.3971      0.8516    0.1484    1.0005
  6       0.8437    0.1563      0.9183    0.0817    1.0000
  7       0.9160    0.0840      0.9464    0.0536    1.0000
  8       0.9449    0.0551      0.9611    0.0389    1.0000
  9       0.9601    0.0399      0.9701    0.0299    1.0000
 10       0.9694    0.0306      0.9762    0.0238    1.0000
 11       0.9756    0.0244      0.9805    0.0195    0.9993
 12       0.9800    0.0200      0.9837    0.0163    1.0000
 13       0.9833    0.0167      0.9862    0.0138    1.0005
 14       0.9859    0.0141      0.9882    0.0118    1.0008
 15       0.9879    0.0121      0.9898    0.0102    1.0000
 16       0.9895    0.0105      0.9911    0.0089    0.9991
 17       0.9909    0.0091      0.9922    0.0078    1.0000
 18       0.9920    0.0080      0.9931    0.0069    1.0009
 19       0.9930    0.0070      0.9939    0.0061    1.0000
 20       0.9938    0.0062      0.9946    0.0054    0.9991
 21       0.9945    0.0055      0.9952    0.0048    1.0000
 22       0.9951    0.0049      0.9957    0.0043    1.0009
 23       0.9957    0.0043      0.9962    0.0038    1.0000
 24       0.9961    0.0039      0.9966    0.0034    0.9991
 25       0.9965    0.0035      0.9970    0.0030    1.0000
 26       0.9969    0.0031      0.9973    0.0027    1.0009
 27       0.9972    0.0028      0.9976    0.0024    1.0000
 28       0.9975    0.0025      0.9978    0.0022    0.9991
 29       0.9978    0.0022      0.9980    0.0020    1.0000
 30       0.9980    0.0020      0.9982    0.0018    1.0009
 31       0.9982    0.0018      0.9984    0.0016    1.0000
 32       0.9984    0.0016      0.9986    0.0014    0.9991
 33       0.9986    0.0014      0.9987    0.0013    1.0000
 34       0.9987    0.0013      0.9989    0.0011    1.0009
 35       0.9989    0.0011      0.9990    0.0010    1.0000
 36       0.9989    0.0011      0.9990    0.0010    0.9991
```

```
                    CASE  8 11/28/72 R M C


FEED STREAM 10.000 MOLS   70.00 DEG C  FEED STAGE   6

BENZEN MOL FRACTION 0.7500   N-BUOH MOL FRACTION 0.2500

DISTILLATE  7.505 MOLS   80.12 DEG C

BENZEN MOL FRACTION 0.9990   N-BUOH MOL FRACTION 0.0010

BOTTOMS      2.495 MOLS  117.25 DEG C

BENZEN MOL FRACTION 0.0010   N-BUOH MOL FRACTION 0.9990

HEAT BALANCE
REBOILER        3808974.  DISTILLATE ENTHALPY    135165.

FEED ENTHALPY     45318.  BOTTOMS    ENTHALPY     25860.

                            PARTIAL CONDENSER      7911.

                           PARALLEL CONDENSER   3685357.

HEAT INPUT      3854292.  HEAT OUTPUT           3854292.
```

```
                     CASE  8A 11/28/72 R M C



                                             FLOW LEAVING STAGE(MOLS)
 STAGE      PRESSURE      TEMPERATURE         LIQUID        VAPOR

   1         760.00          117.25             2.49       200.00
   2         760.00          116.49           202.49       198.11
   3         760.00          112.26           200.61       197.91
   4         760.00           97.72           200.41       230.25
   5         760.00           84.42           232.74       265.10
   6         760.00           81.40           267.59       275.42
   7         760.00           80.71           267.91       279.86
   8         760.00           80.47           272.36       282.16
   9         760.00           80.36           274.65       283.57
  10         760.00           80.30           276.06       284.54
  11         760.00           80.26           277.03       285.23
  12         760.00           80.23           277.72       285.75
  13         760.00           80.21           278.24       286.17
  14         760.00           80.20           278.66       286.50
  15         760.00           80.19           279.00       286.78
  16         760.00           80.18           279.28       287.01
  17         760.00           80.18           279.50       287.20
  18         760.00           80.17           279.69       287.35
  19         760.00           80.17           279.85       287.51
  20         760.00           80.16           280.00       287.63
  21         760.00           80.16           280.12       287.75
  22         760.00           80.16           280.24       287.87
  23         760.00           80.16           280.36       287.95
  24         760.00           80.16           280.45       288.04
  25         760.00           80.16           280.53       288.12
  26         760.00           80.15           280.62       288.21
  27         760.00           80.15           280.70       288.26
  28         760.00           80.15           280.76       288.32
  29         760.00           80.15           280.81       288.37
  30         760.00           80.15           280.87       288.43
  31         760.00           80.15           280.92       288.48
  32         760.00           80.15           280.98       288.54
  33         760.00           80.15           281.03       288.59
  34         760.00           80.15           281.09       288.65
  35         760.00           80.14           281.14         8.10
  36         760.00           80.14             0.59         7.50
```

```
                   CASE  8A 11/28/72 R M C


STAGE  LIQUID MOL FRACTIONS  VAPOR MOL FRACTIONS   SUM Y

           BENZEN   N-BUOH        BENZEN   N-BUOH

  1        0.0010   0.9990        0.0063   0.9937   1.0000
  2        0.0062   0.9938        0.0380   0.9620   1.0000
  3        0.0376   0.9624        0.2006   0.7994   1.0001
  4        0.1981   0.8019        0.6094   0.3906   1.0001
  5        0.6029   0.3971        0.8516   0.1484   1.0000
  6        0.8437   0.1563        0.9183   0.0817   1.0000
  7        0.9160   0.0840        0.9464   0.0536   1.0000
  8        0.9449   0.0551        0.9611   0.0389   1.0000
  9        0.9601   0.0399        0.9701   0.0299   1.0000
 10        0.9694   0.0306        0.9762   0.0238   1.0000
 11        0.9756   0.0244        0.9805   0.0195   1.0000
 12        0.9800   0.0200        0.9837   0.0163   1.0000
 13        0.9833   0.0167        0.9862   0.0138   1.0000
 14        0.9859   0.0141        0.9882   0.0118   1.0000
 15        0.9879   0.0121        0.9898   0.0102   0.9999
 16        0.9895   0.0105        0.9911   0.0089   1.0000
 17        0.9909   0.0091        0.9922   0.0078   1.0000
 18        0.9920   0.0080        0.9931   0.0069   1.0001
 19        0.9930   0.0070        0.9939   0.0061   1.0000
 20        0.9938   0.0062        0.9946   0.0054   1.0000
 21        0.9945   0.0055        0.9952   0.0048   1.0000
 22        0.9951   0.0049        0.9957   0.0043   1.0000
 23        0.9957   0.0043        0.9962   0.0038   1.0000
 24        0.9961   0.0039        0.9966   0.0034   1.0001
 25        0.9965   0.0035        0.9970   0.0030   1.0001
 26        0.9969   0.0031        0.9973   0.0027   1.0001
 27        0.9972   0.0028        0.9976   0.0024   1.0001
 28        0.9975   0.0025        0.9978   0.0022   1.0001
 29        0.9978   0.0022        0.9980   0.0020   1.0001
 30        0.9980   0.0020        0.9982   0.0018   1.0001
 31        0.9982   0.0018        0.9984   0.0016   1.0001
 32        0.9984   0.0016        0.9986   0.0014   1.0001
 33        0.9986   0.0014        0.9987   0.0013   1.0000
 34        0.9987   0.0013        0.9989   0.0011   1.0000
 35        0.9989   0.0011        0.9990   0.0010   1.0000
 36        0.9989   0.0011        0.9990   0.0010   1.0000
```

```
                    CASE  9 11/28/72 R M C



                                              FLOW LEAVING STAGE(MOLS)
STAGE      PRESSURE       TEMPERATURE        LIQUID       VAPOR

  1         760.00          117.25             2.49       100.00
  2         760.00          116.51           102.49        99.05
  3         760.00          112.36           101.55        98.84
  4         760.00           98.11           101.33       114.44
  5         760.00           84.68           116.93       131.91
  6         760.00           81.53           134.41       136.78
  7         760.00           80.77           129.28       139.07
  8         760.00           80.51           131.57       140.24
  9         760.00           80.38           132.74       140.96
 10         760.00           80.32           133.46       141.44
 11         760.00           80.25           133.93       141.82
 12         760.00           80.25           134.31       142.08
 13         760.00           80.25           134.58       142.30
 14         760.00           80.24           134.79       142.44
 15         760.00           80.20           134.93       142.58
 16         760.00           80.16           135.08       142.72
 17         760.00           80.19           135.22       142.83
 18         760.00           80.21           135.32       142.89
 19         760.00           80.18           135.39       142.95
 20         760.00           80.14           135.45       143.04
 21         760.00           80.17           135.53       143.10
 22         760.00           80.20           135.60       143.13
 23         760.00           80.16           135.62       143.16
 24         760.00           80.13           135.65       143.21
 25         760.00           80.16           135.71       143.27
 26         760.00           80.19           135.77       143.28
 27         760.00           80.16           135.78       143.30
 28         760.00           80.12           135.79       143.34
 29         760.00           80.15           135.84       143.39
 30         760.00           80.18           135.88       143.39
 31         760.00           80.15           135.89       143.39
 32         760.00           80.12           135.89       143.43
 33         760.00           80.15           135.93       143.47
 34         760.00           80.18           135.96       143.46
 35         760.00           80.15           135.96       143.46
 36         760.00           80.12           135.96       143.49
 37         760.00           80.15           135.99       143.53
 38         760.00           80.18           136.02       143.52
 39         760.00           80.14           136.01        49.02
 40         760.00           80.11            41.52         7.50
```

```
                    CASE  9 11/28/72 R M C



STAGE  LIQUID MOL FRACTIONS  VAPOR MOL FRACTIONS    SUM Y

          BENZEN   N-BUOH       BENZEN   N-BUOH

  1       0.0010   0.9990       0.0063   0.9937   1.0001
  2       0.0062   0.9938       0.0377   0.9623   1.0003
  3       0.0368   0.9632       0.1969   0.8031   1.0000
  4       0.1921   0.8079       0.6010   0.3990   1.0001
  5       0.5882   0.4118       0.8474   0.1526   1.0009
  6       0.8317   0.1683       0.9144   0.0856   1.0001
  7       0.9095   0.0905       0.9434   0.0566   0.9999
  8       0.9402   0.0598       0.9585   0.0415   1.0000
  9       0.9562   0.0438       0.9678   0.0322   1.0000
 10       0.9660   0.0340       0.9739   0.0261   1.0000
 11       0.9725   0.0275       0.9784   0.0216   0.9992
 12       0.9772   0.0228       0.9817   0.0183   1.0000
 13       0.9807   0.0193       0.9842   0.0158   1.0005
 14       0.9834   0.0166       0.9863   0.0137   1.0009
 15       0.9856   0.0144       0.9880   0.0120   1.0000
 16       0.9874   0.0126       0.9894   0.0106   0.9990
 17       0.9888   0.0112       0.9905   0.0095   1.0000
 18       0.9901   0.0099       0.9915   0.0085   1.0009
 19       0.9911   0.0089       0.9924   0.0076   1.0000
 20       0.9920   0.0080       0.9932   0.0068   0.9991
 21       0.9928   0.0072       0.9938   0.0062   1.0000
 22       0.9935   0.0065       0.9944   0.0056   1.0009
 23       0.9941   0.0059       0.9949   0.0051   1.0000
 24       0.9947   0.0053       0.9954   0.0046   0.9991
 25       0.9952   0.0048       0.9958   0.0042   1.0000
 26       0.9956   0.0044       0.9961   0.0039   1.0009
 27       0.9960   0.0040       0.9965   0.0035   1.0000
 28       0.9963   0.0037       0.9968   0.0032   0.9991
 29       0.9967   0.0033       0.9971   0.0029   1.0000
 30       0.9970   0.0030       0.9973   0.0027   1.0009
 31       0.9972   0.0028       0.9976   0.0024   1.0000
 32       0.9975   0.0025       0.9978   0.0022   0.9991
 33       0.9977   0.0023       0.9980   0.0020   1.0000
 34       0.9979   0.0021       0.9982   0.0018   1.0009
 35       0.9981   0.0019       0.9983   0.0017   1.0000
 36       0.9983   0.0017       0.9985   0.0015   0.9991
 37       0.9985   0.0015       0.9986   0.0014   1.0000
 38       0.9986   0.0014       0.9988   0.0012   1.0009
 39       0.9988   0.0012       0.9989   0.0011   1.0000
 40       0.9989   0.0011       0.9990   0.0010   0.9991
```

```
                        CASE  9 11/28/72 R M C



FEED STREAM 10.000 MOLS   70.00 DEG C  FEED STAGE   6

BENZEN MOL FRACTION 0.7500   N-BUOH MOL FRACTION 0.2500

DISTILLATE  7.505 MOLS   80.11 DEG C

BENZEN MOL FRACTION 0.9990   N-BUOH MOL FRACTION 0.0010

BOTTOMS       2.495 MOLS  117.25 DEG C

BENZEN MOL FRACTION 0.0010   N-BUOH MOL FRACTION 0.9990

HEAT BALANCE
REBOILER          1904490.  DISTILLATE ENTHALPY    135164.

FEED ENTHALPY       45318.  BOTTOMS    ENTHALPY     25860.

                              PARTIAL CONDENSER    546853.

                             PARALLEL CONDENSER   1241931.

HEAT INPUT        1949808.  HEAT OUTPUT           1949808.
























CPU:    24.3
```

```
                         CASE 10 11/28/72 R M C



                                                  FLOW LEAVING STAGE(MOLS)
STAGE       PRESSURE        TEMPERATURE          LIQUID        VAPOR

  1          760.00           117.25               2.49         70.00
  2          760.00           116.52              72.49         69.34
  3          760.00           112.45              71.84         69.12
  4          760.00            98.44              71.62         79.69
  5          760.00            84.87              82.19         91.98
  6          760.00            81.64              94.47         95.20
  7          760.00            80.82              87.70         96.84
  8          760.00            80.54              89.33         97.67
  9          760.00            80.41              90.16         98.18
 10          760.00            80.34              90.67         98.52
 11          760.00            80.27              91.01         98.78
 12          760.00            80.26              91.28         98.97
 13          760.00            80.26              91.47         99.13
 14          760.00            80.26              91.62         99.23
 15          760.00            80.21              91.72         99.32
 16          760.00            80.20              91.82         99.41
 17          760.00            80.19              91.90         99.48
 18          760.00            80.18              91.97         99.54
 19          760.00            80.18              92.03         99.60
 20          760.00            80.17              92.09         99.64
 21          760.00            80.16              92.14         99.69
 22          760.00            80.15              92.18         99.74
 23          760.00            80.17              92.23         99.78
 24          760.00            80.19              92.28         99.80
 25          760.00            80.17              92.29         99.82
 26          760.00            80.14              92.31         99.85
 27          760.00            80.16              92.35         99.89
 28          760.00            80.19              92.38         99.90
 29          760.00            80.16              92.39         99.91
 30          760.00            80.13              92.40         99.94
 31          760.00            80.16              92.43         99.96
 32          760.00            80.18              92.46         99.97
 33          760.00            80.15              92.46         99.97
 34          760.00            80.13              92.47        100.00
 35          760.00            80.15              92.49        100.02
 36          760.00            80.18              92.52        100.02
 37          760.00            80.15              92.51        100.02
 38          760.00            80.12              92.51        100.04
 39          760.00            80.15              92.54        100.06
 40          760.00            80.17              92.56        100.06
 41          760.00            80.15              92.56        100.06
 42          760.00            80.12              92.55        100.08
 43          760.00            80.15              92.57        100.10
 44          760.00            80.17              92.59        100.09
 45          760.00            80.14              92.59         55.66
 46          760.00            80.12              48.16          7.50
```

```
                    CASE 10 11/28/72 R M C



STAGE   LIQUID MOL  FRACTIONS   VAPOR MOL  FRACTIONS    SUM Y

           BENZEN    N-BUOH        BENZEN    N-BUOH

  1        0.0010    0.9990        0.0063    0.9937    1.0001
  2        0.0061    0.9939        0.0373    0.9627    1.0003
  3        0.0361    0.9639        0.1938    0.8062    1.0000
  4        0.1871    0.8129        0.5938    0.4062    1.0001
  5        0.5758    0.4242        0.8438    0.1562    1.0001
  6        0.8215    0.1785        0.9112    0.0888    1.0001
  7        0.9037    0.0963        0.9409    0.0591    0.9998
  8        0.9360    0.0640        0.9563    0.0437    1.0000
  9        0.9527    0.0473        0.9656    0.0344    1.0000
 10        0.9629    0.0371        0.9719    0.0281    1.0000
 11        0.9697    0.0303        0.9764    0.0236    0.9992
 12        0.9745    0.0255        0.9798    0.0202    1.0000
 13        0.9782    0.0218        0.9824    0.0176    1.0006
 14        0.9810    0.0190        0.9845    0.0155    1.0010
 15        0.9833    0.0167        0.9862    0.0138    1.0000
 16        0.9852    0.0148        0.9876    0.0124    1.0000
 17        0.9867    0.0133        0.9888    0.0112    0.9999
 18        0.9880    0.0120        0.9899    0.0101    0.9998
 19        0.9891    0.0109        0.9908    0.0092    0.9997
 20        0.9901    0.0099        0.9916    0.0084    0.9995
 21        0.9910    0.0090        0.9923    0.0077    0.9994
 22        0.9917    0.0083        0.9929    0.0071    0.9992
 23        0.9924    0.0076        0.9935    0.0065    1.0000
 24        0.9930    0.0070        0.9940    0.0060    1.0008
 25        0.9935    0.0065        0.9944    0.0056    1.0000
 26        0.9940    0.0060        0.9948    0.0052    0.9992
 27        0.9945    0.0055        0.9952    0.0048    1.0000
 28        0.9949    0.0051        0.9955    0.0045    1.0008
 29        0.9953    0.0047        0.9959    0.0041    1.0000
 30        0.9956    0.0044        0.9962    0.0038    0.9992
 31        0.9959    0.0041        0.9964    0.0036    1.0000
 32        0.9962    0.0038        0.9967    0.0033    1.0008
 33        0.9965    0.0035        0.9969    0.0031    1.0000
 34        0.9968    0.0032        0.9971    0.0029    0.9992
 35        0.9970    0.0030        0.9974    0.0026    1.0000
 36        0.9972    0.0028        0.9975    0.0025    1.0008
 37        0.9974    0.0026        0.9977    0.0023    1.0000
 38        0.9976    0.0024        0.9979    0.0021    0.9992
 39        0.9978    0.0022        0.9981    0.0019    1.0000
 40        0.9980    0.0020        0.9982    0.0018    1.0008
 41        0.9982    0.0018        0.9984    0.0016    1.0000
 42        0.9983    0.0017        0.9985    0.0015    0.9992
 43        0.9985    0.0015        0.9986    0.0014    1.0000
 44        0.9986    0.0014        0.9988    0.0012    1.0008
 45        0.9988    0.0012        0.9989    0.0011    1.0000
 46        0.9989    0.0011        0.9990    0.0010    0.9992
```

```
                         CASE 10 11/28/72 R M C



    FEED STREAM 10.000 MOLS   70.00 DEG C  FEED STAGE   6

    BENZEN MOL FRACTION 0.7500   N-BUOH MOL FRACTION 0.2500

    DISTILLATE  7.505 MOLS   80.12 DEG C

    BENZEN MOL FRACTION 0.9990   N-BUOH MOL FRACTION 0.0010

    BOTTOMS      2.495 MOLS  117.25 DEG C

    BENZEN MOL FRACTION 0.0010   N-BUOH MOL FRACTION 0.9990

    HEAT BALANCE
    REBOILER        1333145.  DISTILLATE ENTHALPY    135165.

    FEED ENTHALPY     45318.  BOTTOMS    ENTHALPY     25860.

                                PARTIAL CONDENSER    634309.

                               PARALLEL CONDENSER    583129.

    HEAT INPUT      1378463.  HEAT OUTPUT           1378463.
















CPU:   23.8

READY
BYE

OFF AT 21:16
```

```
                         CASE 11 11/28/72 R M C



                                                FLOW LEAVING STAGE(MOLS)
STAGE      PRESSURE      TEMPERATURE      LIQUID      VAPOR

  1         760.00         117.25           2.49      50.00
  2         760.00         116.53          52.49      49.53
  3         760.00         112.56          52.03      49.31
  4         760.00          98.86          51.81      56.54
  5         760.00          85.17          59.04      65.34
  6         760.00          81.78          67.83      67.49
  7         760.00          80.89          59.98      68.68
  8         760.00          80.59          61.17      69.28
  9         760.00          80.45          61.77      69.65
 10         760.00          80.37          62.14      69.88
 11         760.00          80.29          62.38      70.07
 12         760.00          80.29          62.57      70.21
 13         760.00          80.28          62.70      70.30
 14         760.00          80.25          62.80      70.39
 15         760.00          80.21          62.88      70.47
 16         760.00          80.22          62.96      70.53
 17         760.00          80.24          63.03      70.58
 18         760.00          80.21          63.07      70.62
 19         760.00          80.18          63.12      70.66
 20         760.00          80.20          63.16      70.70
 21         760.00          80.21          63.20      70.72
 22         760.00          80.19          63.22      70.74
 23         760.00          80.16          63.24      70.78
 24         760.00          80.18          63.27      70.81
 25         760.00          80.20          63.30      70.82
 26         760.00          80.18          63.31      70.83
 27         760.00          80.15          63.33      70.86
 28         760.00          80.17          63.35      70.88
 29         760.00          80.19          63.38      70.89
 30         760.00          80.17          63.38      70.90
 31         760.00          80.15          63.39      70.91
 32         760.00          80.17          63.41      70.93
 33         760.00          80.18          63.43      70.94
 34         760.00          80.16          63.43      70.94
 35         760.00          80.14          63.44      70.96
 36         760.00          80.16          63.45      70.98
 37         760.00          80.18          63.47      70.98
 38         760.00          80.16          63.47      70.98
 39         760.00          80.14          63.47      70.99
 40         760.00          80.16          63.49      71.01
 41         760.00          80.18          63.50      71.01
 42         760.00          80.15          63.50      71.01
 43         760.00          80.13          63.51      71.02
 44         760.00          80.15          63.52      71.04
 45         760.00          80.17          63.53      71.04
 46         760.00          80.15          63.53      71.04
 47         760.00          80.13          63.53      71.05
 48         760.00          80.15          63.54      71.06
 49         760.00          80.17          63.56      71.06
 50         760.00          80.15          63.55      71.06
```

```
                    CASE II  11/20/72

                                                     FLOW LEAVING STAGE(MOLS)
  STAGE      PRESSURE       TEMPERATURE       LIQUID       VAPOR

   51          760.00           80.13          63.55        71.07
   52          760.00           80.15          63.57        71.08
   53          760.00           80.17          63.58        71.08
   54          760.00           80.15          63.58        71.08
   55          760.00           80.13          63.57        71.09
   56          760.00           80.15          63.59        71.10
   57          760.00           80.17          63.60        71.10
   58          760.00           80.15          63.59        71.10
   59          760.00           80.12          63.59        71.11
   60          760.00           80.14          63.60         8.76
   61          760.00           80.16           1.25         7.50
```

```
                         CASE 11  11/28/72  R M C



STAGE  LIQUID MOL  FRACTIONS   VAPOR MOL  FRACTIONS    SUM Y

          BENZEN     N-BUOH        BENZEN     N-BUOH

  1       0.0010     0.9990        0.0063     0.9937     1.0001
  2       0.0060     0.9940        0.0369     0.9631     1.0003
  3       0.0352     0.9648        0.1898     0.8102     1.0000
  4       0.1807     0.8193        0.5842     0.4158     1.0001
  5       0.5596     0.4404        0.8389     0.1611     1.0005
  6       0.8080     0.1920        0.9071     0.0929     1.0003
  7       0.8957     0.1043        0.9375     0.0625     0.9997
  8       0.9299     0.0701        0.9531     0.0469     1.0000
  9       0.9475     0.0525        0.9626     0.0374     1.0000
 10       0.9582     0.0418        0.9690     0.0310     1.0000
 11       0.9653     0.0347        0.9735     0.0265     0.9991
 12       0.9705     0.0295        0.9769     0.0231     1.0000
 13       0.9743     0.0257        0.9796     0.0204     1.0006
 14       0.9773     0.0227        0.9817     0.0183     1.0000
 15       0.9797     0.0203        0.9835     0.0165     0.9993
 16       0.9816     0.0184        0.9849     0.0151     1.0000
 17       0.9833     0.0167        0.9862     0.0138     1.0007
 18       0.9846     0.0154        0.9872     0.0128     1.0000
 19       0.9858     0.0142        0.9882     0.0118     0.9993
 20       0.9869     0.0131        0.9890     0.0110     1.0000
 21       0.9878     0.0122        0.9897     0.0103     1.0007
 22       0.9886     0.0114        0.9904     0.0096     1.0000
 23       0.9893     0.0107        0.9909     0.0091     0.9993
 24       0.9900     0.0100        0.9915     0.0085     1.0000
 25       0.9906     0.0094        0.9920     0.0080     1.0007
 26       0.9911     0.0089        0.9924     0.0076     1.0000
 27       0.9916     0.0084        0.9928     0.0072     0.9993
 28       0.9921     0.0079        0.9932     0.0068     1.0000
 29       0.9925     0.0075        0.9935     0.0065     1.0007
 30       0.9929     0.0071        0.9938     0.0062     1.0000
 31       0.9932     0.0068        0.9942     0.0058     0.9993
 32       0.9936     0.0064        0.9944     0.0056     1.0000
 33       0.9939     0.0061        0.9947     0.0053     1.0006
 34       0.9942     0.0058        0.9950     0.0050     1.0000
 35       0.9945     0.0055        0.9952     0.0048     0.9994
 36       0.9947     0.0053        0.9954     0.0046     1.0000
 37       0.9950     0.0050        0.9956     0.0044     1.0006
 38       0.9952     0.0048        0.9958     0.0042     1.0000
 39       0.9955     0.0045        0.9960     0.0040     0.9994
 40       0.9957     0.0043        0.9962     0.0038     1.0000
 41       0.9959     0.0041        0.9964     0.0036     1.0006
 42       0.9961     0.0039        0.9966     0.0034     1.0000
 43       0.9963     0.0037        0.9967     0.0033     0.9994
 44       0.9965     0.0035        0.9969     0.0031     1.0000
 45       0.9967     0.0033        0.9971     0.0029     1.0006
 46       0.9968     0.0032        0.9972     0.0028     1.0000
 47       0.9970     0.0030        0.9974     0.0026     0.9994
 48       0.9972     0.0028        0.9975     0.0025     1.0000
 49       0.9973     0.0027        0.9976     0.0024     1.0006
 50       0.9975     0.0025        0.9978     0.0022     1.0000
```

```
STAGE  LIQUID MOL  FRACTIONS   VAPOR MOL  FRACTIONS    SUM Y

          BENZEN     N-BUOH        BENZEN     N-BUOH

  51      0.9976     0.0024        0.9979     0.0021    0.9994
  52      0.9978     0.0022        0.9980     0.0020    1.0000
  53      0.9979     0.0021        0.9982     0.0018    1.0006
  54      0.9981     0.0019        0.9983     0.0017    1.0000
  55      0.9982     0.0018        0.9984     0.0016    0.9994
  56      0.9983     0.0017        0.9985     0.0015    1.0000
  57      0.9985     0.0015        0.9986     0.0014    1.0006
  58      0.9986     0.0014        0.9988     0.0012    1.0000
  59      0.9987     0.0013        0.9989     0.0011    0.9994
  60      0.9989     0.0011        0.9990     0.0010    1.0000
  61      0.9989     0.0011        0.9990     0.0010    1.0006
```

```
                         CASE 11 11/28/72 R M C


FEED STREAM 10.000 MOLS   70.00 DEG C  FEED STAGE   6

BENZEN MOL FRACTION 0.7500   N-BUOH MOL FRACTION 0.2500

DISTILLATE  7.505 MOLS   80.16 DEG C

BENZEN MOL FRACTION 0.9990   N-BUOH MOL FRACTION 0.0010

BOTTOMS      2.495 MOLS  117.25 DEG C

BENZEN MOL FRACTION 0.0010   N-BUOH MOL FRACTION 0.9990

HEAT BALANCE
REBOILER         952248.  DISTILLATE ENTHALPY    135179.

FEED ENTHALPY     45318.  BOTTOMS    ENTHALPY     25860.

                            PARTIAL CONDENSER     16478.

                           PARALLEL CONDENSER    820049.

HEAT INPUT       997566.  HEAT OUTPUT            997566.
```

```
CPU:    30.2
```

```
                       CASE 12 11/25/72 R M C



                                                    FLOW LEAVING STAGE(MOLS)
STAGE      PRESSURE       TEMPERATURE              LIQUID       VAPOR

  1         760.00           99.96                  8.67        50.00
  2         760.00           99.60                 58.67        49.66
  3         760.00           96.18                 58.33        48.84
  4         760.00           85.66                 57.51        49.55
  5         760.00           80.26                 48.22        50.00
  6         760.00           78.95                 48.67         2.49
  7         760.00           78.51                  1.15         1.33
STAGE   LIQUID MOL  FRACTIONS   VAPOR MOL  FRACTIONS    SUM Y

           ETOH       WATER           ETOH       WATER

  1       0.0001     0.9999          0.0014     0.9986     1.0000
  2       0.0012     0.9988          0.0154     0.9846     1.0001
  3       0.0131     0.9869          0.1396     0.8604     1.0000
  4       0.1186     0.8814          0.4603     0.5397     0.9998
  5       0.4523     0.5477          0.6379     0.3621     1.0005
  6       0.6348     0.3652          0.7213     0.2787     1.0002
  7       0.6882     0.3118          0.7500     0.2500     0.9998
```

```
                   CASE 12 11/25/72 R M C


FEED STREAM 10.000 MOLS  100.00 DEG C  FEED STAGE   4

ETOH   MOL FRACTION 0.1000   WATER  MOL FRACTION 0.9000

DISTILLATE  1.332 MOLS   78.51 DEG C

ETOH   MOL FRACTION 0.7500   WATER  MOL FRACTION 0.2500

BOTTOMS      8.668 MOLS   99.96 DEG C

ETOH   MOL FRACTION 0.0001   WATER  MOL FRACTION 0.9999

HEAT BALANCE
REBOILER         874874.  DISTILLATE ENTHALPY     27535.

FEED ENTHALPY     33634.  BOTTOMS    ENTHALPY     28124.

                            PARTIAL CONDENSER     20201.

                           PARALLEL CONDENSER    832649.

HEAT INPUT       908508.  HEAT OUTPUT            908508.
```

```
CPU:   15.9
```

```
                         CASE 13 11/25/72 R M C



                                                  FLOW LEAVING STAGE(MOLS)
STAGE       PRESSURE       TEMPERATURE         LIQUID       VAPOR

  1          760.00           99.96              8.67       20.00
  2          760.00           99.67             28.67       19.88
  3          760.00           97.23             28.55       19.50
  4          760.00           88.25             28.17       19.50
  5          760.00           82.27             28.17       19.96
  6          760.00           79.51             18.63       20.08
  7          760.00           78.76             18.75        1.53
  8          760.00           78.44              0.20        1.33
STAGE   LIQUID MOL  FRACTIONS   VAPOR MOL  FRACTIONS     SUM Y

            ETOH        WATER          ETOH       WATER

  1         0.0001      0.9999         0.0014     0.9986     1.0000
  2         0.0010      0.9990         0.0129     0.9871     1.0001
  3         0.0090      0.9910         0.1027     0.8973     0.9999
  4         0.0711      0.9289         0.3870     0.6130     0.9993
  5         0.2679      0.7321         0.5605     0.4395     1.0009
  6         0.5469      0.4531         0.6789     0.3211     1.0002
  7         0.6738      0.3262         0.7420     0.2580     1.0009
  8         0.6882      0.3118         0.7500     0.2500     0.9998
```

```
                        CASE 13 11/25/72 R M C


       FEED STREAM 10.000 MOLS  100.00 DEG C  FEED STAGE   5

       ETOH   MOL FRACTION 0.1000   WATER  MOL FRACTION 0.9000

       DISTILLATE  1.332 MOLS   78.4 DEG C

       ETOH   MOL FRACTION 0.7500   WATER  MOL FRACTION 0.2500

       BOTTOMS      8.668 MOLS  100.0 DEG C

       ETOH   MOL FRACTION 0.0001   WATER  MOL FRACTION 0.9999

       HEAT BALANCE
       REBOILER          349951.  DISTILLATE ENTHALPY     27533.

       FEED ENTHALPY      33634.  BOTTOMS    ENTHALPY     28124.

                                    PARTIAL CONDENSER      3462.

                                   PARALLEL CONDENSER    324467.

       HEAT INPUT        383585.  HEAT OUTPUT            383585.
```

```
    CPU:    18.1
```

```
                     CASE 14 11/25/72 R M C



                                                    FLOW LEAVING STAGE(MOLS)
STAGE      PRESSURE      TEMPERATURE      LIQUID      VAPOR

  1         760.00          99.96           8.67      30.00
  2         760.00          99.63          38.67      29.81
  3         760.00          96.71          38.48      29.27
  4         760.00          86.83          37.94      29.41
  5         760.00          81.45          38.07      29.95
  6         760.00          79.28          28.62      16.56
  7         760.00          78.65          15.23       1.33
STAGE   LIQUID MOL  FRACTIONS   VAPOR MOL  FRACTIONS     SUM Y

           ETOH      WATER          ETOH      WATER

  1        0.0001    0.9999         0.0014    0.9986    1.0000
  2        0.0011    0.9989         0.0141    0.9859    1.0001
  3        0.0110    0.9890         0.1211    0.8789    0.9999
  4        0.0935    0.9065         0.4275    0.5725    0.9996
  5        0.3302    0.6698         0.5877    0.4123    1.0000
  6        0.5802    0.4198         0.6943    0.3057    1.0001
  7        0.6894    0.3106         0.7500    0.2500    1.0003
```

```
                      CASE 14 11/25/72 R M C



FEED STREAM 10.000 MOLS  100.00 DEG C  FEED STAGE   5

ETOH   MOL FRACTION 0.1000   WATER  MOL FRACTION 0.9000

DISTILLATE  1.332 MOLS   78.65 DEG C

ETOH   MOL FRACTION 0.7500   WATER  MOL FRACTION 0.2500

BOTTOMS      8.668 MOLS   99.96 DEG C

ETOH   MOL FRACTION 0.0001   WATER  MOL FRACTION 0.9999

HEAT BALANCE
REBOILER          524925.  DISTILLATE ENTHALPY     27539.

FEED ENTHALPY      33634.  BOTTOMS    ENTHALPY     28124.

                              PARTIAL CONDENSER   266173.

                             PARALLEL CONDENSER   236724.

HEAT INPUT        558559.  HEAT OUTPUT            558559.
```

```
                       CASE 15 11/25/72 R M C



                                                  FLOW LEAVING STAGE(MOLS)
STAGE      PRESSURE      TEMPERATURE      LIQUID      VAPOR

  1         760.00          99.96           8.67      10.00
  2         760.00          99.73          18.67       9.95
  3         760.00          98.22          18.62       9.77
  4         760.00          91.97          18.43       9.63
  5         760.00          84.73          18.30       9.98
  6         760.00          80.32           8.65      10.06
  7         760.00          79.04           8.72       3.36
  8         760.00          78.57           2.02       1.33
STAGE   LIQUID MOL  FRACTIONS   VAPOR MOL  FRACTIONS    SUM Y

            ETOH       WATER          ETOH       WATER

  1        0.0001     0.9999         0.0014     0.9986    1.0000
  2        0.0008     0.9992         0.0102     0.9898    1.0000
  3        0.0055     0.9945         0.0670     0.9330    0.9999
  4        0.0355     0.9645         0.2770     0.7230    0.9994
  5        0.1458     0.8542         0.4869     0.5131    1.0005
  6        0.4464     0.5536         0.6354     0.3646    1.0009
  7        0.6179     0.3821         0.7127     0.2873    1.0000
  8        0.6882     0.3118         0.7500     0.2500    0.9998
```

```
                              CASE 15 11/25/72 R M C


    FEED STREAM 10.000 MOLS  100.00 DEG C  FEED STAGE   5

    ETOH   MOL FRACTION 0.1000   WATER  MOL FRACTION 0.9000

    DISTILLATE  1.332 MOLS   78.57 DEG C

    ETOH   MOL FRACTION 0.7500   WATER  MOL FRACTION 0.2500

    BOTTOMS      8.668 MOLS   99.96 DEG C

    ETOH   MOL FRACTION 0.0001   WATER  MOL FRACTION 0.9999

    HEAT BALANCE
    REBOILER         174976.  DISTILLATE ENTHALPY     27536.

    FEED ENTHALPY     33634.  BOTTOMS    ENTHALPY     28124.

                                PARTIAL CONDENSER     35403.

                               PARALLEL CONDENSER    117547.

    HEAT INPUT       208610.  HEAT OUTPUT            208610.




CPU:    18.1
```

```
                         CASE 16 11/25/72 R M C



                                               FLOW LEAVING STAGE(MOLS)
STAGE      PRESSURE      TEMPERATURE        LIQUID     VAPOR

  1         760.00           99.96            8.67     10.00
  2         750.00           99.37           18.67      9.94
  3         740.00           97.47           18.61      9.75
  4         730.00           90.83           18.41      9.60
  5         720.00           83.26           18.27      9.97
  6         710.00           78.54            8.64     10.05
  7         700.00           76.93            8.71      3.20
  8         690.00           76.11            1.87      1.33
STAGE  LIQUID MOL FRACTIONS  VAPOR MOL FRACTIONS     SUM Y

           ETOH      WATER         ETOH      WATER

  1        0.0001    0.9999        0.0014    0.9986    1.0000
  2        0.0008    0.9992        0.0103    0.9897    1.0002
  3        0.0055    0.9945        0.0673    0.9327    0.9999
  4        0.0357    0.9643        0.2789    0.7211    0.9994
  5        0.1466    0.8534        0.4891    0.5109    1.0005
  6        0.4489    0.5511        0.6372    0.3628    1.0009
  7        0.6199    0.3801        0.7139    0.2861    1.0000
  8        0.6883    0.3117        0.7500    0.2500    0.9998
```

```
                    CASE 16 11/25/72 R M C


FEED STREAM 10.000 MOLS  100.00 DEG C  FEED STAGE   5

ETOH   MOL FRACTION 0.1000   WATER  MOL FRACTION 0.9000

DISTILLATE  1.332 MOLS   76.11 DEG C

ETOH   MOL FRACTION 0.7500   WATER  MOL FRACTION 0.2500

BOTTOMS      8.668 MOLS   99.96 DEG C

ETOH   MOL FRACTION 0.0001   WATER  MOL FRACTION 0.9999

HEAT BALANCE
REBOILER         175199.  DISTILLATE ENTHALPY      27468.

FEED ENTHALPY     33634.  BOTTOMS    ENTHALPY      28124.

                            PARTIAL CONDENSER      32848.

                           PARALLEL CONDENSER     120394.

HEAT INPUT       208834.  HEAT OUTPUT             208834.




CPU:    17.7
```

```
                     CASE 17 11/25/72 R M C



                                                   FLOW LEAVING STAGE(MOLS)
STAGE      PRESSURE       TEMPERATURE        LIQUID       VAPOR

  1         760.00           99.96             8.67        5.00
  2         750.00           99.44            13.67        4.97
  3         740.00           98.33            13.64        4.90
  4         730.00           95.07            13.57        4.77
  5         720.00           88.74            13.44        4.70
  6         710.00           83.93            13.37        5.02
  7         700.00           79.05             3.69        5.05
  8         690.00           77.01             3.72        5.07
  9         680.00           76.00             3.74        1.92
 10         670.00           75.31             0.59        1.33
STAGE   LIQUID MOL  FRACTIONS   VAPOR MOL  FRACTIONS    SUM Y

           ETOH      WATER           ETOH      WATER

  1       0.0001    0.9999          0.0014    0.9986    1.0000
  2       0.0006    0.9994          0.0075    0.9925    1.0002
  3       0.0028    0.9972          0.0357    0.9643    1.0002
  4       0.0130    0.9870          0.1392    0.8608    0.9994
  5       0.0495    0.9505          0.3317    0.6683    1.0000
  6       0.1168    0.8832          0.4602    0.5398    1.0007
  7       0.3555    0.6445          0.5995    0.4005    1.0008
  8       0.5456    0.4544          0.6788    0.3212    0.9990
  9       0.6535    0.3465          0.7312    0.2688    0.9998
 10       0.6883    0.3117          0.7500    0.2500    0.9998
```

```
                    CASE 17 11/25/72 R M C


FEED STREAM 10.000 MOLS  100.00 DEG C  FEED STAGE   6

ETOH   MOL FRACTION 0.1000   WATER  MOL FRACTION 0.9000

DISTILLATE  1.332 MOLS   75.31 DEG C

ETOH   MOL FRACTION 0.7500   WATER  MOL FRACTION 0.2500

BOTTOMS      8.668 MOLS   99.96 DEG C

ETOH   MOL FRACTION 0.0001   WATER  MOL FRACTION 0.9999

HEAT BALANCE
REBOILER          87652.  DISTILLATE ENTHALPY     27445.

FEED ENTHALPY     33634.  BOTTOMS    ENTHALPY     28124.

                            PARTIAL CONDENSER     10292.

                           PARALLEL CONDENSER     55426.

HEAT INPUT       121286.  HEAT OUTPUT            121286.




CPU:    18.8
```

```
                          CASE 18  1/13/73 R M C



                                                       FLOW LEAVING STAGE(MOLS)
      STAGE       PRESSURE        TEMPERATURE           LIQUID        VAPOR

        1          760.00            44.65               0.00         70.00
        2          760.00            44.23              70.00         68.84
        3          760.00            44.20              68.84         68.72
        4          760.00            44.20              68.72         68.73
        5          760.00            44.21              68.73         68.75
        6          760.00            44.21              68.75         68.77
        7          760.00            44.21              68.77         68.79
        8          760.00            44.22              68.79         68.80
        9          760.00            44.22              68.80         68.81
       10          760.00            44.22              68.81         68.82

      STAGE                  LIQUID MOL FRACTIONS                   SUM Y

                         MEOH        ACETON       DMBUT

        1               0.4000       0.3000       0.3000           1.0006
        2               0.2608       0.2532       0.4859           1.0005
        3               0.2430       0.2389       0.5181           0.9998
        4               0.2435       0.2329       0.5236           1.0000
        5               0.2457       0.2288       0.5256           1.0001
        6               0.2476       0.2256       0.5268           1.0003
        7               0.2492       0.2230       0.5278           1.0004
        8               0.2504       0.2210       0.5286           1.0006
        9               0.2514       0.2194       0.5292           1.0007
       10               0.2522       0.2181       0.5297           1.0008













   CPU:    15.2

   READY
```

```
                      CASE 19 3/22/73 R M C



                                                 FLOW LEAVING STAGE(MOLS)
    STAGE      PRESSURE      TEMPERATURE      LIQUID       VAPOR

      1         760.00          44.73           0.00        70.00
      2         760.00          44.26          70.00        71.18
      3         760.00          44.22          71.18        71.24
      4         760.00          44.22          71.24        71.21
      5         760.00          44.22          71.21        71.18
      6         760.00          44.21          71.18        71.16
      7         760.00          44.21          71.16        71.13
      8         760.00          44.20          71.13        71.11
      9         760.00          44.20          71.11        71.09
     10         760.00          44.20          71.09        71.07

    STAGE            LIQUID MOL FRACTIONS                 SUM Y

                  MEOH        ACETON       DMB

      1          0.1000       0.1000      0.8000         1.0000
      2          0.2650       0.1514      0.5837         1.0005
      3          0.2818       0.1646      0.5536         0.9998
      4          0.2789       0.1729      0.5482         1.0000
      5          0.2750       0.1797      0.5452         1.0001
      6          0.2717       0.1855      0.5428         1.0001
      7          0.2688       0.1903      0.5408         1.0001
      8          0.2664       0.1943      0.5392         1.0000
      9          0.2645       0.1977      0.5379         0.9999
     10          0.2628       0.2004      0.5367         0.9998













CPU:    11.1

READY
BYE
```

```
                         CASE 20 3/22/73 R M C



                                                 FLOW LEAVING STAGE(MOLS)
STAGE      PRESSURE       TEMPERATURE       LIQUID        VAPOR

  1         760.00           44.73            0.00         70.00
  2         760.00           44.26           70.00         71.18
  3         760.00           44.22           71.18         71.24
  4         760.00           44.22           71.24         71.21
  5         760.00           44.22           71.21         71.18
  6         760.00           44.21           71.18         71.16
  7         760.00           44.21           71.16         71.13
  8         760.00           44.20           71.13         71.11
  9         760.00           44.20           71.11         71.09
 10         760.00           44.20           71.09         71.07
 11         760.00           44.19           71.07         71.05
 12         760.00           44.19           71.05         71.04
 13         760.00           44.18           71.04         71.03
 14         760.00           44.18           71.03         71.02
 15         760.00           44.18           71.02         71.02
 16         760.00           44.20           71.02         71.02
 17         760.00           44.22           71.02         71.01
 18         760.00           44.20           71.01         71.01
 19         760.00           44.18           71.01         71.01
 20         760.00           44.20           71.01         71.01

STAGE             LIQUID MOL FRACTIONS                      SUM Y

                MEOH       ACETON      DMB

  1            0.1000      0.1000      0.8000              1.0000
  2            0.2650      0.1514      0.5837              1.0005
  3            0.2818      0.1646      0.5536              0.9998
  4            0.2789      0.1729      0.5482              1.0000
  5            0.2750      0.1797      0.5452              1.0001
  6            0.2717      0.1855      0.5428              1.0001
  7            0.2688      0.1903      0.5408              1.0001
  8            0.2664      0.1943      0.5392              1.0000
  9            0.2645      0.1977      0.5379              0.9999
 10            0.2628      0.2004      0.5367              0.9998
 11            0.2615      0.2027      0.5358              0.9997
 12            0.2603      0.2046      0.5351              0.9995
 13            0.2594      0.2061      0.5345              0.9994
 14            0.2587      0.2073      0.5340              0.9993
 15            0.2580      0.2083      0.5336              0.9991
 16            0.2575      0.2092      0.5333              1.0000
 17            0.2572      0.2098      0.5330              1.0008
 18            0.2569      0.2104      0.5327              1.0000
 19            0.2566      0.2108      0.5326              0.9992
 20            0.2563      0.2112      0.5325              1.0000




CPU:    14.4
```