

THESIS



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**OPTIMUM FEED PLATE LOCATION
IN MULTICOMPONENT DISTILLATION**

by

RUSSELL HOWARD FOY

A THESIS

**Submitted to the College of Engineering
Michigan State University of Agriculture and
Applied Science in partial fulfillment of
the requirements for the degree of**

MASTER OF SCIENCE

Department of Chemical Engineering

1959

To my wife
their patience

0308
0-24-66

DEDICATION

**To my wife, Janet, and daughter, Beth, for
their patience and understanding.**

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IN MULTICOMPONENT DISTILLATION**

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RUSSELL HOWARD FOY

AN ABSTRACT

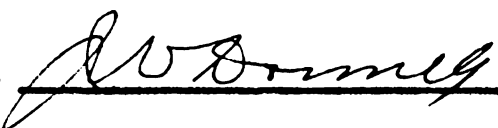
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THE UNIVERSITY OF CHICAGO

ABSTRACT

In a multiple component distillation design, it is evident that there exists an optimum feed plate location somewhere between the inoperative conditions of top or bottom plate, except in the case of an abbreviated column such as a stripper.

The two most commonly used methods for locating the optimum feed plate are those of Gilliland and Montrose-Scheibel.

Gilliland's method consists of choosing the feed plate so that the ratio of the key components on the feed plate is equal to the ratio of the key components in the feed. The method has been checked by far too few problems because of the long and tedious plate to plate calculations required. Several problems involving eleven plates have been checked by Gilliland's method and agree fairly well with the correlation developed in this investigation.

The method of Montrose and Scheibel is based on an empirical equation which involves the use of the ratio of the key components on the feed plate at total and minimum reflux. The equation appears to be based on only semi-rigorous calculations since the simplifying assumptions of constant relative volatility and latent heats were made to

reduce the labor of calculation. This empirical equation also makes use of the less than rigorous terms of minimum reflux and minimum number of plates. No attempt was made to check if the method agreed with the results of this investigation, as the Montrose and Scheibel assumptions are too general.

It was the purpose of this work to obtain an empirical multicomponent optimum feed plate location relation based upon a considerable number of truly rigorous plate to plate calculations. A rigorous plate to plate calculation is one which takes into consideration both the variation of equilibrium constant with temperature and an enthalpy or heat balance about each plate. To perform these rigorous calculations, a method of solution suited for a high speed computer was developed and programmed. The electronic digital computer used was the Michigan State University 40 cathode ray tube, single address machine.

The computer was used to solve several hundred problems rigorously. The results of these problems were then used to study the effect of certain variables such as reflux ratio, feed composition, and number of plates upon the relative optimum feed plate location. It was found that reflux

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ratio, number of plates, and feed temperature had very little effect on the location of the optimum feed plate. A function of $\frac{x_{HK} x_{LK}}{x_{HK} + x_{LK}}$ was found to fit the data of various feed compositions very well, and a correlation based on relative optimum feed plate location versus this function was made.

Although many problems were solved in this investigation, no claim is made that all possible combinations of feed composition, as well as types of components, i.e., relative volatilities, will have the optimum feed plate location as found using this correlation. However, most commercial applications will be covered. It is probable that when non-adjacent key components are used the optimum feed plate location is more sensitive than when employing adjacent keys. Since this investigation did not cover non-adjacent keys, care should be exercised when attempting to use the correlation for such systems.

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Thanks are also extended to the Computer Laboratory staff of Michigan State University for their cooperation in making the MISTIC and the auxiliary equipment available for use in this investigation.

INTRODUCTION

INTRODUCTION

The unit operation of distillation is an old one, dating back to the early days of the alcohol stills. Through the years, the use of distillation as a means of separating a mixture of liquids into desired products has been growing steadily. The petroleum industry, perhaps, has been the largest contributor in the expansion of distillation techniques and applications. It has been estimated that two-thirds of the total investment in petroleum refineries is in distillation equipment.

The solution of binary distillation problems was first analyzed and organized into a systematic approach by Sorel (15) in 1893. His solution consisted of making energy and material balances around each plate and assuming that equilibrium is attained on each plate.

Practically all distillation calculations today use the theoretical plate concept; that is, the assumption that equilibrium is attained on each calculated plate. Then one applies the theoretical calculations to actual design by using an efficiency factor to obtain the number of physical plates to use. For example, if a plate of certain design is known to give fifty per cent efficiency on the liquid-vapor

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system in question, then two plates must be used for each theoretical one. Henceforth then, subsequent distillation discussions in this paper will be confined to the theoretical plate approach.

Sorel's rigorous method involves starting at either end of the distillation tower and using end products (obtained by a material balance and product specification) to calculate downward (or upward) plate by plate until the other end of the tower is reached. The composition of the liquid on a tray is obtained from vapor-liquid equilibrium data. Then the amount and composition of the vapor entering this tray from the tray below is calculated by a material and heat balance around the tray in question. This last calculation is made by assuming a certain vapor rate and checking from known latent and specific heat data for each component to see if this heat data will allow the amount of vapor assumed to enter the plate in question. This, then, is seen to involve a trial and error procedure - a tedious process.

Ponchon (14) however, developed a graphical method which can be used to execute the Sorel plate to plate

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calculation for binary systems in a rigorous fashion in a relatively short time. The method involves plotting an enthalpy versus composition (mole fraction or weight fraction) diagram for both saturated liquid and saturated vapor. This diagram is then used to satisfy equilibrium relationships and to make material balances. The method takes into account the change in liquid and vapor rates from plate to plate, which is what the Sorel method accomplishes.

McCabe and Thiele's (13) graphical method has become the most popular method of solution for binary mixtures; in fact, it has become a classic. This method, as many others before and after it, makes certain simplifying assumptions to handle problems more easily. The primary assumptions one must make when applying a solution such as this are:

1. Negligible sensible heat effects of liquids and vapors as compared to latent heats.
2. Latent heats of vaporization per mole of both components are equal and do not vary with temperature.
3. Negligible heat losses to surroundings.
4. No heats of mixing.

The latter two assumptions are two which are standard assumptions to nearly all methods of solution; and well they might be, for both effects are very small in comparison to the large amounts of heat being considered in a column. The first assumption is usually a good one to make. However, the second assumption is the one that could be greatly in error, and thus cause incorrect results. For most mixtures of two components which are members of the same homologous series, the assumption of equal molal heats of vaporization is a reasonable one, and the McCabe-Thiele method provides a very quick and accurate method of solution. The McCabe-Thiele method can also be modified to handle cases where the heats of vaporization are unequal. In this case, the method is slower but still gives good results.

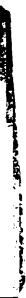
The mechanics of the McCabe-Thiele method consist of plotting the equilibrium diagram for the components in question on a vapor-liquid composition graph. Plotted on the same graph are the operating lines, i.e., the upper operating line starts with the top product

composition and has a slope equal to the ratio of liquid to vapor rates in the top of the tower, while the bottom operating line starts with the composition of the bottom product and has a slope equal to the ratio of liquid to vapor rates below the feed plate. The lines represent material balance equations and relate the composition of the vapor leaving a plate to the composition of the liquid leaving the plate above it. The number of plates required can be determined by alternately moving from the operating line horizontally to the equilibrium line, and from the equilibrium line vertically downward to the operating line, and so on until the bottom composition is reached. The procedure may be reversed and, starting with the bottom product, take vertical and horizontal steps until the top product composition is reached. Either way, each pair of horizontal and vertical steps represent a plate. If constant heats of vaporization are assumed, the operating lines referred to above are straight lines. If the heats of vaporization are not assumed to be equal, then the operating lines will not be straight, but curved. One method of plotting the curved operating lines would be

to make use of a Ponchon diagram in conjunction with the McCabe-Thiele diagram. But rather than do that, one might just as well use a Ponchon diagram by itself, which accomplishes the same purpose in a simpler fashion.

The solution of multicomponent distillation problems is closely related to the solution of binary distillation problems, in that they are both based on theoretical plates, material balances, and heat balances. The procedure for the solution of a multicomponent problem is different, however, because the boiling points of the liquids are no longer a function of one component composition as was the case in binary mixtures. In multicomponent mixtures (three or more components) the liquid on a given plate may have an infinite number of boiling points corresponding to a certain composition for one component, depending upon the composition of the other components in the mixture.

In the previous discussion of binary distillation, the McCabe-Thiele graphical method was referred to as a classic because it gives rigorous (if curved operating lines are used) yet rapid and clear solutions to most



binary distillation problems. There is no similar method which is simple enough for multicomponent calculations. Plate to plate calculations are therefore widely recognized as the standard method for multicomponent systems. The other methods of solution may be roughly broken down into the categories of

- 1) graphical solutions, 2) overall equations, and
- 3) empirical solutions. Several examples of each category will now be outlined briefly.

The two most common plate to plate methods used are the Lewis-Matheson (12) which makes the major assumption of constant liquid and vapor rates, and the Thiele-Geddes (16) which uses heat balances as a major calculating tool.

The Lewis-Matheson method consists of starting with the desired end products and calculating the number of theoretical plates required. Plate to plate calculations from both extremes of the column to the feed plate are carried out by using material balances and equilibrium relationships and by making successive approximations as to the temperature on each plate. The reflux ratio must also be found by trial and error.

The calculations in detail are carried out as follows. The reflux ratio is first approximated and the composition of the vapor leaving the top tray is calculated. For a total condenser this step would not be necessary, since the composition of the vapor would be the same as that of the top product. By using some sort of equilibrium relationship such as Raoult's law, relative volatility, or K values (where $y = Kx$ and equilibrium is attained when $\sum y = 1$, $K = f(T,P)$) the liquid composition and the temperature on the top plate are found by assuming values for the temperature until the sum of the mole fractions, as calculated from the equilibrium relationship, is unity. Similarly, the temperature of the still and the composition of the vapors rising from it are calculated. Reflux is assumed not to change from one end of the column to the other, except at the feed plate where the reflux is increased by the amount of liquid in the feed. By use of a material balance and the dew point equation, the temperatures and compositions on each plate are calculated plate by plate.

By studying the composition determined by working up from the bottom, a suitable feed plate is chosen.

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The composition of the light key (highest boiling component which does not come out in bottom product) on the feed plate is calculated. The computation is continued until the heavy key (lowest boiling component which does not appear in appreciable amounts in the overhead product) is of negligible concentration. If the compositions thus determined correspond substantially with those determined by calculating down the column, the problem is solved. If not, the composition on the feed plate must be re-estimated and the last series of calculations repeated.

The most important contribution of Lewis and Matheson was to demonstrate that multicomponent systems could be solved by using a plate to plate calculation similar to that used for binary mixtures.

Because the method starts with the distillate and bottoms composition, the method is not readily applicable to mixtures that have two or three components which appear in both product streams. It will be pointed out later that there are not enough degrees of freedom to specify the exact product composition together with the number of plates. This is the most serious disadvantage of the

method. The Lewis-Matheson method can be made more rigorous by taking into consideration the changing liquid and vapor rates by applying the principles used by Sorel, i.e., heat balances.

The method introduced by Thiele and Geddes in 1933 is a rigorous plate to plate calculation in which it is not necessary to know or assume the products. It is, however, necessary to start with the number of equilibrium plates and the reflux ratio. These constitute the primary assumptions. The secondary assumptions are the temperatures on each plate. The method makes use of mole fraction ratios; that is, the ratio of the mole fraction of a component in either the liquid or vapor phase to the mole fraction of the same component in the end product stream. Above the feed the ratios are with respect to the distillate, below the feed with respect to the bottom product.

Calculations are performed from both extremes of the tower toward the feed plate, making use of the previously mentioned mole fraction ratios. When the feed plate is reached, these ratios are meshed to find the composition of the products. After the feed plate mesh

is accomplished, one must go back and calculate the compositions on each plate, which in turn are used to calculate the corresponding temperatures. If the calculated temperatures do not agree with those assumed, the process is repeated using the new assumptions, until the temperatures for all the plates agree on two successive trials. It should be stressed that all temperatures must agree, since an incorrect temperature at any point will invalidate all of the calculations.

The Thiele-Geddes method is a very good method for multicomponent systems. Its main advantage over the Lewis-Matheson method is the manner in which the unequal molal overflow is taken into account, as well as not having to start with the composition of the products.

In 1935, Gilliland (7) published a shortcut method for solution of multicomponent problems by using relative volatility, as well as a new function of relative operability. Equilibrium relationships are written for the two key components in terms of relative volatility. By writing component material balances around a plate for each key component, and by dividing one component balance by the other, Gilliland uses the resulting

equation to define relative operability. He then combines the relative operability with relative volatility to give the relative changes in composition for one complete equilibrium stage, i.e., from liquid on one plate to liquid on the next. By expanding the above relationship for total plates in each section, he obtains relative composition changes across both the enriching and stripping sections. The method is a rapid approximation that can be used with a fair degree of accuracy for sharp separations. However, using this method, it is necessary to know the composition on the feed plate.

The limitations of the method are that there are too many simplifying assumptions. For instance, if the relative volatility or operability varies from one end of the column to the other, an arithmetic average is used. It is, nevertheless, a good method for giving quick approximations, which could be used as a first estimate in a more rigorous method.

Some investigators, such as Lewis and Cope (11) and Jenny (10), developed graphical solutions comparable to the McCabe-Thiele method.

The Lewis and Cope method consists of constructing a separate plot of y vs. x for each component. Assuming an equilibrium relationship of $y = Kx$, with K dependent on temperature only, equilibrium lines are plotted for several temperatures, and the correct temperature determined by trial and error. This process is repeated for each plate. The method is very cumbersome and also requires a knowledge of the composition of the products.

Jenny proposed a graphical method utilizing a x vs. y diagram similar to the McCabe-Thiele diagram, which involves constructing a modified equilibrium line, which is supposed to allow for the non-volatile lighter than key and heavier than key components. The equilibrium line is plotted by making a few plate to plate calculations. Separate diagrams are used for both the stripping and enriching sections, using the light key for the enriching section and the heavy key for the stripping section. The operating lines are assumed to be straight. This method requires knowing the composition on the feed plate.

A method based on overall equations for both sections of the tower was proposed by Edmister (5). The equations are based on the use of absorption and stripping factors

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Many so-called empirical solutions have been proposed, based on various correlations of past calculations. Several of these correlations will now be discussed.

In 1939, Brown and Martin (1) proposed a method for obtaining the number of equilibrium plates required for a given separation at a specified reflux ratio. The method is based upon an empirical correlation and the variables plotted are actual reflux divided by minimum reflux versus the actual plates divided by the minimum plates. Key components and pinch-point concepts are used. The correlation was developed from the results of rigorous calculations for a number of separations. Most of the systems were binary, with some multicomponent systems.

About the same time that Brown and Martin published their method, Gilliland (2) proposed a method very similar, although developed independently. This correlation plotted the actual minus the minimum plates divided by one plus

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the actual plates versus the actual minus the minimum reflux divided by one plus the actual reflux. The variables are plotted on log-log scales.

Gilliland's correlation was also the result of rigorous calculations for a number of binary mixtures. The correlation was also checked for a few multi-component systems. The correlation of Gilliland is a little simpler to use than that of Brown and Martin.

In 1950, Donnell and Cooper (4) proposed a correlation which involved plotting the ratio of actual plates to minimum plates versus the logarithm of the ratio of actual boil up to minimum boil up. The equations of Fenske (6) and Underwood (17) are used to obtain values for the minimum plates and minimum vapor load. One of the most important advantages of this correlation is that the curve approaches a straight line in the region of minimum reflux. This is of importance since most optimum conditions lie in this range near the minimum reflux. Thus, it is desirable to be able to read the graph easily, or even interpolate if necessary.

Several other investigators made correlations similar to those already discussed. Included is the group

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In, 1940, Gilliland (8) published a method for determining the optimum feed plate location. This method consists of placing the feed plate so that the ratio of the mole fractions of the key components in the feed is between the ratio of the key components on the plate above and below the feed plate. According to Gilliland's method, there is a slight variation if the feed is partially vaporized or all vapor.

Montrose and Scheibel in 1946 (3a) offer a method for optimum feed plate location. This method is based on an empirical equation which involves the use of the ratio of the key components on the feed plate at total and minimum reflux. The equation appears to be based on only semi-rigorous calculations since the simplifying assumptions of constant relative volatility and latent heats were made to reduce the labor of calculation. This empirical equation also makes use of the less than rigorous terms of minimum reflux and minimum number of plates. No attempt was made to check if the method agreed with the results of this investigation, as the Montrose and Scheibel assumptions are too general.

STATEMENT OF THE PROBLEM

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The need of a rigorous solution to multicomponent distillation problems is not a new idea. It was stated some years back by Colburn (2) that what the engineering profession needs in multicomponent calculations is "either an exact solution, even though it is difficult, or an approximate solution, if it is easy." With the advent of high speed computers, the challenge to see who could develop an exact solution first has grown considerably. This investigation was undertaken to: 1) develop an exact solution using a high speed computer as a tool to perform the calculations, and 2) use the exact solution to study the effect of feed tray location on the degree of separation in multicomponent mixtures.

When a distillation column is designed and built, it is desired that for a given number of plates, reflux ratio, and feed composition, the maximum separation be obtained. It is desirable, then, to locate the feed plate so that the optimum separation is obtained.

To illustrate the necessity for the optimum feed plate location, consider the following binary problem.

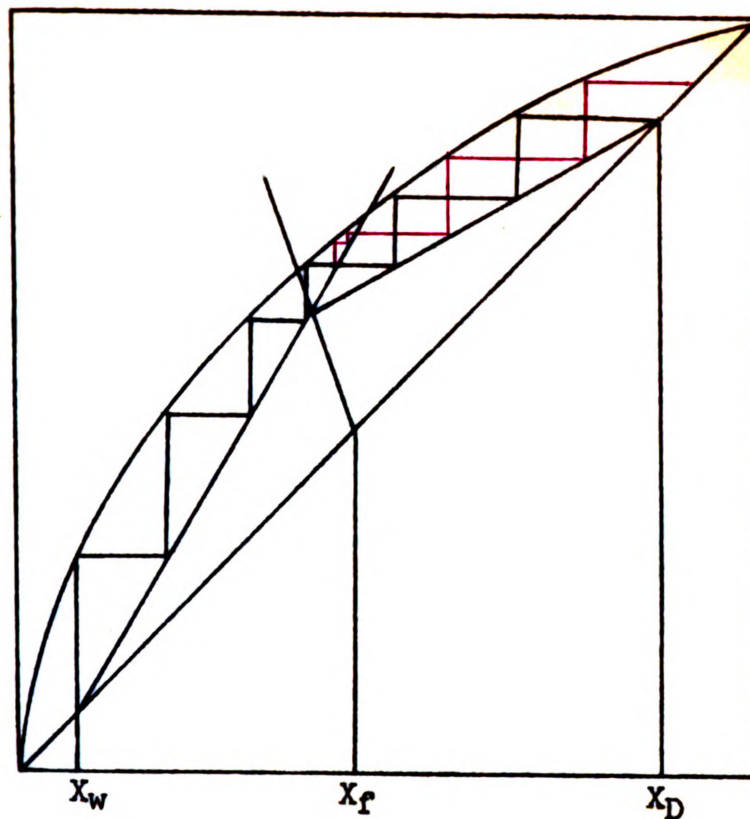


Figure 1

If the feed plate were not located on the fourth plate from the bottom, but higher up, it would require more plates to do the same job of separation, or a worse separation would be obtained, if the same number of plates were used.

The red line in Figure 1 illustrates the case where the feed plate is not the fourth but the sixth plate from the bottom. In this case, it would take two more plates to do the same job of separation. Similarly, if the feed plate were located lower than the fourth plate from the bottom, the same situation would arise.

Multicomponent systems are not so easy to illustrate as the foregoing binary one, but the same type of relationship exists. That is, there exists an optimum feed plate location, or series of locations, so that a maximum separation is obtainable.

In attempting to study the effect of feed tray location, it becomes necessary to work out many problems to see how the optimum varies with number of plates, reflux ratio, and feed composition. In a study such as this, a rigorous solution should be used in order to get a more accurate picture of the variables involved. Thus, this investigation utilized a high speed computer to solve many problems in a rigorous fashion (that is, taking into account changing vapor and liquid rates and perfect matching at the feed plate.)

NEED FOR HIGH SPEED COMPUTER

NEED FOR HIGH SPEED COMPUTER

The importance of greater and greater accuracy has been brought out as one reason why more rigorous methods of solution must be employed. The more rigorous a problem, the more trial and error calculations are required, until finally it is conceivable that an engineer working a rigorous multicomponent distillation problem might take weeks to solve the problem. Most of that time would be spent doing the rather routine trial and error calculations to make sure that all compositions, amounts, and temperatures were consistent with the material balances, heat balances, and equilibrium data. The answer to the engineer's dream is a high speed electronic computer. Of course, the engineer would still be required to set the problem up, but the computer would do all the calculations in a very short period of time.

The same problem that might take an engineer a week to solve could be solved using a computer in a few hours or less.

The great speed at which computers operate is also important from an economic standpoint. Once a program has been written for a problem, it can be used over and over for the solution of many similar problems. Although

the cost of buying or renting a computer is quite high (rentals run on the order of \$200 per hour) the cost is still substantially lower than paying the salary of an engineer for the time necessary to work out the problem by hand.

As was pointed out previously, the study of the effect of feed tray location on the separation obtained is one which requires many problems to be solved. This lends itself to computer application very nicely, since the computer can perform a rigorous solution in a short period of time.

Not only does the computer provide a means of studying the effect of feed tray location, but also it affords a detailed study of other variables which enter into the problem. One of the variables now being studied is the effect of condition of feed, i.e., pre-heated or cold, on the tower performance. Another important study is being made on the relationship between number of plates and reflux ratio to obtain a desired separation.

Another important advantage of the use of computers is their reliability. Although some might argue this to

be a trivial point, it is nevertheless an important one. The reliability of computers is certainly better than an engineer running a slide rule or desk calculator. It must be admitted that computers do occasionally make a mistake. However, when a mistake is made, it is almost always so obvious that it is immediately noticed. On the other hand, an engineer could easily carry a mistake on and on without it being noticed.

In the discussion of previous methods used in solving multicomponent distillation problems, it was mentioned that some methods use the ratio of the so-called key components as a criterion for convergence of the feed plate mesh. This, of course, is only an approximation and serves to shorten the calculations. Once again, the computer can perform these calculations exactly and thus eliminate the need for the assumption. It may be argued that this advantage of the computer is merely due to the speed at which the machine operates. However, there is more to a computer than speed and accuracy. It enables one to solve lengthy and complex problems that could not be worked without the use of such a computer. Many of these seemingly

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impossible solutions are now being handled very nicely by computers.

There are two alternative approaches to the problem of applying computers to solve distillation problems. The first alternative would be to adapt one of the well-known and accepted calculation methods presented by other authors to a computer. The second alternative would be to develop a calculation method particularly suited to automatic calculation. The latter alternative was chosen since it is felt that none of the existing calculation methods are suitable to automatic computation, either because of the method itself or because of certain simplifying assumptions which the method required, which were felt unnecessary to make.

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DERIVATION OF EQUATIONS

The solution of a multicomponent distillation problem is one of trial and error. This is even more pronounced if the simplifying assumptions of constant liquid and vapor rates are not made. The three tools with which we are armed to obtain a solution are: 1) Vapor-liquid equilibrium conditions, 2) material balances, and 3) energy balances.

At this point, it is well to point out that from any given feed, the problem of product specification is quite different in a multicomponent mixture than it is in a binary mixture. In a binary mixture, the product desired may be fixed by specifying the composition of one component, since the composition of the other component will then also be fixed. However, in a multicomponent mixture the product cannot be specified for all the components. Instead, only the composition with respect to one component may be specified.

The situation of not being able to specify the products and the fact that computers are limited as to the number of simultaneous equations they can solve, leads directly to a trial and error solution. The solution becomes, then, an iterative process of assuming the composition of the products, working through the problem, and correcting the product compositions until the assumptions prove correct.

The primary variables which must be known before starting the solution of a problem are: 1) Feed composition and condition of the feed, 2) Reflux ratio, L/D , 3) number of plates above and below the feed plate, and 4) tower pressure. The latter is necessary for equilibrium and enthalpy data.

There are two types of problems which may arise. The first would be the problem of designing a new column with the proper number of plates to give a desired separation. The desired separation, of course, must be in accordance with the foregoing discussion on product specification.

The second type of problem would be the utilization of an existing column and the desire to determine the products obtainable with a given feed. Actually, both types of problems would be solved utilizing the same method of solution. The problem of determining the number of plates necessary to obtain a desired product requires an estimate of the number of plates, working through the problem, and checking the results with the desired products. If the results agree, then the number of plates assumed will be sufficient. If the results do not agree, then a new estimate of the number of plates must be made, and the problem reworked until the

products obtained are acceptable. The problem with the number of plates already known and the products unknown is solved using the same method of solution as for the above type problem, except that the number of plates need not be assumed since it is already known. Therefore, the solution of both types of problems will be handled as one, and the number of plates in the column will be taken as a known variable.

The general solution of the problem will be to assume one of the product compositions and quantities (the top product in this solution) and calculate from both extremities of the tower toward the middle until the feed plate is reached from both directions. At this point a mesh, or comparison, of the compositions obtained from both directions is made. If the compositions are equal, to a specified degree of accuracy, then the products assumed are correct and the solution is complete. If the compositions do not mesh, then the assumed product is modified in proportion to the variation of the mesh, and the calculations are carried out again until the feed plate mesh is satisfactory.

In the development of the method, frequent reference to previous equations already developed will occur, and so are

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numbered to help identify them. A diagram is provided to help picture the problem and also to refer to as to nomenclature.

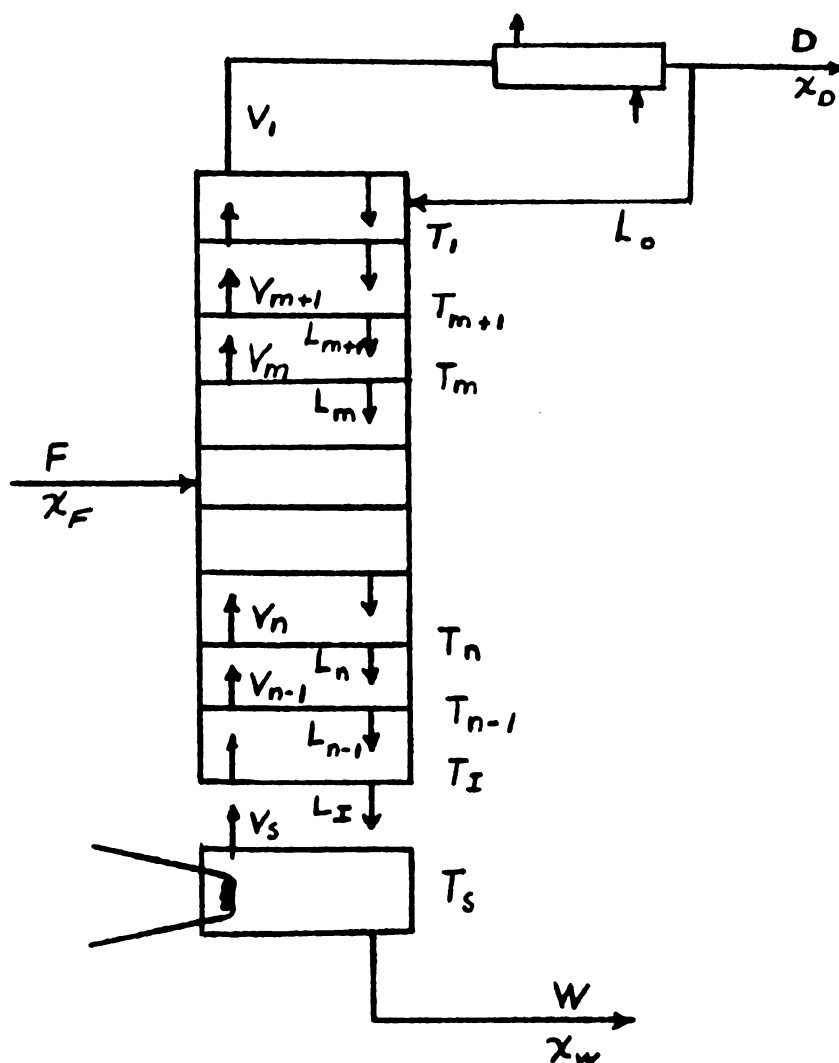


Figure 2

For simplification purposes, a basis of one mole of feed is chosen. This allows the composition of the feed, expressed in mole fractions, to be the moles of each component in the feed. It also provides an easy, quick estimate of the amount and composition of the top product by estimating

the number of moles of each component which will be produced overhead. The first estimate of top product, as well as estimates of the top temperature, bottom temperature, and amount of vapor in the bottom section, are read into the computer as data. In the section on the actual computer programming, the entire list of data necessary to work a problem will be outlined.

The statement and derivation of the algebraic procedure used in the problem follows:

- 1) Calculate the amount of overhead product.

$$D = \sum_1 D \times D_1$$

For the first iteration this step is unnecessary, since the top product has been assumed. However, in later iterations the top product will be altered, making it necessary to perform this calculation.

- 2) Calculate the amount of bottom product.

$$W = F - D = 1 - D$$

- 3) Calculate the bottom composition.

$$x_{w1} = \frac{F x_{f1} - D x_{d1}}{W}$$

- 4) Using the assumed moles ($D x_{d1}$) of each component and the D from step 1, calculate the overhead

composition. $x_{d1} = \frac{D x_{d1}}{D}$

5) Calculate V_1 and L_o from given reflux ratio and D

calculated in 1.

$$V_1 = D(R+1)$$

$$L_o = R \cdot D$$

6) Determine the temperature on the top and bottom plate, using the bubble point and dew point calculations as shown below.

$$T_1 \text{ at top when } \sum_i \frac{x_{oi}}{K_i} = 1$$

$$T_s \text{ at bottom when } \sum_i K_i x_{wi} = 1$$

The values of K_i are obtained from a third degree polynomial in temperature. The K values are assumed to be dependent on temperature and pressure only. When the correct temperatures are found, then $K_i X_{wi} = Y_{wi}$ and each Y_{wi} is saved for later calculations.

7) Determine the dew point of the overhead product as follows:

$$T_o \text{ when } \sum_i K_i x_{oi} = 1$$

8) Calculate heat flux in top of column by subtracting enthalpy of reflux from enthalpy of top vapor, thusly:

$$h_o = L_o \sum_i \bar{h}_{oi} x_{oi} \text{ at } T_o$$

$$H_1 = V_1 \sum_i \bar{H}_{1i} x_{oi} \text{ at } T_1$$

$$Q_a = H_1 - h_o$$

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Note that this solution is for a total condenser. It would have to be modified slightly for the use of a partial condenser.

- 9) Assuming no heat losses to surroundings, calculate Q_r from enthalpy of the feed and Q_a . The enthalpy of the feed is read in as data and is calculated in the same manner as all other enthalpies, i.e., the enthalpy of a mixture is the sum of the individual products of mole fraction and enthalpy of pure component. The enthalpy of each pure component is calculated from a third degree polynomial in temperature.

Make a heat balance around the entire column:

$$\begin{aligned} h_F + h_S &= h_C + h_D + h_W \\ h_F &= (h_W - h_S) + (h_C + h_D) \\ (h_S - h_W) &= (h_C + h_D) - h_F \end{aligned}$$

A heat balance around the top and bottom section separately gives:

$$\begin{aligned} \text{Top section} \quad H &= h_D + h_C + h \\ \text{or} \quad H - h &= h_D + h_C = Q_A \\ \text{Bottom section} \quad H + h_W &= h + h_S \\ \text{or} \quad H - h &= h_S - h_W = Q_r \\ \text{Thus} \quad Q_r &= Q_a - h_F \end{aligned}$$

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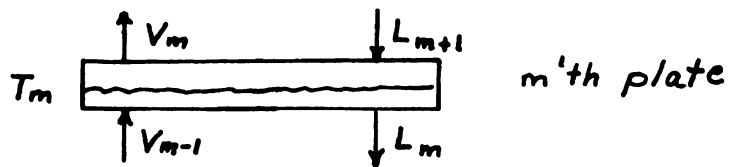


Figure 3

The general case of plate m will be illustrated. By looking at the second plate from the top in Figure 2, it is easy to see just what is known and what is unknown. The same will apply to the m 'th plate as one works downward. The composition and temperature of L_{m+1} are known, while V_m , y_{mi} , T_m , $L_{(m+1)}$, and x_{mi} are all unknown. Actually, V_{m-1} , T_{m-1} , and $y_{(m-1)i}$ are unknown also, but come into consideration on the next plate. If there are i components present, then there are $2i+3$ unknowns to solve for. The equations available for their solution are: 1) total material balance above m 'th plate and around top of tower, 2) i component material balances around same portion of tower, 3) heat balance around above mentioned section of the tower, 4) dew point equation, and 5) i equilibrium equations. It is well to point out that if a set of simultaneous equations were set up for the whole tower, it would involve equations which would number $(2i+3)$ times the number of plates in the column. It is conceivable to have

a column with fifty plates and ten components, which would require the solution of 1150 equations and 1150 unknowns. Very few, if any, computers even approach a capacity large enough to handle such a problem except by an iterative process. Even if a computer were large enough to handle the 1150 equations, it is doubtful if a solution could be obtained, since it is unlikely that all the equations would have constant coefficients.

The procedure used here to solve the $(2i+3)$ equations, one plate at a time, is a trial and error method based on assuming values for T_m and L_{m+1} and using Newton's method to arrive at better values for the assumed variables. This is done until the correction factor for T_m and L_{m+1} becomes arbitrarily close to zero.

10) Choose a temperature T_m and a liquid rate L_{m+1} .

A good first estimate is to use the values obtained as answers to the previous plate. After the first iteration through the column this step will be altered by using the temperature and liquid rate for the previous iteration as the first guess, since they will be a better approximation than the temperature and liquid rate for the preceeding plate.

- 11) Calculate V_m from D and the assumed L_{m+1} by an overall material balance around top of tower.

$$V_m = L_{m+1} + D$$

- 12) Calculate y_{mi} from a component material balance around top of tower.

$$y_{mi} = \frac{L_{m+1} x_{(m+1)i} + D x_{0i}}{V_m}$$

- 13) Calculate ϕ using assumed T_m . This also gives the values of x_{mi} .

$$\phi = 1 - \sum y_m / K_m$$

Note that ϕ will approach zero as the correct temperature is found.

- 14) Using assumed T_m , y_{mi} , and x_{mi} as calculated in 12 and 13, find H_m .

$$H_m = \sum \bar{H}_m y_m$$

- 15) Calculate h_{m+1} from temperature of plate above, T_{m+1} .

$$h_{m+1} = \sum \bar{h}_{m+1} x_{m+1}$$

- 16) Making a neat balance around top of column, find ϕ' .

$$\phi' = 1 - \frac{V_m H_m - L_{m+1} h_{m+1}}{\phi_a}$$

ϕ' must also tend to zero as the proper T_m and L_{m+1} are obtained.

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The Newton technique for quick convergence of iterations consists of substituting the slopes, or derivatives of the function at the point in question, for the new variables. A correction factor is calculated which must be subtracted from the previous T_m and L_{m+1} estimates to improve their accuracy. The equations for the derivatives are:

$$\begin{aligned} 17) \quad \frac{\partial \phi}{\partial T_m} &= \rho_1 = \frac{\partial}{\partial T_m} \left(\sum y_m / K_m \right) \\ &= \sum \frac{x_m}{K_m} (b_k + 2 c_k T_m + 3 d_k T_m^2) \end{aligned}$$

$$\begin{aligned} \frac{\partial \phi}{\partial L_{m+1}} &= \rho_2 = \frac{\partial}{\partial L_{m+1}} \left(\sum y_m / K_m \right) \\ &= - \frac{1}{V_m} \sum \frac{x_{m+1} - y_m}{K_m} \end{aligned}$$

$$\begin{aligned} \frac{\partial \phi'}{\partial T_m} &= \rho_3 = \frac{\partial}{\partial T_m} \left(1 - \frac{V_m H_m - L_{m+1} h_{m+1}}{\phi_a} \right) \\ &= - \frac{V_m}{\phi_a} \sum (b_h + 2 c_h T_m + 3 d_h T_m^2) y_m \end{aligned}$$

$$\begin{aligned} \frac{\partial \phi'}{\partial L_{m+1}} &= \rho_4 = \frac{\partial}{\partial L_{m+1}} \left(1 - \frac{V_m H_m - L_{m+1} h_{m+1}}{\phi_a} \right) \\ &= - \frac{1}{\phi_a} \left[\sum \bar{H}_m x_{m+1} - \sum \bar{h}_{m+1} x_{m+1} \right] \end{aligned}$$

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18) The correction equations are:

$$\rho_1 \Delta T_m + \rho_2 \Delta L_{m+1} = \phi$$

$$\rho_3 \Delta T_m + \rho_4 \Delta L_{m+1} = \phi'$$

rewriting and solving for ΔT_m and ΔL_{m+1} :

$$\Delta T_m = \frac{\phi \rho_4 - \rho_2 \phi'}{\rho_4 \rho_1 - \rho_2 \rho_3}$$

$$\Delta L_{m+1} = \frac{\phi - \rho_3 \Delta T_m}{\rho_4}$$

19) The new estimates for T_m and L_{m+1} are obtained by subtracting the correction factor from the previous estimates:

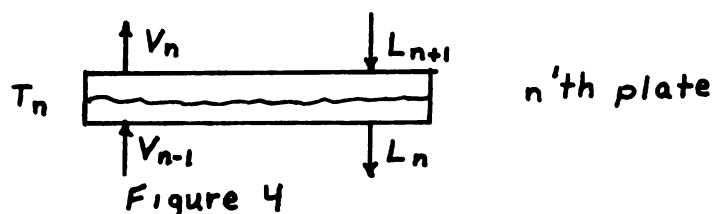
$$T_m(\text{new}) = T_m(\text{old}) - \Delta T_m$$

$$L_{m+1}(\text{new}) = L_{m+1}(\text{old}) - \Delta L_{m+1}$$

These new values for T_m and L_{m+1} are used to go through steps 11 - 19 again until they satisfy all the equations.

After steps 11 - 19 are solved, the solution for the m 'th plate is complete, at least for the first iteration through the column. Steps 10 - 19 are repeated M times until the feed plate is reached. The composition of the liquid leaving the feed plate as calculated above is then saved for the feed plate mesh later.

The calculations are now performed on the bottom of the tower in much the same manner as for the top of the tower.



By looking at the reboiler of Figure 2 and considering it a theoretical plate, one can see that the known quantities for the solution of the n' th plate will be the composition and temperature of the vapor entering the plate from below, i.e., plate $n-1$. The unknown quantities are V_{n-1} , L_n , X_{n1} , T_n , and $Y_{(n-1)1}$. Once again, there are actually more unknowns in $L_{(n+1)}$, $T_{(n+1)}$, and $X_{(n+1)1}$ but they will be solved for on the $(n+1)$ th plate. The same equations as used for the section above the feed plate are used in this section below the feed plate, except that the bubble point equation is substituted for the dew point equation. The Newton method is used here also, with the alteration that T_n and V_{n-1} are the two variables which are estimated.

- 20) Choose a first estimate of the temperature, T_n , and the vapor rate, V_{n-1} . Use as a first estimate the temperature and vapor rate from the solution of the previous plate. After the first iteration through the tower, this step will be altered the same as was step 10 in the other section of the column.

For the first plate above the reboiler, the original estimate cannot be obtained from the plate calculated below it, and so must be a good, qualified approximation. The vapor rate can be approximated quite well by considering the reflux ratio and the condition of the feed, i.e., liquid or vapor, superheated or supercooled.

- 21) Find K_{ni} using assumed T_n :

$$K_{ni} = a_{Ki} + b_{Ki} T_n + c_{Ki} T_n^2 + d_{Ki} T_n^3$$

- 22) Calculate the liquid rate from a material balance:

$$L_n = V_{n-1} + W$$

- 23) Calculate the composition of liquid on the n'th plate using a component material balance:

$$x_{ni} = \frac{W x_{wi} + V_{n-1} y_{(n-1)i}}{L_n}$$

For the first plate $y_{(n-1)i}$ was calculated in step 6 when $\sum K_n x_w = 1$. For succeeding plates $y_{(n-1)i}$ will be calculated in step 24 of the previous plate.

- 24) Calculate Θ (bubble point equation.)

$$\Theta = 1 - \sum K_n x_n$$

- 25) From the assumed T_n , and the temperature of the plate below, calculate H_{n-1} and h_n .

$$H_{n-1} = \sum \bar{H}_{n-1} y_{n-1}$$

$$h_n = \sum \bar{h}_n x_n$$

26) Calculate Θ' (heat balance.)

$$\Theta' = 1 + \frac{L_n h_n - V_{n-1} H_{n-1}}{Q_r}$$

27) The Newton method is used in the same manner here as for section above the feed plate and the equations for the slopes will not be derived.

Find $q_1 - q_4$

$$q_1 = - \sum y_n (b_K + 2 c_K T_n + 3 d_K T_n^2)$$

$$q_2 = - \frac{1}{L_n} \sum K_n (y_{n-1} - x_n)$$

$$q_3 = - L_n / Q_r \sum (b_h + 2 c_h T_n + 3 d_h T_n^2) x_n$$

$$q_4 = - \frac{1}{Q_r} [\sum \bar{H}_{n-1} y_{n-1} - \sum \bar{h}_n y_n]$$

28) Determine the correction factors ΔT_n and ΔV_{n-1} .

$$\Delta T_n = \frac{\Theta q_4 - q_2 \Theta'}{q_1 q_4 - q_2 q_3}$$

$$\Delta V_{n-1} = \frac{\Theta' - q_3 \Delta T_n}{q_4}$$

29) Determine the new values of T_n and V_{n-1} to put back into step 21. Steps 21 - 29 are repeated until the correction factors become arbitrarily close to zero.

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$$T_n \text{ (new)} = T_n \text{ (old)} - \Delta T_n$$

$$V_{n-1} \text{ (new)} = V_{n-1} \text{ (old)} - \Delta V_{n-1}$$

Steps 20 - 29 represent the solution of one plate, and so must be repeated N times. When the feed plate is reached, the compositions of the liquid stream leaving the feed plate, as calculated from the condenser down and the reboiler up, are compared to see if convergence has been attained.

The feed plate mesh consists of taking the ratio of the composition of the liquid leaving the feed plate as calculated from the condenser down to the composition calculated from the reboiler up. This is done for all components.

$$r_i = \frac{X_{fi} \text{ (down)}}{X_{fi} \text{ (up)}}$$

This ratio r_i should, of course, approach unity. The convenient property of r is that it not only tells whether or not one has convergence but also gives an indication of the size and direction the correction on the assumed products should be made. If r is greater than unity, then the amount of that component coming out overhead has been assumed too great. Conversely, if r is less than one, the quantity of that component in the overhead has been assumed too small.

The magnitude of r also indicates the magnitude of the error in the assumed products.

The important thing is that the ratios be used to correct the products in such a manner so as to conform with the overall material balance. In order to be able to apply the ratios to all components, it is very important that some quantity of each component be assumed going out in each product. This can be illustrated by taking the case where one component was assumed to come out in only one product, i.e., top or bottom product. If this were so, then when the assumed product for that particular component was multiplied (or divided) by the feed mesh ratio, the amount of product would still be zero, and thus unchanged. It should be pointed out that the components will always be corrected in the product stream where their composition is the smaller. The product stream containing the larger composition of the component is then corrected using an overall material balance.

For the components which tend to leave in the overhead, the following equations are used for correcting the assumed products:

$$\begin{aligned} W x_{wi} (\text{revised}) &= r_i \cdot W x_{wi} (\text{previous}) \\ D x_{Di} (\text{revised}) &= F x_{fi} - W x_{wi} (\text{revised}) \end{aligned}$$

For components which tend to leave in the bottom product the following correction equation is used:

$$Dx_{Di}(\text{revised}) = \frac{1}{r_i} Dx_{Di}(\text{previous})$$

The fact that the revised W/x_{wi} is not calculated here for the components which tend to leave in the bottoms is explained by pointing out that when re-iterating through the entire problem, one must go all the way back to step 1. It can be seen that in steps 2 and 3 the new W and x_{wi} are calculated, and thus need not be calculated here.

If the feed plate mesh ratio is arbitrarily close to one for all components, the solution is complete, at least for the number of plates used. However, if the problem is of the type where one wants to determine the number of plates necessary to obtain a desired separation, then the solution may not be complete. That is if the products do not meet the desired specifications, then a new number of plates must be chosen, and the problem worked through again.

This is the advantage of using a computer, since it can calculate the new conditions very quickly, while without such a machine one must be satisfied with trying to set approximate specifications.

COMPUTER USED

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COMPUTER USED

Throughout this investigation, the computer owned by Michigan State University was used exclusively. The computer is named "The Michigan State Integral Computer," better known as MISTIC. The computer operates in the binary number system and makes use of punch tape input and output. IBM card input and output are also available but were not used in this investigation.

The storage or memory consists of forty cathode ray tubes and the associated circuitry. At the present time, the capacity of the computer is rather limited, with only 1024 storage locations. However, this will soon be altered to well over 16,000 locations, when the new magnetic core memory is installed.

MISTIC is a single address machine, i.e., each instruction carries only one address. Orders for the MISTIC contain two symbols from the decimal digits 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, and the letters K, S, N, J, F, L, and one decimal number between 0 and 1023. The two symbols form the operation code, while the number is an identification number (address) for one of the 1024 electrostatic memory locations. In essence, the operation code tells the computer what to do and the

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Two orders constitute one word and are referred to as an order pair. There is a lefthand order and a righthand order in each word. The orders are obeyed in sequence left to right.

Since the MISTIC is a binary machine, the address in each order must be in binary form before entering the machine. This would require a tremendous amount of work by the programmer; and, fortunately, there is an input program available to convert the decimal addresses to sexadecimal automatically. This program is known as the Decimal Order Input (DOI) and is used in all problems.

When using the DOI, each order must contain a two digit operation code, an address between 0 and 1023, and a termination symbol. The termination symbols are K, S, N, J, F, and L.

Because of the complexity of the method of solution of the distillation problem, it was decided to use the floating point subroutine even though the subroutine actually causes the computer to perform the calculations at a much slower

speed. However, by using the floating point routine, hereafter referred to as A₁, the tedious task of scaling the numbers was bypassed, since this subroutine keeps track of the decimal point automatically. To use ordinary MISTIC orders would require that all numbers be scaled so that they are between plus one and minus one. This scaling must also consider all numbers which will be calculated, making sure that they, too, would lie in the proper range.

Almost the entire distillation program is written in A₁, with a few orders being in ordinary MISTIC language. For any questions that arise concerning the few MISTIC orders, reference should be made to the MISTIC Programming Manual. In the appendix of this thesis is an outline of the orders encountered in using the A₁ subroutine. This may prove helpful as a reference when reading through the program.

DETAILED CODING PROCEDURE

DETAILED CODING PROCEDURE

This section will be devoted to outlining the problems of programming a problem for use on a high speed computer, as well as the detailed coding of the main program used. It is intended that such a detailed coding of the program might aid the reader in visualizing the method of calculation used.

Liquid vapor equilibrium data used throughout this investigation was of the type $y = Kx$. It was assumed that K depended only on temperature and pressure. In order to quickly calculate a desired K value at a given temperature, third degree polynomials of the form $K = a_k + b_k T + c_k T^2 + d_k T^3$ were used to describe the variation of K with temperature. The four constants were evaluated for various components, using the method of least squares on the data of Cooper and Donnell, and Maxwell. These polynomials were prepared at various pressures within the range of operation for a distillation column.

Enthalpy of liquids and vapors of each component were also represented by third order polynomials in temperature. The data used was from Maxwell. The enthalpy of a mixture was assumed to be the sum of the individual products of mole fraction and enthalpy of pure product.

Before one reads through the detailed coding of any program, it is well to point out that in many cases, calculations are set up in a far different manner and order for a computer than would be done if a person were to do the same calculations by hand or with a desk calculator. It should also be pointed out that in programming such a problem for a computer, there are quite often several choices of orders one could use. Thus, a person reading this program might well find places where orders could be changed or possibly even left out. This is especially true in the program illustrated here. Due to the complexity of the problem, there were many changes to be made after the program was put together. In order to conserve time, the program was altered in sort of a piecemeal affair. However, this in no way affects the principles involved, nor the calculations which are being carried out.

Before getting into the main program, it should be pointed out that the enthalpy polynomial subroutine (HSR) and the equilibrium constant subroutine (KSR) will not be outlined. They simply involve the calculation of the K values and the enthalpy values for a given compound from a third degree polynomial. The factored form of the

polynomial is used to decrease the number of orders required. For instance, $K = [(d_K T + c_K) T + b_K] T + a_K$. This way, the constants for the polynomials must be input in reverse order; that is, in the order d, c, b, and a for each component. The constants must be changed for each different tower pressure as well as for when different components are in the feed.

Whenever control is transferred to HSR or KSR from the main program, the K values or enthalpy values are calculated, then control is transferred automatically back to the next order in the main program. In other words, both HSR and KSR are closed subroutines.

The outline of the program shall be broken down into three sections: 1) Specification of Parameters, 2) Outline of Data, and 3) Main Program.

Specification of Parameters

This involves specifying various parameters before the problem can be worked. These parameters are essential to the solution of the problem. The parameters are used in conjunction with the S termination symbol to specify certain addresses within the program. The parameters which must be specified and stored in locations 3 - 11 are:

- 3) Specifies floating register for floating point subroutine
- 4) Number of components
- 5) Plates above feed plate
- 6) Plates below feed plate
- 7) Number of components x 4
- 8) Number of components x 8
- 9) Total number of plates less feed plate
- 10) Number of components expected in overhead product in appreciable amount
- 11) Number of components expected in bottom product in appreciable amount

For this program, location 3 is always the same and specifies location 28 as the floating register. All the other parameters may vary with the particular problem being worked. Perhaps the parameters specified in locations 10 and 11 should be made a little clearer. An example will be given to illustrate their use. In a given problem, there are eight components in the feed, and it is to be split in two products, the top product containing essentially the three most volatile components and the bottom product containing essentially the other five components. It is evident

that some of the light components will appear in the bottom product and some of the heavy components will appear in the top product, but in small amounts. In this case, location 10 will specify three components in overhead product and location 11 will specify five components in bottom product. The sum of locations 10 and 11 must always be equal to the total number of components in the feed. In the case of a component which will appear in both products in appreciable amounts, it won't matter where it is assumed to be in the greater amount.

The parameters are used primarily for the reading in of the program to the computer; and many of them are destroyed by storing other results in the same locations, once the program has been read in.

Outline of Data

There are certain bits of data that are necessary to work a problem, such as feed composition, feed condition, as well as initial estimates of certain variables which are to be determined by trial and error. Following is a list of essential data and the locations in which it is stored.

- 647-654 Assumed moles of each component leaving in
 overhead product
- 655 Initial estimate of still temperature
- 656 Integer one
- 657 Constant for bubble point and dew point
 convergence tests
- 658 Constant for temperature convergence
- 659 Reflux ratio (L/D)
- 660 Initial estimate of top temperature
- 661-663 Any other constants which are necessary when
 program alterations are made
- 664 Initial estimate of vapor rate in stripping
 section
- 665-672 Mole fraction of each component in feed
- 673 Enthalpy of feed (BTU per mole)
- 674 Constant for ratio r convergence
- 675 Same as 661-663

The maximum number of components this program will handle is eight. If more memory space were available, the program could easily be altered to handle as many components as desired. The constants which must be specified for various convergence tests will depend on just how accurate an

answer is desired. For example, in finding the temperature on a certain plate, the temperature is changed until the sum of the mole fractions is unity. However, to actually obtain unity might require very much time when a value of $1 \pm .001$ would serve just as well. In this case, then, the constant in location 657 would be .001.

When a feed is used which contains less than eight components, the remaining memory locations must be filled with some arbitrary constants. The reason being that the computer, in reading in the data, stores it consecutively. Thus, if the blank locations are not filled, the data following will be stored in a different location than specified. For the same reason, all data locations must be filled. It is also essential that in the feed composition, assumed $D \times_0$, and in the KSR and HSR the components are always in the same order.

Main Program

Outline of Storage Space

0, 1, 2	Temporary storage
3-11*	Parameter specification
10	Temperature storage for equilibrium and enthalpy subroutines

11-18	Storage of K and H values
20-27	Storage of h values
28-29	Floating accumulator (Specified by 3)
30-300	Program
300-356	Answer storage
357-398	Equilibrium constant subroutine
399-478	Enthalpy subroutine
479-646	Floating point subroutine
647-675	Data
676-686	Space for program alterations
687-706	Program
707-719	Space for program alterations
720-1023	Answer storage

*The parameters specified in locations 10 and 11 are destroyed after program is read in.

Outline of Answer Storage

300	D
301	W
302	$(\sum x_o/K) - 1, (\sum K x_w) - 1$
303	Qa
304	Qr
305	$-\phi', \Delta T_m, -\theta, \Delta T_n$
306	$\sum h_{m+1} L_{m+1}, -\phi', \Delta L_{m+1}, \sum V_{n-1} H_{n-1}, \theta', \Delta V_{n-1}$

1

307	Temperature storage in calculating $p_1 - p_4$, $q_1 - q_4$
308	$\Sigma H_m x_{m+1}$, $\Sigma H_{n-1} y_{n-1}$
309	$\Sigma h_{m+1} x_{m+1}$, $\Sigma h_n y_n$
310	p_1 , $-q_1$
311	$-p_2$, $-q_2$
312	$-p_3$, $-q_3$
313	p_4 , q_4
314	Constant for testing iterations through top of column
315	Used over and over for various sums
316	Constant for testing iterations through bottom of column
317-324	x_{0i}
325-332	x_{wi}
333-340	x_f as calculated from condenser downward
341-348	$y_{(n-1)i}$
349-356	x_{mi}
720-808	Temperature on various plates
813-905	Vapor rates from each plate
906-998	Liquid rates from each plate
999-1007	K values, r values
1008-1015	y_{mi} , y_{ni}
1016-1023	$x_{(m+1)i}$, x_{ni}

0030K

- 0) 41 314F Put a zero in location 314
- 50 L Standard entry to subroutine
- 1) 26 479F Enter floating point subroutine
- 1K 29F Set box 1 counter at 29
- 2) 88 F Read in floating point fraction
- 1S 647F Store fraction in location 647
- 3) 13 2L Loop to left side of location 2L
- 85 660F Bring in T_1
- 4) 8S 720F Store T_1 in location 720
- 85 655F Bring in T_2
- 5) 8S 721S5 Store T_2 in location 721S5
- 85 664F Bring in V_1
- 6) 8S 813S5 Store V_1 in location 813S5
- 5K F Waste order (change for program alteration)
- 7) 8K F Put zero in accumulator
- 8S 316F Store zero in location 316
- 8) 0K S5 Set box 0 for number of plates above feed
- 1K 84 Set box 1 for number of components
- 9) 8K F Put zero in accumulator
- 14 647F Add $D \times \alpha_i$ to accumulator
- 10) 12 9L Loop to right side 9L
- 8S 300F Place $\sum D \times \alpha_0$ in location 300

1

- 11) 87 659F Multiply $\mathbb{M}$ by $\mathbb{R}$
 8S 906F Place $\mathbb{DR} = \mathbb{L}_0$ in location 906
- 12) 84 300F Add $\mathbb{D}$ to $\mathbb{DR}$
 8S 813F Place $\mathbb{D}(\mathbb{R} + 1) = \mathbb{V}$, in location 813
- 13) 85 656F Bring in integer 1
 80 300F Subtract $\mathbb{D}$
- 14) 8S 301F Store $1 - \mathbb{D} = \mathbb{W}$ in location 301
 1K S4 Set box 1 counter at S4
- 15) 15 665F Bring in x_f
 10 647F Subtract $\mathbb{D} x_0$
- 16) 86 301F Divide by $\mathbb{W}$
 1S 325F Store $\frac{x_f - \mathbb{D} x_0}{\mathbb{W}} = x_w$ in location 325
- 17) 13 15F Loop to left side of location 15L
 1K S4 Set box 1 at S4
- 18) 15 647F Bring in $\mathbb{D} x_0$
 86 300F Divide by $\mathbb{D}$
- 19) 1S 317F Store $\mathbb{D} x_0 / \mathbb{D} = x_0$ in location 317
 13 18L Loop to left side of location 18L
- 20) 85 720F Bring in $\mathbb{T}_1$
 8S 10F Place $\mathbb{T}_1$ in location 10 for KSR
- 21) 1K S4 Set box 1 at S4
 8J 22L Leave $\mathbb{A}$, go to left side of location 22L

- 22) 41 315F Put zero in location 315
50 22L Standard entry to KSR
- 23) 26 357F Transfer control to KSR
15 317F Bring in X_0 (equals y_1)
- 24) 16 11F Divide by K
1S 1016F Store $y_1/K = X_1$ in location 1016
- 25) 84 315F Add contents of location 315
8S 315F Store sum back in location 315
- 26) 12 23L Loop to right side of location 23L
80 656F Subtract 1 from $\sum x_i$
- 27) 8S 302F Store $\sum x_i - /$ in location 302
85 657F Bring in convergence test constant
- 28) 8N 302F Subtract absolute value of $(\sum x_i - /)$
83 34L If positive (convergence) go to left side
of 34L; if minus, go on
- 29) 85 302F Bring in $(\sum x_i - /)$
83 32L If positive (temperature too low) go to left
side 32L
- 30) 85 720F (Temperature too high) bring in T_1
80 658F Subtract temperature convergence constant
- 31) 8S 720F Store new T_1 in location 720
82 20L T_1 always positive, so transfer to right side
20L

- 32) 85 720F Bring in T_1 (temperature too low)
84 658F Add temperature convergence constant
- 33) 88 720F Store new T_1 in location 720
82 20L Transfer control to right side 20L
- 34) 85 721S5 Bring in T_5
88 10F Place in location 10 for KSR
- 35) 1K S4 Set box 1 counter at S4
8J 36L Leave A_1 , transfer to left side location 36L
- 36) 41 315F Place zero in location 315
50 36L Standard entry to KSR
- 37) 26 357F Transfer control to KSR
15 325F Bring in X_w
- 38) 17 11F Multiply by K
18 341F Place $X_w \cdot K = Y_5$ in location 341
- 39) 84 315F Add contents of location 315
88 315F Store sum in location 315
- 40) 12 37L Loop to right side location 37L
80 656F Subtract 1 from $\sum y_s$
- 41) 88 302F Store $-(1 - \sum y_s)$ in location 302
85 657F Bring in convergence test constant
- 42) 8N 302F Subtract absolute of $-(1 - \sum y_s)$
83 48L If positive (convergence) go to left side 48L

- 43) 85 302F Bring in $-(1 - \sum y_s)$
83 46L If plus (temperature too high) go to
left side 48L
- 44) 85 721S5 Bring in T_s
84 658F Add temperature convergence constant
- 45) 8S 721S5 Store new T_s in location 721S5
82 34L Transfer to right side of 34L
- 46) 85 721S5 Bring in T_s
80 658F Subtract temperature convergence constant
- 47) 8S 721S5 Store new T_s in location 721S5
82 34L Transfer to right side 34L
- 48) 85 660F Bring in initial estimate of T_i
8S 10F Place in location 10 for KSR
- 49) 1K S4 Set box 1 counter at S4
8J 50L Leave A, , and go to left side of 50L
- 50) 41 315F Store zero in location 315
50 50L Standard entry to KSR
- 51) 26 357F Transfer control to KSR
15 11F Bring in K_i
- 52) 17 317F Multiply by X_{0i}
84 315F Add contents of location 315
- 53) 8S 315F Place sum in location 315
12 51L Loop to right side of 51L

- 54) 80 656F Subtract 1 from $\sum K X_0$
8S 302F Store $-(1 - \sum K x_0)$ in location 302
- 55) 85 657F Bring in convergence test constant
8N 302F Subtract absolute of $-(1 - \sum K x_0)$
- 56) 82 61L If plus (convergence) transfer to right side 61L
85 302F Bring in $-(1 - \sum K x_0)$
- 57) 82 59L If plus (temperature too high) go to right side 59L
85 660F Bring in T_c
- 58) 84 658F Add temperature convergence constant
8S 660F Store new T_c in location 660
- 59) 82 48L Transfer to right side of 48L
85 660F Bring in T_c
- 60) 80 658F Subtract temperature convergence constant
8S 660F Store new T_c in 660
- 61) 82 48L Transfer to right side of 48L
85 660F Bring in T_c
- 62) 8S 10F Store in location 10 for HSR
8J 63L Leave A_1 , transfer to right side 63L
- 63) 41 315F Place zero in location 315
50 63L Standard entry to HSR

- 64) 26 399F Transfer control to HSR
 1K S4 Set box 1 at S4
- 65) 15 20F Bring in $\bar{h}$
 17 317F Multiply by X_0
- 66) 84 315F Add contents of location 315
 88 315F Place sum in location 315
- 67) 13 65L Loop to left side location 65L
 87 906F Multiply h_c by L_0
- 68) 8S 315F Store $h_c L_0$ in location 315
 8K 2F Place interger 2 in accumulator
- 69) 83 687F Transfer control to left side 687
 8K F Waste order
- 70) 05 721F Bring in T_m
 8S 10F Place in location 10 for KSR
- 71) 1K S4 Set box 1 counter at S4
 8J 72L Leave A_i , transfer to left side 72L
- 72) 41 315F Place zero in location 315
 50 72L Standard entry to KSR
- 73) 26 357F Transfer control to KSR
 15 11F Bring in K_i
- 74) 1S 999F Store K_i in location 999
 12 73L Loop to right side of location 73L

- 75) 05 907F Bring in L_{m+1}
84 300F Add D
- 76) 0S 814F Store $L_{m+1} + D = V_m$ in location 814
1K S4 Set box 1 counter at S4
- 77) 05 907F Bring in L_{m+1}
17 1016F Multiply by X_{m+1}
- 78) 14 647F Add X_0
06 814F Divide by V_m
- 79) 1S 1008F Store Y_m in location 1008
13 77L Loop to left side location 77L
- 80) 1K S4 Set box 1 counter at S4
15 1008F Bring in Y_m
- 81) 16 999F Divide by K
1S 349F Store $Y_m / K_m = X_m$ in location 349
- 82) 84 315F Add contents of location 315
8S 315F Store sum in location 315
- 83) 12 80L Loop to right side of location 80L
80 656F Subtract 1 from $\sum X_m$
- 84) 8S 305F Store $-1 + \sum X_m = -\phi$ in location 305
05 720F Bring in T_{m+1}
- 85) 8S 10F Place T_{m+1} in location 10 for HSR
8J 86L Leave A, , transfer to left side of 86L

- 86) 41 309F Place zero in location 309
50 86L Standard entry to HSR
- 87) 26 399F Transfer control to HSR
4K S4 Set box 4 counter at S4
- 88) 45 20F Bring in $\bar{h}$
47 1016F Multiply by X_{m+1}
- 89) 84 309F Add contents of location 309
8S 309F Store sum in location 309
- 90) 43 88L Loop to left side of location 88L
07 907F Multiply by L_{m+1}
- 91) 8S 306F Store $L_{m+1} \cdot h_{m+1}$ in location 306
05 721F Bring in T_m
- 92) 8S 10F Place T_m in location 10 for HSR
8J 93L Leave A, , transfer to left side of 93L
- 93) 41 315F Place zero in location 315
50 93L Standard entry to HSR
- 94) 26 399F Transfer control to HSR
4K S4 Set box 4 counter at S4
- 95) 8K F Bring in zero
8S 308F Store zero in location 308
- 96) 45 11F Bring in $\bar{H}_m$
47 1016F Multiply by X_{m+1}

1

- 97) 84 308F Add contents of location 308
8S 308F Place sum in location 308
- 98) 45 11F Bring in $\bar{h}_m$
47 1008F Multiply by Y_m
- 99) 84 315F Add contents of location 315
8S 315F Place sum in location 315
- 100) 43 96L Loop to left side of location 96L
07 814F Multiply by V_m
- 101) 80 306F Subtract L_{m+1} h_{m+1}
86 303F Divide by Q_a
- 102) 80 656F Subtract integer 1
8S 306F Store- ϕ' in location 306
- 103) 1K 4F Set box 1 counter at 4
8K F Place zero in accumulator
- 104) 1S 310F Place zero in location 310
13 104L Loop to left side of 104L
- 105) 1K F Set box 1 counter at zero
2K S4 Set box 2 counter at S4
- 106) 8K 3F Bring in integer 3
17 367F Multiply by d_K
- 107) 07 721F Multiply by T_m
8S 307F Store $3dkT_m$ in location 307

- 108) 8K 2F Bring in integer 2
17 368F Multiply by c_K
- 109) 84 307F Add $3d_K T_m$
07 721F Multiply by T_m
- 110) 14 369F Add b_K
27 349F Multiply by X_m
- 111) 84 310F Add contents of location 310
8S 310F Store sum in location 310
- 112) 1L 4F Increase increment of box 1 by 4
23 106L Loop to left side of location 106L
- 113) 1K S4 Set box 1 counter at S4
15 1016F Bring in X_{m+1}
- 114) 10 1008F Subtract Y_m
16 999F Divide by K_m
- 115) 84 311F Add contents of location 311
8S 311F Store sum in location 311
- 116) 12 113L Loop to right side of 113L
06 814F Divide by V_m
- 117) 8S 311F Store $-p_2$ in location 311
1K F Set box 1 counter at zero
- 118) 2K S4 Set box 2 counter at S4
8K 3F Bring in integer 3

- 119) 17 416F Multiply by d_h
07 721F Multiply by T_m
- 120) 8S 307F Store in location 307
8K 2F Bring in integer 2
- 121) 17 417F Multiply by c_h
84 307F Add $3d_h T_m$
- 122) 07 721F Multiply by T_m
14 418F Add b_h
- 123) 27 1008F Multiply by Y_m
84 312F Add contents of location 312
- 124) 8S 312F Store sum in location 312
1L 4F Increase increment of box 1 by 4
- 125) 22 118L Loop to right side of location 118L
07 814F Multiply by V_m
- 126) 86 303F Divide by Q_a
8S 312F Store $-p_3$ in location 312
- 127) 85 309F Bring in $\sum \bar{h}_{m+1} x_{m+1}$
80 308F Subtract $\sum \bar{H}_m x_{m+1}$
- 128) 86 303F Divide by Q_a
8S 313F Store p_4 in location 313
- 129) 85 311F Bring in $-p_2$
87 312F Multiply by $-p_3$

- 130) 8S 308F Store $p_2 p_3$ in location 308
85 313F Bring in p_4
- 131) 87 310F Multiply by p_1
80 308F Subtract $p_2 p_3$
- 132) 8S 308F Store $p_4 p_1 - p_2 p_3$ in location 308
85 311F Bring in $-p_2$
- 133) 87 306F Multiply by $-\phi'$
8S 309F Store $p_2 \phi'$ in location 309
- 134) 81 305F Bring in ϕ
87 313F Multiply by p_4
- 135) 80 309F Subtract $p_2 \phi'$
86 308F Divide by $p_4 p_1 - p_2 p_3$
- 136) 8S 305F Store ΔT_m in location 305
85 312F Bring in $-p_3$
- 137) 87 305F Multiply by ΔT_m
80 306F Subtract $-\phi'$
- 138) 86 313F Divide by p_4
8S 306F Store ΔL_{m+1} in location 306
- 139) 05 721F Bring in old T_m
80 305F Subtract ΔT_m
- 140) 0S 721F Store new T_m in location 721
05 907F Bring on old L_{m+1}

- 141) 80 306F Subtract ΔL_{m+1}
0S 907F Store new L_{m+1} in location 907
- 142) 85 305F Bring in ΔT_m
8N 658F Subtract absolute of temperature
convergence constant
- 143) 82 69L If plus not convergence, transfer to right
side 69L
85 306F Bring in ΔL_{m+1}
- 144) 8N 657F Subtract absolute of temperature convergence
constant
82 69L If plus not convergence, go to right side 69L
- 145) 1K S4 Set box 1 counter at S4
15 349F Bring in X_m
- 146) 1S 1016F Store X_m in 1016 (now becomes X_{m+1})
12 145L Loop to right side 145L
- 147) 02 695F Next plate, loop to right side 695
1K S4 Set box 1 counter at S4
- 148) 15 349F Bring in X_m (feed plate composition)
1S 333F Store in location 333
- 149) 13 148L Loop to left side 148L
8K 2F Bring in integer 2
- 150) 83 181F Transfer to left side location 181
83 181F Waste order

00181K

- 0) 0K S6 Set box 0 counter at S6
8J 1L Leave A_1 , transfer to left side 1L
- 1) 1S 316F Bring in loop counter constant
L0 6F Subtract number of plates below feed
- 2) 36 7L If plus, go to left side 7L
F3 316F Bring in loop constant and add 1 to it
- 3) 40 316F Store new loop constant at 316
50 3L Standard entry to A_1
- 4) 26 479F Transfer control to A_1
05 721S5 Bring in T_s
- 5) 08 722S5 Store T_n in location 722S5
05 813S5 Bring in V_{n-1}
- 6) 08 814S5 Store V_{n-1} in 814S5
82 7L Transfer control to right side 7L
- 7) 22 704F (MISTIC) transfer to right side 704
05 814S4 Bring in V_{n-1}
- 8) 84 301F Add W
08 907S5 Store $V_{n-1} + W = L$ in location 907S5
- 9) 1K S4 Set box 1 counter at S4
15 341F Bring in Y_{n-1}
- 10) 07 814S5 Multiply by V_{n-1}
1S 1016F Store in 1016

- 11) 85 301F Bring in W
- 17 325F Multiply by X_w
- 12) 14 1016F Add V_{n-1} y_{n-1}
- 06 907S5 Divide by L_n
- 13) 1S 1016F Store X_n ; in location 1016
- 12 9L Loop to right side of 9L
- 14) 05 722S5 Bring in T_n
- 8S 10F Place T_n in location 10 for KSR
- 15) 1K S4 Set box 1 counter at S4
- 8J 16L Leave A, , go to right side of 16L
- 16) 41 315F Place zero in 315
- 50 16L Standard entry to KSR
- 17) 26 357F Transfer control to KSR
- 15 11F Bring in K
- 18) 1S 999F Store K at location 999
- 17 1016F Multiply by X_n
- 19) 1S 1008F Store Y_n in location 1008
- 84 315F Add contents of location 315
- 20) 8S 315F Place sum in location 315
- 12 17L Loop to right side of 17L
- 21) 80 656F Subtract 1
- 8S 305F Store $(\sum y_n - 1) = -\Theta$ in location 305

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- 22) 05 721S5 Bring in T_{n-1}
8S 10F Store T_{n-1} in location 10 for HSR
- 23) 1K S4 Set box 1 counter at S4
8J 24L Leave A_1 , go to left side 24L
- 24) 41 308F Place zero in location 308
50 24L Standard entry to HSR
- 25) 26 399F Transfer control to HSR
15 11F Bring in $\bar{H}$
- 26) 17 341F Multiply by y_{n-1}
84 308F Add contents of location 308
- 27) 8S 308F Store sum in location 308
12 25L Loop to right side of location 25L
- 28) 07 814S5 Multiply by V_{n-1}
8S 306F Store $H_{n-1} \cdot V_{n-1}$ in location 306
- 29) 05 722S5 Bring in T_n
8S 10F Store T_n in location 10 for HSR
- 30) 1K S4 Set box 1 counter at S4
8J 31L Leave A_1 , transfer to left side 31L
- 31) 41 315F Store zero in location 315
50 31L Standard entry to HSR
- 32) 26 399F Transfer control to HSR
8K F Put zero in accumulator

- 33) 8S 309F Store zero in location 309
15 20F Bring in $\bar{h}$
- 34) 17 1008F Multiply by y_n
84 309F Add contents of location 309
- 35) 8S 309F Store sum in location 309
15 20F Bring in $\bar{h}$
- 36) 17 1016F Multiply by X_n
84 315F Add contents of location 315
- 37) 8S 315F Store sum in location 315
12 33L Loop to right side of location 33L
- 38) 07 907S5 Multiply by L_n
80 306F Subtract $V_{n-1} H_{n-1}$
- 39) 86 304F Divide by Q_n
84 656F Add integer 1
- 40) 8S 306F Store Θ' in location 306
1K 4F Set box 1 counter at 4
- 41) 8K F Bring in zero
1S 310F Store zero in location 310
- 42) 12 41L Loop to right side location 41L
1K F Set box 1 counter at zero
- 43) 2K S4 Set box 2 counter at S4
8K 3F Bring in integer 3

- 44) 17 367F Multiply by d_k
 07 722S5 Multiply by T_n
- 45) 8S 307F Store $3d_k T_n$ in location 307
 8K 2F Bring in integer 2
- 46) 17 368F Multiply by c_k
 84 307F Add $3d_k T_n$
- 47) 07 722S5 Multiply by T_n
 14 369F Add b_k
- 48) 27 1008F Multiply by Y_n
 84 310F Add contents of location 310
- 49) 8S 310F Store sum in location 310 ($-q_1$)
 1L 4F Increase box 1 counter by 4
- 50) 22 43L Loop to right side of location 43L
 1K S4 Set box 1 counter at S4
- 51) 15 341F Bring in Y_{n-1}
 10 1016F Subtract X_n
- 52) 17 999F Multiply by K_n
 84 311F Add contents of location 311
- 53) 8S 311F Store sum in location 311
 13 51L Loop to left side of location 51L
- 54) 06 90785 Divide by L_n
 8S 311F Store $-q_2$ in location 311

- 55) 1K F Set box 1 counter at zero
 2K S4 Set box 2 counter at S4
- 56) 8K 3F Bring in integer 3
 17 416F Multiply by d_h
- 57) 07 722S5 Multiply by T_n
 8S 307F Store $3d_h T_n$ in location 307
- 58) 8K 2F Bring in integer 2
 17 417F Multiply by c_h
- 59) 84 307F Add $3d_h T_n$
 07 722S5 Multiply by T_n
- 60) 14 418F Add b_h
 27 1016F Multiply by X_n
- 61) 84 312F Add contents of location 312
 8S 312F Store sum in location 312
- 62) 1L 4F Increase box 1 counter by 4
 23 56L Loop to left side of location 56L
- 63) 86 304F Divide by Q_r
 07 907S5 Multiply by L_n
- 64) 8S 312F Store $-q_3$ in location 312
 85 309F Bring in $h_n Y_n$
- 65) 80 308F Subtract $\bar{H}_{n-1} Y_{n-1}$
 86 304F Divide by Q_r

- 66) 8S 313F Store q_4 in location 313
8S 311F Bring in $-q_2$
- 67) 87 312F Multiply by $-q_3$
8S 307F Store q_2q_3 in location 307
- 68) 81 310F Bring in q_1
87 313F Multiply by q_4
- 69) 80 307F Subtract q_2q_3
8S 307F Store in location 307
- 70) 81 305F Bring in Θ
87 313F Multiply by q_4
- 71) 8S 305F Store Θq_4 in location 305
8S 311F Bring in $-q_2$
- 72) 87 306F Multiply by Θ'
84 305F Add Θq_4
- 73) 86 307F Divide by $q_1q_4 - q_2q_3$
8S 305F Store ΔT_n in location 305
- 74) 8S 312F Bring in $-q_3$
87 305F Multiply by ΔT_n
- 75) 84 306F Add Θ'
86 313F Divide by q_4
- 76) 8S 306F Store ΔV_{n-1} in location 306
0S 722S5 Bring in T_n (old)
- 77) 80 305F Subtract ΔT_n
0S 722S5 Store new T_n in location 722S5

78) 05 814S5 Bring in old V_{n-1}
80 306F Subtract ΔV_{n-1}
79) 08 814S5 Store new V_{n-1} in location 814S5
85 305F Bring in ΔT_n
80) 8N 658F Subtract temperature convergence constant
82 7L If plus (not convergence) loop to right side
7L
81) 85 306F Bring in ΔV_{n-1}
8N 657F Subtract convergence test constant
82) 82 7L If plus (not convergence) loop to right side
7L
1K S4 Convergence, so set box 1 counter at S4
83) 11 1008F Bring in y_n
1S 341F Store y_n in location 341 (now becomes Y_{n-1})
84) 13 83L Loop to left side of location 83L
02 181F Next plate, loop to right side location 181
85) 1K SK Set box 1 counter at SK
15 333F Bring in X_f as calculated from condenser
downward
86) 16 1016F Divide by X_f as calculated from reboiler
upward
1S 999F Store r in location 999

- 87) 87 301F Multiply by W
17 325F Multiply by X_w
- 88) 88 302F Store $r W/X_w$ in location 302
81 302F Bring in $- r W/X_w$
- 89) 14 665F Add X_f (also equals $F X_f$)
18 647F Store revised $D x_0$ in location 647
- 90) 12 85L Loop to right side of location 85L
1K SS Set box 1 counter at SS
- 91) 15 333SK Bring in X_f as calculated from top down
15 1016SK Divide by X_f as calculated from bottom up
- 92) 18 999SK Store r in location 999SK
15 647SK Bring in previous $D x_0$
- 93) 16 999SK Divide by r
18 647SK Store $D x_0$ revised in location 647SK
- 94) 13 91L Loop to left side of location 91L
1K S4 Set box 1 counter at S4
- 95) 15 999F Bring in r
80 656F Subtract integer one
- 96) 8N 674F Subtract absolute of convergence constant
82 98L If plus must iterate, transfer to right side 98L
- 97) 13 95L If above minus component converged, test next component
8K 2F Bring in integer 2 to make plus

- 98) 82 99L Transfer control to right side location 99L
8K 2F Make plus for next order to be obeyed
- 99) 83 38F Reiterate through entire tower
8K F Bring in zero
- 100) 8S 314F Store zero in location 314 (for additional
reflux ratios)
8K F Waste order
- 101) 1K 1S5 Set box 1 counter at 1S5
15 720F Bring in temperatures above feed plate
- 102) 8 96F Output temperature
12 101L Loop to right side of location 101L
- 103) 1K S6 Set box 1 counter at S6
15 720S9 Bring in temperatures below feed (in
reverse order)
- 104) 89 6F Output temperature
1L 1022F Used to output temperatures in forward
order
- 105) 12 103L Loop to right side of location 103L
1K 1S5 Set box 1 counter at 1S5
- 106) 15 906F Bring in liquid rates above feed plate
89 6F Output liquid rates
- 107) 13 106L Loop to left side of location 106L
1K S6 Set box 1 counter at S6

- 108) 15 906S9 Bring in liquid rates below feed
(reverse order)
89 6F Output liquid rate
- 109) 1L 1022F Used to output liquid rates in forward
order
13 108L Loop to left side of location 108L
- 110) 1K 1S5 Set box 1 counter at 1S5
15 813F Bring in vapor rates above feed
- 111) 89 6F Output vapor rate
12 110L Loop to right side of location 110L
- 112) 1K S6 Set box 1 counter at S6
15 813S9 Bring in vapor rates below feed
(reverse order)
- 113) 89 6F Output vapor rates
1L 1022F Used to output vapor rates in forward
order
- 114) 12 112L Loop to right side of location 112L
1K 16F Set box 1 counter at 16
- 115) 15 317F Bring in X_D and X_W
89 6F Output X_D and X_W
- 116) 13 115L Loop to left side of location 115L
85 300F Bring in D

117) 89 6F Output D
 8J 118L Leave A₁ , transfer to location 118L
118) 0F F Shuts machine off
 0F F Waste order

00 687K

0) 85 720F Bring in T₁
 8S 10F Store T₁ in location 10 for HSR
1) 1K S4 Set box 1 counter at S4
 8J 2L Leave A₁ , transfer to left side 2L
2) 41 303F Store zero in location 303
 50 2L Standard entry to HSR
3) 26 399 Transfer control to HSR
 15 11F Bring in $\bar{H}$ ₁
4) 17 317F Multiply by X₀
 84 303F Add contents of location 303
5) 8S 303F Store sum in location 303
 12 3L Loop to right side of location 3L
6) 87 813F Multiply by L₀
 80 315F Subtract h₀
7) 8S 303F Store Q_a in location 303
 80 673F Subtract H_f
8) 8S 304F Store Q_r in location 304
 8J 9L Leave A₁ , transfer to 9L

- 9) 15 314F (MISTIC) Bring in loop counter
 10 5F Subtract contents of location 5
- 10) 32 15L If plus go to right side of 15L
 F5 314F Bring in contents of 314 and add one
- 11) 40 314F Store in location 314
 50 11L Standard entry to A₁
- 12) 26 479F Enter A₁
 05 900F Bring in V_n
- 13) 03 907F Store in location 907
 05 720F Bring in T_n
- 14) 05 721F Store in location 721
 8K 2F Bring in integer 2
- 15) 82 16L Transfer to right side 16L
 50 15L Standard entry to A₁
- 16) 26 479F Transfer control to A₁
 8K 2F Bring in integer 2 (makes plus)
- 17) 83 100F Transfer to left side location 100
 50 17L Standard entry to A₁
- 18) 26 479F Enter A₁
 8K 2F Bring in integer 2
- 19) 82 188F Transfer to location 188
 82 188F Waste order

There are many ways in which the foregoing program may be altered to perform a desired calculation. Several of the possible desirable alterations which have been made shall now be discussed.

In an investigation such as this where many problems must be solved, the program as it stands would only allow one problem to be worked, then the computer would shut off. If more problems were desired to be run, the new problem would then have to be read into the computer. It is desirable, then, to be able to put five, ten, or even twenty problems on one tape, and let the computer solve them all one after the other. The only major change which must be made is to remove the order which instructs the machine to shut off and to replace it by a transfer of control order to some location where the program alterations are to be stored.

If one desires a given problem to be worked for various values of reflux ratio, holding everything else constant, this may be accomplished very simply by changing the right hand order in location 36 to be $SK(n)F$, where (n) is the number of various reflux ratios to be run. Then it would only require a few new orders which would change the reflux

ratio as desired and start the problem over using the new reflux ratio. This could be accomplished by either instructing the computer to read in more tape (on which the new reflux ratio would be) or by changing R in a stepwise manner, such as by increasing it by five each time.

As mentioned in the section on the MISTIC computer itself, it is necessary to use DOI when reading in more tape. Because of the limited storage space in the computer, the DOI has been overwritten and thus destroyed. Before anything can be read in again, DOI must be read once again and stored in its proper locations. Thus, whenever the main program is altered to read in more data instead of shutting off, the DOI must be the first thing on the tape. The computer may be instructed to read the DOI by writing a bootstrap start in the program alteration. Even though the DOI, when read in again, will destroy some of the stored answers, nothing is hurt since the solution was already completed and the new problem will simply store its answers overtop the new DOI just read in.

Other variables which can be changed by slight program alterations are: 1) number of plates in the column, or simply the location of the feed plate, and 2) the feed

composition. If any changes are desired in the data to the program, such as feed composition or reflux ratio, the entire set of data must be made up, even though many of the things remain the same.

If it is desired to change the number of plates or the feed plate location, then only the orders which use the S termination symbol followed by a 5, 6, or 9 must be repeated. This is because they are the only orders which will be changed in this case. Because this change in number of plates was a common occurrence in this investigation, a special tape containing only the orders which would change (S5, S6, and S9 orders) was made up and used frequently.

Another program alteration which was used mainly at first to see if the program was working was to instruct the computer to punch out the composition of liquid on each plate for each iteration. By doing this, one can see how fast the problem is converging and also see how many iterations are required.

Through the cooperation of the computer laboratory staff, problems for this investigation were many times run off at night. In these instances, the foregoing program alterations were made use of to prepare problems which would run all night and require no watching. Many times, tapes were prepared

which contained several combinations of feed composition, reflux ratio, number of plates, and feed plate location.

One improvement which could be made in this program, if more storage space were available, would be to include various tests and checks to make sure certain physical laws are not broken, such as negative equilibrium constants. The computer could be instructed to shut off if such a thing occurred, or could go on to the next problem, if a program alteration were used to run a series of problems.

DATA AND DISCUSSION OF RESULTS

At first glance at the data, the reaction one might have is that it does not matter much where the feed plate is located. This, in a majority of cases, results in overdesign if the optimum feed location is not used and the column still carries out the desired separation. Of course, only in special cases such as stripping columns, will the optimum location be near either extreme of the column.

The variables which were studied to see if optimum location changed were: 1) feed composition, 2) reflux ratio, 3) number of plates, 4) condition of feed, and 5) tower pressure.

It was generally found that for most feed compositions, the optimum location for the feed plate varied from 55-75% of the way from the bottom of the column upward. If either extreme of mostly all light key or heavy key in the feed were approached, the optimum would be near the top of the column for high heavy key concentrations and near the bottom for high light key concentrations.

The method of determining the degree of separation in a multicomponent problem may take on different forms depending

upon what is being attempted in the column. The criterion for separation used in this investigation was concerned with: 1) the highest purity of light key in the overhead product (with particular attention paid to the amount of heavy key there also) and 2) the maximum recovery of light key in the overhead and the heavy key in the residue. The maximum recovery was taken as the maximum of the sums of the recovery of light key out the overhead and the recovery of heavy key out in the residue. This criterion was found to agree very well with the criterion of purity of products. The various variables involved will now be discussed individually.

Composition of Feed

This was without a doubt the most studied variable of those involved. Many different feed compositions were tested to see how the optimum feed plate location might change with composition.

Key components are those components between which the actual separation is made, and not the components which may be specified in attempting to obtain a desired product. The key components depend upon pressure, condenser duty, and top and bottom temperatures. Upon fixing these variables, the key components are fixed and one has no choice but to take

what separation is obtained for a given number of plates. The key components in all the calculations made were butane and isopentane.

Table I

	Temp	O_p	Feed Composition					$\frac{X_{HK}X_{LK}}{X_{LK}X_{HK}}$
			1-But.	n-But.	1-Pent.	n-Pent.	Hex.	
Feed A	126		.20	.25	.15	.20	.20	.72
Feed B	128		.10	.30	.30	.20	.10	.65
Feed C	125		.10	.50	.20	.10	.10	.86
Feed D	117		.10	.60	.10	.10	.10	.94
Feed E	109		.05	.70	.10	.10	.05	.96
Feed F	137		.30	.30	.15	.15	.10	.77
Feed G	113		.10	.20	.40	.20	.10	.47
Feed H	123		.10	.15	.50	.15	.10	.35
Feed I	100		.30	.30	.15	.15	.10	.77
Feed J*	137		.30	.30	.15	.15	.10	.77

*Feed J at 150 psi, all others at 100 psi.

It has been previously mentioned that for the extreme cases of nearly all light key or heavy key in the feed, the optimum location of feed plate would approach the bottom or the top of the column. To take advantage of this, the function $\frac{X_{HK}X_{LK}}{X_{LK}X_{HK}}$ was used as the means of defining the composition of the feed in terms of the key

DATA AND DISCUSSION OF RESULTS

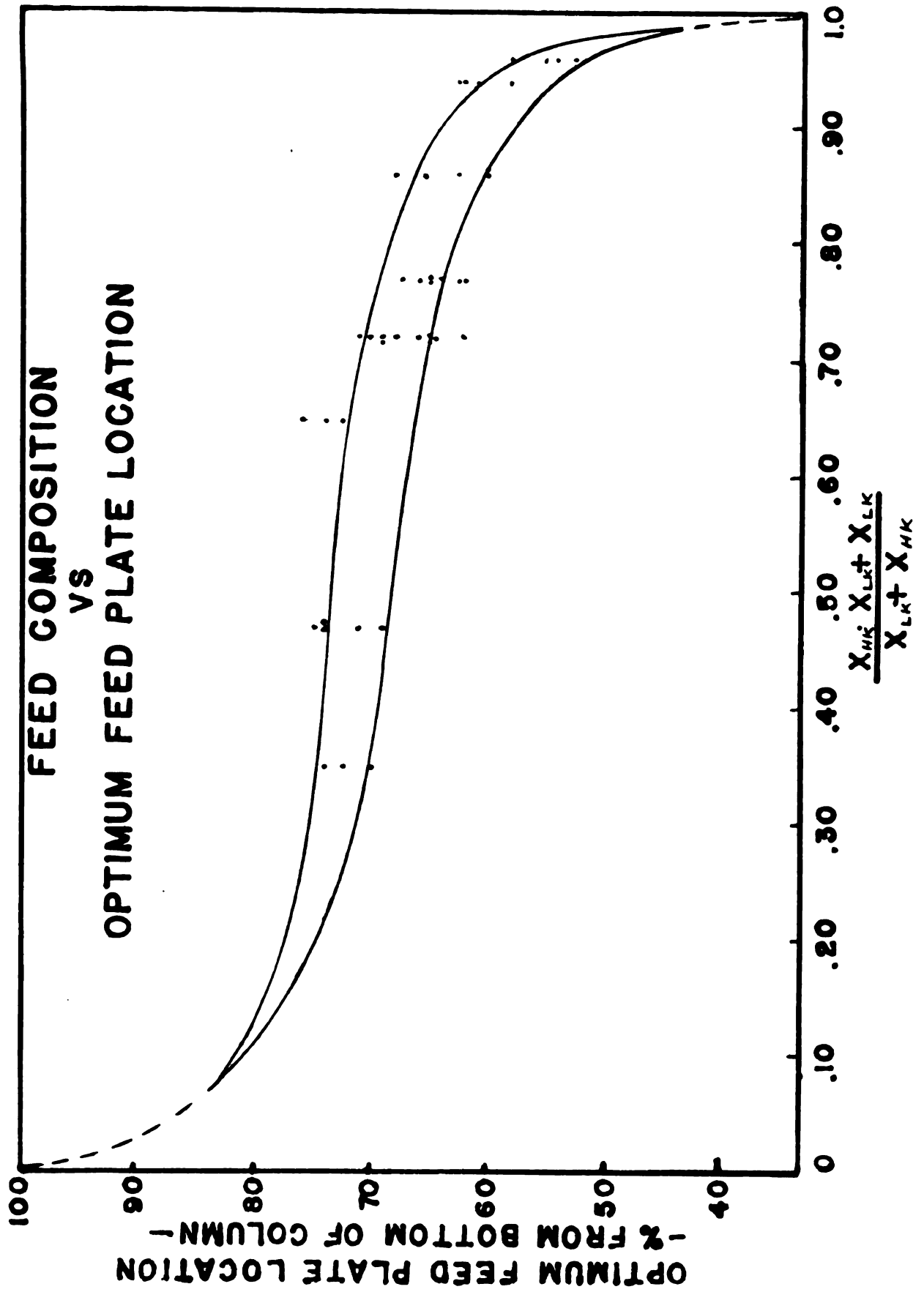


Figure 3

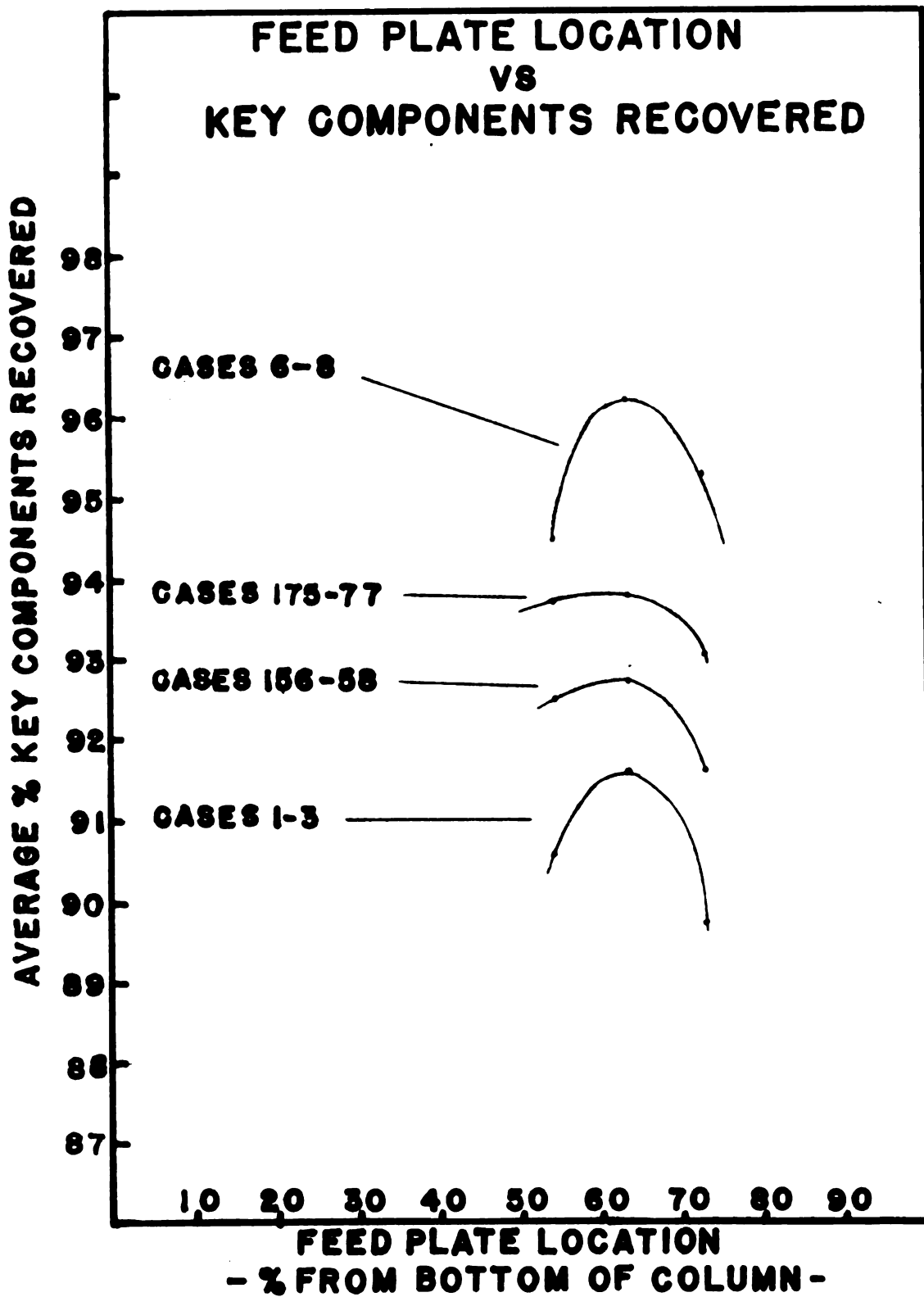


Figure 6

components. Figure 5 shows the results of plotting this function versus optimum feed plate location expressed in percentages from the bottom of the column. The data does not cover the entire range of feed composition; but does, however, cover most cases which will normally be met (see Table I). The ends of the curve are dotted since they are strictly empirical. By examining the abscissa of Figure 5, it can be seen that when the feed is all light key ($X_{HK} = 0$) then the function goes to 1 and the optimum location of feed plate should approach the bottom of the column. When the feed is all heavy key ($X_{LK} = 0$) then the function goes to zero and the optimum feed plate location approaches the top of the column.

Figure 5 was determined using the data of Table II (see Appendix). The maximum separation, and thus the optimum location of feed plate, was determined by plotting the average of the per cent light key recovered out the overhead and the per cent heavy key recovered out the bottom, versus feed plate location. Typical plots are shown in Figure 6. The optimum feed plate location was then plotted versus the function describing the feed composition in Figure 5. The band was drawn in to include the points scattered, due

to changes in reflux ratio, feed condition, and column pressure, as well as to include the "band" of optimum locations observed for several columns.

It is felt that the most important variable not investigated was that of variation of relative volatility between the key components. Although some problems were solved using a six-component feed, nearly all the problems solved in this investigation had a feed composed of the same five hydrocarbons. Any future work in this field should include this variable, as well as including components other than aliphatic hydrocarbons.

Reflux Ratio

By examining Table II for cases 1-81 and cases 82-155, which illustrate variation of reflux ratio, it can be seen that the degree of separation increases with reflux ratio. This is true up to a high value of reflux ratio, and then the products obtained remain the same with increasing reflux ratio. From plots of the type shown in Figure 6, it was found that the optimum feed plate location remained nearly the same for various reflux ratios. There is only a slight shift of the optimum feed plate location upward in the column with increased reflux ratio.

Number of Plates

Once again, the number of plates in a column has very little effect on the relative optimum feed plate location, that is, the feed plate location expressed as a percentage, such as used in Figure 5. In towers with a small number of plates (11) the optimum location sometimes resulted in a specific location, rather than a band of feed plate locations, which occurred in many columns with more plates. This band occurred due to the flat shape of the separation versus feed plate location curve (Figure 6.)

The columns with 21 and 31 plates which were calculated often had pinch points where the composition and temperatures did not change from one plate to the next. One set of problems was solved using 41 plates and the same relative optimum feed plate location was obtained as for columns with 21 and 31 plates. However, because of the increased number of plates in the pinch region, the optimum location band was slightly widened.

Condition of Feed

To determine if the optimum feed plate location changed with the condition of feed, that is, hot or cold feed, the same feed composition was used at two different temperatures. Feed F was at 137°F and Feed I at 100°F. Cases 211-222 and 254-268

are the solutions applicable here. In this case, the optimum location was not affected by the change of feed condition. It seems safe to generalize that, at least for all liquid feed, the condition of the feed will not affect the relative optimum feed plate location. However, caution should be used in extending this generalization to include vapor feeds.

Tower Pressure

Since the tower pressure is not an independent variable in commercial design but must be compatible with condenser temperature and product specifications, it is difficult to determine the effect of pressure on the optimum feed plate location.

The only check was the comparison of Feed F with Feed J (cases 211-222 and 269-282.) Feed J was used in a column at 150 psi pressure while the column for Feed F and all other cases were at 100 psi.

Although slightly different products were obtained, no appreciable change in optimum feed plate location was found.

CONCLUSIONS

CONCLUSIONS

1. A rigorous method for the solution of multicomponent distillation problems has been developed and programmed for a high speed digital computer.
2. Several hundred problems have been solved rigorously to use in making a correlation of optimum feed plate location.
3. From these numerous solutions, a correlation between the optimum feed plate location and the feed composition has been made. The function $\frac{x_{HK}x_{LK}}{x_{HK} + x_{LK}}$ was found to give a good correlation of feed composition.
4. The effects of other variables such as reflux ratio, tower pressure, feed condition, and number of plates, upon relative optimum feed plate location, have also been studied and found to be very small.

APPENDIX

Table II

CASE	FEED	REFLUX RATIO	PLATES ABOVE FEED PLATE	PLATES BELOW FEED PLATE	Mole Fraction of Distillate					
					$i C_4$	C_4	$i C_5$	C_5	C_6	D
1	A	2	3	7	.4525	.5095	.0263	.0111	.0007	.4261
2	A	2	4	6	.4397	.5194	.0307	.0099	.0003	.4441
3	A	2	5	5	.4257	.5130	.0476	.0136	.0002	.4604
4	A	2	6	4	.4065	.4935	.0763	.0236	.0002	.4812
5	A	2	7	3	.3813	.4639	.1106	.0440	.0002	.5100
6	A	6	3	7	.4532	.5345	.0095	.0027	.0001	.4359
7	A	6	4	6	.4418	.5394	.0157	.0031	.0000	.4499
8	A	6	5	5	.4297	.5327	.0319	.0056	.0000	.4642
9	A	6	6	4	.4094	.5075	.0680	.0151	.0000	.4861
10	A	6	7	3	.3805	.4719	.1130	.0345	.0001	.5220
11	A	10	3	7	.4534	.5385	.0065	.0016	.0001	.4370
12	A	10	4	6	.4422	.5424	.0131	.0023	.0000	.4504
13	A	10	5	5	.4297	.5327	.0319	.0056	.0000	.4642
14	A	10	6	4	.4098	.5095	.0067	.0140	.0000	.4867
15	A	10	7	3	.3803	.4731	.1137	.0328	.0001	.5239
16	A	14	3	7	.4534	.5401	.0053	.0011	.0000	.4374
17	A	14	4	6	.4424	.5437	.0120	.0019	.0000	.4506
18	A	14	5	5	.4299	.5336	.0312	.0053	.0000	.4643
19	A	14	6	4	.4100	.5103	.0662	.0136	.0000	.4869

20	A	14	7	3	.3801	.4735	.1141	.0323	.0000	.5247
21	A	18	3	7	.4535	.5409	.0047	.0009	.0000	.4376
22	A	18	4	6	.4425	.5443	.0115	.0017	.0000	.4506
23	A	18	5	5	.4300	.5341	.0309	.0051	.0000	.4644
24	A	18	6	4	.4100	.5106	.0660	.0134	.0000	.4871
25	A	18	7	3	.3800	.4736	.1143	.0321	.0000	.5253
26	A	2	4	16	.5337	.4592	.0054	.0017	.0001	.3672
27	A	2	6	14	.4438	.5464	.0082	.0015	.0000	.4501
28	A	2	8	12	.4375	.5453	.0156	.0016	.0000	.4569
29	A	2	10	10	.4178	.5209	.0156	.0057	.0000	.4785
30	A	2	12	8	.3842	.4790	.1158	.0210	.0000	.5201
31	A	2	14	6	.3661	.4554	.1403	.0383	.0000	.5450
32	A	6	4	16	.5230	.4750	.0016	.0004	.0000	.3790
33	A	6	6	14	.4450	.5541	.0009	.0001	.0000	.4494
34	A	6	8	12	.4421	.5525	.0051	.0003	.0000	.4524
35	A	6	10	10	.4267	.5332	.0383	.0019	.0000	.4687
36	A	6	12	8	.3829	.4784	.1279	.0108	.0000	.5223
37	A	10	4	16	.5225	.4763	.0009	.0002	.0000	.3801
38	A	10	6	14	.4450	.5545	.0004	.0000	.0000	.4494
39	A	10	8	12	.4425	.5531	.0043	.0002	.0000	.4520
40	A	10	10	10	.4274	.5342	.0369	.0015	.0000	.4679
41	A	10	12	8	.3821	.4775	.1308	.0097	.0000	.5235

42	A	14	4	16	.5227	.4764	.0007	.0002	.0000	.3802
43	A	14	6	14	.4451	.5546	.0003	.0000	.0000	.4493
44	A	14	8	12	.4426	.5532	.0040	.0001	.0000	.4519
45	A	14	10	10	.4275	.5343	.0369	.0014	.0000	.4679
46	A	14	12	8	.3814	.4767	.1326	.0093	.0000	.5243
47	A	18	4	16	.5228	.4766	.0005	.0001	.0000	.3804
48	A	18	6	14	.4451	.5547	.0002	.0000	.0000	.4493
49	A	18	8	12	.4427	.5533	.0039	.0001	.0000	.4518
50	A	18	10	10	.4274	.5342	.0371	.0013	.0000	.4680
51	A	18	12	8	.3808	.4760	.1343	.0090	.0000	.5252
52	A	2	5	25	.4644	.5225	.0104	.0026	.0000	.4300
53	A	2	6	24	.4501	.5412	.0074	.0014	.0000	.4442
54	A	2	7	23	.4448	.5493	.0051	.0007	.0000	.4496
55	A	2	9	21	.4435	.5537	.0026	.0002	.0000	.4510
56	A	2	12	18	.4403	.5503	.0091	.0003	.0000	.4542
57	A	2	15	15	.4161	.5200	.0614	.0025	.0000	.4807
58	A	2	18	12	.3753	.4690	.1367	.0190	.0000	.5329
59	A	6	5	25	.4548	.5437	.0013	.0003	.0000	.4397
60	A	6	6	24	.4469	.5524	.0007	.0001	.0000	.4475
61	A	6	9	21	.4444	.5555	.0001	.0000	.0000	.4500
62	A	6	12	18	.4435	.5544	.0020	.0000	.0000	.4509
63	A	6	15	15	.4272	.5339	.0384	.0005	.0000	.4682

64	A	10	5	25	.4541	.5451	.0006	.0001	.0000	.4404
65	A	10	6	24	.4467	.5529	.0003	.0000	.0000	.4477
66	A	10	9	21	.4444	.5555	.0000	.0000	.0000	.4500
67	A	10	12	18	.4437	.5546	.0017	.0000	.0000	.4508
68	A	10	15	15	.4282	.5352	.0362	.0004	.0000	.4671
69	A	14	5	25	.4539	.5456	.0004	.0001	.0000	.4405
70	A	14	6	24	.4467	.5531	.0002	.0000	.0000	.4477
71	A	14	9	21	.4445	.5555	.0000	.0000	.0000	.4500
72	A	14	12	18	.4437	.5546	.0017	.0000	.0000	.4508
73	A	14	15	15	.4282	.5353	.0362	.0003	.0000	.4671
74	A	18	5	25	.4538	.5458	.0003	.0001	.0000	.4406
75	A	18	6	24	.4467	.5532	.0001	.0000	.0000	.4477
76	A	18	9	21	.4445	.5555	.0000	.0000	.0000	.4500
77	A	18	12	18	.4437	.5546	.0017	.0000	.0000	.4508
78	A	18	15	15	.4281	.5351	.0365	.0003	.0000	.4672
79	A	2	8	32	.4451	.5510	.0035	.0004	.0000	.4493
80	A	2	12	28	.4441	.5551	.0007	.0000	.0000	.4503
81	A	2	16	24	.4421	.5526	.0052	.0001	.0000	.4524
82	B	2	2	8	.2202	.6386	.1092	.0302	.0018	.4498
83	B	2	3	7	.2204	.6406	.1125	.0259	.0008	.4486
84	B	2	4	6	.2137	.6245	.1340	.0273	.0004	.4624
85	B	2	5	5	.2030	.5951	.1682	.0335	.0003	.4861



86	B	2	6	4	.883	.5532	.2122	.0460	.0002	.5225
87	B	6	2	8	.2353	.6917	.0608	.0117	.0005	.4231
88	B	6	3	7	.2318	.6859	.0716	.0105	.0002	.4298
89	B	6	4	6	.2230	.6626	.1014	.0130	.0001	.4471
90	B	6	5	5	.2095	.6237	.1479	.0189	.0001	.4757
91	B	6	6	4	.1915	.5706	.2073	.0305	.0001	.5200
92	B	6	7	3	.1723	.5135	.2628	.0514	.0001	.5770
93	B	10	3	7	.2345	.6960	.0619	.0075	.0001	.4255
94	B	10	4	6	.2248	.6700	.0947	.0105	.0001	.4440
95	B	10	5	5	.2108	.6294	.1433	.0164	.0000	.4734
96	B	10	6	4	.1921	.5740	.2060	.0278	.0000	.5192
97	B	10	7	3	.1721	.5142	.2658	.0479	.0000	.5792
98	B	14	3	7	.2356	.7004	.0577	.0062	.0001	.4236
99	B	14	4	6	.2255	.6729	.0922	.0094	.0000	.4428
100	B	14	5	5	.2113	.6314	.1419	.0154	.0000	.4726
101	B	14	7	3	.1924	.5752	.2058	.0266	.0000	.5190
102	B	14	7	3	.1718	.5139	.2680	.0462	.0000	.5807
103	B	18	3	7	.2363	.7029	.0552	.0055	.0001	.4225
104	B	18	4	6	.2259	.6743	.0910	.0088	.0000	.4422
105	B	18	5	5	.2115	.6323	.1414	.0148	.0000	.4724
106	B	18	6	4	.1924	.5758	.2057	.0261	.0000	.5190
107	B	18	7	3	.1717	.5140	.2687	.0455	.0000	.5812
108	B	2	4	16	.2382	.7028	.0497	.0091	.0002	.4193

109	B	2	6	14	.2356	.7031	.0550	.0064	.0000	.4243
110	B	2	8	12	.2224	.6653	.1024	.0098	.0000	.4494
111	B	2	10	10	.2023	.6054	.1740	.0182	.0000	.4949
112	B	2	12	8	.1791	.5359	.2492	.0358	.0000	.5580
113	B	2	14	6	.1634	.4884	.2867	.0615	.0000	.6112
114	B	6	4	16	.2484	.7420	.0084	.0011	.0000	.4024
115	B	6	6	14	.2468	.7399	.0126	.0007	.0000	.4052
116	B	6	8	12	.2362	.7084	.0532	.0021	.0000	.4233
117	B	6	10	10	.2111	.6330	.1500	.0060	.0000	.4738
118	B	6	12	8	.1761	.5280	.2788	.0172	.0000	.5679
119	B	10	4	16	.2495	.7459	.0041	.0005	.0000	.4007
120	B	10	6	14	.2480	.7437	.0081	.0003	.0000	.4033
121	B	10	8	12	.2379	.7135	.0472	.0015	.0000	.4204
122	B	10	10	10	.2122	.6365	.1468	.0045	.0000	.4713
123	B	10	12	8	.1750	.5249	.2858	.0143	.0000	.5714
124	B	14	4	16	.2499	.7471	.0027	.0003	.0000	.4002
125	B	14	6	14	.2484	.7449	.0065	.0002	.0000	.4026
126	B	14	8	12	.2383	.7148	.0458	.0012	.0000	.4197
127	B	14	10	10	.2124	.6371	.1466	.0039	.0000	.4708
128	B	14	12	8	.1742	.5224	.2903	.0013	.0000	.5741
129	B	18	4	16	.2500	.7477	.0020	.0002	.0000	.3999
130	B	18	6	14	.2486	.7455	.0057	.0002	.0000	.4023

131	B	18	8	12	.2384	.7151	.0454	.0011	.0000	.4195
132	B	18	10	10	.2123	.6370	.1471	.0036	.0000	.4709
133	B	18	12	8	.1737	.5210	.2928	.0125	.0000	.5757
134	B	2	6	24	.2425	.7226	.0314	.0035	.0000	.4124
135	B	2	9	21	.2421	.7259	.0304	.0016	.0000	.4130
136	B	2	12	18	.2292	.6875	.0799	.0034	.0000	.4362
137	B	2	15	15	.2067	.6120	.1641	.0095	.0000	.4839
138	B	2	18	12	.1774	.5320	.2614	.0292	.0000	.5637
139	B	6	6	24	.2496	.7481	.0022	.0002	.0000	.4007
140	B	6	9	21	.2494	.7482	.0024	.0001	.0000	.4010
141	B	6	12	18	.2435	.7306	.0255	.0044	.0000	.4106
142	B	6	15	15	.2170	.6510	.1303	.0017	.0000	.4608
143	B	6	18	12	.1665	.4994	.3253	.0088	.0000	.6007
144	B	10	6	24	.2499	.7491	.0009	.0001	.0000	.4002
145	B	10	9	21	.2497	.7491	.0012	.0000	.0000	.4005
146	B	10	12	18	.2448	.7344	.0206	.0002	.0000	.4085
147	B	10	15	15	.2189	.6568	.1232	.0011	.0000	.4568
148	B	14	6	24	.2499	.7494	.0006	.0000	.0000	.4000
149	B	14	9	21	.2498	.7493	.0009	.0000	.0000	.4003
150	B	14	12	18	.2450	.7351	.0197	.0002	.0000	.4081
151	B	14	15	15	.2192	.6576	.1223	.0009	.0000	.4562
152	B	18	6	24	.2500	.7496	.0004	.0000	.0000	.4000
153	B	18	9	21	.2498	.7495	.0007	.0000	.0000	.4003

154	B	18	12	18	.2451	.7353	.0194	.0001	.0000	.4080
155	B	18	15	15	.2192	.6575	.1225	.0008	.0000	.4563
156	C	2	3	7	.1689	.7972	.0293	.0043	.0003	.5822
157	C	2	4	6	.1681	.8010	.0278	.0031	.0001	.5846
158	C	2	5	5	.1656	.7974	.0340	.0030	.0000	.5932
159	C	2	6	4	.1611	.7823	.0525	.0041	.0000	.6092
160	C	2	7	3	.1540	.7512	.0871	.0077	.0000	.6346
161	C	6	3	7	.1703	.8176	.0110	.0011	.0001	.5826
162	C	6	4	6	.1686	.8192	.0114	.0008	.0000	.5890
163	C	6	5	5	.1661	.8159	.0171	.0009	.0000	.5987
164	C	6	6	4	.1622	.8021	.0339	.0018	.0000	.6134
165	C	6	7	3	.1555	.7711	.0690	.0044	.0000	.6388
166	C	6	5	15	.1689	.8293	.0017	.0001	.0000	.5917
167	C	6	6	14	.1673	.8317	.0010	.0001	.0000	.5977
168	C	6	8	12	.1664	.8315	.0021	.0000	.0000	.6011
169	C	6	10	10	.1631	.8153	.0213	.0003	.0000	.6131
170	C	6	8	22	.1588	.7940	.0465	.0007	.0000	.6297
171	C	6	10	20	.1667	.8332	.0001	.0000	.0000	.6001
172	C	6	11	19	.1666	.8332	.0002	.0000	.0000	.6001
173	C	6	13	17	.1664	.8318	.0019	.0000	.0000	.6011
174	C	6	15	15	.1669	.8331	.0000	.0000	.0000	.5991
175	D	6	3	7	.1474	.8381	.0111	.0032	.0002	.6690
176	D	6	4	6	.1467	.8413	.0101	.0020	.0001	.6731

177	D	6	5	5	.1447	.8414	.0121	.0018	.0000	.6821
178	D	6	6	4	.1422	.8446	.0121	.0011	.0000	.7006
179	D	6	7	3	.1388	.8277	.0300	.0035	.0000	.7174
180	D	6	5	15	.1456	.8536	.0007	.0001	.0000	.6865
181	D	6	6	14	.1438	.8557	.0004	.0000	.0000	.6951
182	D	6	8	12	.1429	.8567	.0004	.0000	.0000	.6998
183	D	6	10	10	.1422	.8533	.0044	.0001	.0000	.7031
184	D	6	12	8	.1375	.8251	.0366	.0008	.0000	.7271
185	D	6	10	20	.1429	.8571	.0000	.0000	.0000	.7000
186	D	6	11	19	.1429	.8571	.0000	.0000	.0000	.7000
187	D	6	13	17	.1428	.8571	.0001	.0000	.0000	.7000
188	D	6	15	15	.1425	.8548	.0027	.0000	.0000	.7019
189	E	2	3	7	.0708	.9166	.0097	.0028	.0001	.6915
190	E	2	4	6	.0704	.9201	.0079	.0017	.0000	.6952
191	E	2	5	5	.0698	.9217	.0074	.0011	.0000	.7003
192	E	2	6	4	.0690	.9214	.0086	.0010	.0000	.7066
193	E	2	7	3	.0681	.9176	.0130	.0013	.0000	.7141
194	E	6	3	7	.0708	.9252	.0032	.0007	.0000	.6977
195	E	6	4	6	.0700	.9271	.0025	.0004	.0000	.7059
196	E	6	5	5	.0692	.9281	.0025	.0002	.0000	.7151
197	E	6	6	4	.0682	.9281	.0034	.0003	.0000	.7258
198	E	6	7	3	.0673	.9258	.0064	.0005	.0000	.7368

199	E	6	5	15	.0739	.9252	.0007	.0001	.0000	.6743
200	E	6	6	14	.0705	.9290	.0004	.0000	.0000	.7074
201	E	6	8	12	.0673	.9326	.0001	.0000	.0000	.7431
202	E	6	10	10	.0667	.9330	.0002	.0000	.0000	.7495
203	E	6	12	8	.0664	.9294	.0042	.0000	.0000	.7530
204	E	6	14	6	.0639	.8942	.0410	.0008	.0000	.7823
205	E	6	10	20	.0669	.9331	.0000	.0000	.0000	.7474
206	E	6	11	19	.0667	.9333	.0000	.0000	.0000	.7493
207	E	6	13	17	.0667	.9333	.0000	.0000	.0000	.7499
208	E	6	15	15	.0667	.9333	.0001	.0000	.0000	.7500
209	E	6	17	13	.0666	.9322	.0012	.0000	.0000	.7509
210	E	6	19	11	.0656	.9184	.0160	.0000	.0000	.7622
211	F	6	3	7	.5022	.4732	.0190	.0054	.0002	.5875
212	F	6	4	6	.4934	.4876	.0169	.0022	.0000	.6063
213	F	6	6	14	.5008	.4986	.0005	.0001	.0000	.5989
214	F	6	8	12	.4990	.4989	.0020	.0001	.0000	.6011
215	F	6	10	10	.4889	.4888	.0218	.0005	.0000	.6136
216	F	6	12	8	.4489	.4488	.0980	.4043	.0000	.6682
217	F	6	7	23	.5092	.4905	.0002	.0000	.0000	.5890
218	F	6	9	21	.5039	.4961	.0001	.0000	.0000	.5953
219	F	6	11	19	.5000	.5000	.0001	.0000	.0000	.6000
220	F	6	13	17	.4994	.4994	.0011	.0000	.0000	.6007

221	F	6	15	15	.4937	.4937	.0125	.0001	.0000	.6077
222	F	6	17	13	.4608	.4608	.0078	.0006	.0000	.6510
223	G	6	2	8	.3044	.5876	.0925	.0148	.0007	.3258
224	G	6	3	7	.3022	.5881	.0974	.0122	.0003	.3258
225	G	6	4	6	.2983	.5828	.1077	.0111	.0001	.3325
226	G	6	5	5	.2936	.5738	.1218	.0107	.0001	.3370
227	G	6	6	4	.2890	.5632	.1367	.0110	.0000	.3405
228	G	6	4	16	.3275	.6520	.0186	.0018	.0000	.3053
229	G	6	6	14	.3269	.6528	.0193	.0010	.0000	.3058
230	G	6	8	12	.3240	.6470	.0281	.0009	.0000	.3086
231	G	6	10	10	.3199	.6380	.0412	.0009	.0000	.3125
232	G	6	12	8	.3143	.6254	.0593	.0010	.0000	.3177
233	G	6	6	24	.3318	.6634	.0045	.0003	.0000	.3014
234	G	6	8	22	.3323	.6644	.0032	.0001	.0000	.3010
235	G	6	9	21	.3322	.6643	.0035	.0001	.0000	.3011
236	G	6	10	20	.3320	.6639	.0041	.0001	.0000	.3012
237	G	6	11	19	.2962	.5923	.1091	.0025	.0000	.3377
238	H	6	2	8	.3681	.5103	.1094	.0115	.0008	.2663
239	H	6	3	7	.3643	.5173	.1092	.0088	.0003	.2702
240	H	6	4	6	.3591	.5153	.1178	.0077	.0001	.2741
241	H	6	5	5	.3531	.5086	.1310	.0072	.0001	.2777
242	H	6	6	4	.3470	.4989	.1469	.0071	.0000	.2803

243	H	6	4	16	.3895	.5781	.0304	.0019	.0000	.2566
244	H	6	6	14	.3876	.5793	.0319	.0011	.0000	.2579
245	H	6	8	12	.3825	.5718	.0447	.0010	.0000	.2613
246	H	6	10	10	.3754	.5601	.0634	.0010	.0000	.2661
247	H	6	12	8	.3662	.5443	.0884	.0010	.0000	.2723
248	H	6	6	24	.3957	.5933	.0107	.0004	.0000	.2527
249	H	6	7	23	.3959	.5938	.0100	.0003	.0000	.2526
250	H	6	8	22	.3956	.5933	.0109	.0002	.0000	.2528
251	H	6	9	21	.3942	.5911	.0145	.0002	.0000	.2537
252	H	6	10	20	.3942	.5911	.0145	.0002	.0000	.2537
253	H	6	11	19	.3426	.5138	.1413	.0023	.0000	.2919
254	I	6	3	7	.5056	.4860	.0068	.0013	.0000	.5885
255	I	6	4	6	.5041	.4883	.0067	.0009	.0000	.5909
256	I	6	5	5	.5024	.4893	.0075	.0008	.0000	.5928
257	I	6	6	4	.5010	.4894	.0088	.0008	.0000	.5937
258	I	6	7	3	.5001	.4887	.0104	.0009	.0000	.5926
259	I	6	5	15	.5044	.4946	.0008	.0001	.0000	.5944
260	I	6	6	14	.5009	.4986	.0005	.0000	.0000	.5988
261	I	6	8	12	.4992	.4990	.0018	.0000	.0000	.6010
262	I	6	10	10	.4897	.4896	.0203	.0005	.0000	.6127
263	I	6	7	23	.5012	.4986	.0002	.0000	.0000	.5986
264	I	6	11	19	.5000	.5000	.0001	.0000	.0000	.6000

J

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265	I	6	13	17	.4999	.4999	.0001	.0000	.0000	.6001
266	I	6	15	15	.4999	.4999	.0002	.0000	.0000	.6001
267	I	6	17	13	.4999	.4999	.0003	.0000	.0000	.6002
268	I	6	19	11	.4998	.4998	.0004	.0000	.0000	.6002
269	J	6	3	7	.4920	.4872	.0154	.0053	.0001	.6079
270	J	6	4	6	.4907	.4864	.0174	.0055	.0000	.6094
271	J	6	5	5	.4893	.4851	.0196	.0059	.0000	.6107
272	J	6	6	4	.4878	.4834	.0223	.0066	.0000	.6115
273	J	6	7	3	.4863	.4811	.0253	.0073	.0000	.6109
274	J	6	6	14	.5012	.4984	.0003	.0001	.0000	.5984
275	J	6	8	12	.4996	.4994	.0009	.0001	.0000	.6004
276	J	6	10	10	.4950	.4949	.0089	.0011	.0000	.6060
277	J	6	12	8	.4981	.4977	.0038	.0004	.0000	.6022
278	J	6	11	19	.5001	.4999	.0000	.0000	.0000	.5998
279	J	6	13	17	.5001	.4999	.0000	.0000	.0000	.5999
280	J	6	15	15	.5000	.5000	.0000	.0000	.0000	.6000
281	J	6	17	13	.5000	.5000	.0000	.0000	.0000	.6000
282	J	6	19	11	.5000	.5000	.0000	.0000	.0000	.5999

COMPUTER LABORATORY

LIBRARY ROUTINE A 1 - 63

TITLE Floating Decimal Arithmetic Routine

TYPE Interpretive routine with 18 interpretive orders, entered as a closed routine, left by an 8J interpretive order.

NUMBER OF WORDS 168

PURPOSE This routine manipulates numbers in the floating decimal form, that is, numbers which are represented as $A \times 10^P$. It is of the interpretive type. This means that it selects parameters called interpretive orders which are written by the user one at a time and performs a calculation corresponding to each interpretive order. Interpretive orders carry out normal arithmetic operations such as addition and multiplication and some red tape operations such as counting and address changing.

In general, one will use this routine to do computations which do not require the full speed of the computer but which are too time-consuming to be done by hand. It is especially effective for problems with scaling difficulties. In a sense, one may think of the floating decimal routine as converting the MISTIC to a medium speed floating

decimal computer having a very convenient order code.

ACCURACY About 9 decimals

TEMPORARY STORAGE 0, 1, 2

PRESET PARAMETERS S3 is used to specify two locations of non-temporary storage, S3 and 1S3, which are used for the floating decimal accumulator.

METHOD OF USE The floating decimal routine is entered as a standard subroutine. Following the entry, i.e., after the transfer of control to the subroutine, one begins writing interpretive orders. These orders each occupy one-half word and consist of a pair of function digits followed by a single address. They, therefore, have the same form as standard machine orders and may be read by the Decimal Order Input with full use of the conventional terminating symbols.

The first of the two function digits of an interpretive order describes the group characteristics of the order and may take values 0, 1, ..., 8. Normal arithmetic interpretive orders have this digit equal to 8. The second of the two function digits describes the type of interpretive order.

INTERPRETIVE ORDER LIST WITH FIRST FUNCTION DIGIT b = 8

Let F be the floating decimal number in the floating accumulator and let $F(n)$ be the floating decimal number in location n .

- 80 N Replace F by $F - F(n)$.
- 81 n Replace F by $-F(n)$.
- 82 n Transfer control to the right hand interpretive order
in n if $F \geq 0$.
- 83 n Transfer control to the left hand interpretive order
in n if $F \geq 0$.
- 84 n Replace F by $F + F(n)$.
- 85 n Replace F by $F(n)$.
- 86 n Replace F by $F/F(n)$.
- 87 n Replace F by $F \times F(n)$.
- 88 0 Replace F by one number read from the input tape
punched as sign, any number of decimal digits, sign,
and two decimal digits to represent the exponent.
For example, $.8971 \times 10^{10}$ would be punched as
+ 8971 + 10.
- 89 n Punch or print F as a sign, n decimal digits, sign,
two decimal digits to represent the exponent and
two spaces. This print out may be reread by this
routine. After F has been punched or printed, it
may not remain in the floating accumulator unmodified.
n can take values 2 to 9.
- 8K n Replace F by n if $0 \leq n < 200$.

- 88 n Replace $F(n)$ by F .
- 8N n Replace F by $|F| - |F(n)|$.
- 8J n Transfer control to the ordinary Illiac order on the left hand side of n . This used to escape from the floating decimal subroutine.
- 8F n Give a carriage return and line feed and start a new block of printing having n columns. This order is only obeyed once for a particular block of printing. At this time, a counter is set up which will cause a carriage return and line feed to occur automatically from then on after every set of numbers that is printed.

INTERPRETIVE ORDERS WITH $b \neq 8$.

If the first function digit of an interpretive order is 0, 1, ..., 7, it will refer to one of a set of control registers or b - registers in the floating decimal routine which are similarly numbered. These registers are used for counting the number of passages through loops or cycles and for advancing addresses on successive passages. For this purpose, a particular b - register which may be used in a particular cycle contains two counting indices g_b and c_b . These are both intergers in the range 0 to 1023. The index

c_b is used for counting purposes to determine the number of passages through a loop. The index g_b is used for advancing the addresses of interpretive arithmetic orders. Although the interpretive order with first function digit b is not actually altered in the memory, it is obeyed as if g_b is increased by one upon each passage through the cycle. The multiplicity of b - registers allows one to program many loops within loops.

ORDER LIST WITH $n \neq 8$

b0 n Replace F by $F - F(n+g_b)$.

b1 n Replace F by $-F(n+g_b)$.

b2 n Replace g_b, c_b by $g_b + 1, c_b + 1$.

Then transfer control to the right hand (if $b2\ n$) or left hand interpretive (if $b3\ n$) order is n if $c_b + 1$

b3 n is negative. This transfer is used at the end of a loop.

b4 n Replace F by $F + F(n + g_b)$.

b5 n Replace F by $F(n + g_b)$.

b6 n Replace F by $F/F(n+g_b)$.

b7 n Replace F by $F \times F(n + g_b)$.

bK n Replace g_b, c_b by $0, -n$. This interpretive order is used for preparing to cycle around a loop n times.

b8 n Replace $F(n + g_b)$ by F .

- bN n** Replace F by $|F| - |F(n + g_b)|$.
- bL n** Replace g_b, c_b by $g_b + n, c_b$. This interpretive order is used when one wishes to step addresses by some increment other than +1 in a loop. If one places **bL 1022** in a loop, the effect will be to decrease addresses by one on each passage. **bL 1** will increase them by 2, etc.
- 8L n** Replace g_b, c_b by n, c_b , where b is the last b -register referred to by some previous interpretive order.

DURATION OF INDIVIDUAL INTERPRETIVE ORDERS

8N	5 milliseconds + $m \times (3/2)$. Where m is the number of
80	
84	shifts required to convert A, p back to standard form.
81	2 milliseconds
85	
82	3 milliseconds
83	
87	5 milliseconds
86	6 milliseconds
8K	3 milliseconds
8S	3 milliseconds
8F	3 milliseconds
8L	2 milliseconds
8J	3 milliseconds



When an interpretive order is preceded by b # 8, add one millisecond to the above times.

When one wishes to repeat a cycle of interpretive orders n times, the interpretive order bK n may be written before entering the loop to set the counter c_b to -n. The interpretive orders in the loop will be obeyed n times if the loop is terminated by b2 or b3 interpretive order to transfer control to the beginning of the loop. This transfer of control interpretive order will be obeyed n-1 times and disobeyed the nth time.

Use of Auxiliary Routines. It is often convenient to be able to leave the floating decimal routine so as to modify interpretive orders or to perform calculations which may be done more effectively outside of floating point. To leave the floating decimal routine one uses an 8J n order. (All standard floating decimal auxiliaries are entered in this way.) To return to floating decimal, one should transfer control to the left hand side of word 29 of the floating decimal routine. The interpretive order following the 8J n order which was last obeyed will then be obeyed and so on. In this way, it is not necessary to plant a link in auxiliary subroutines. One may, in fact, think of the 8J n order as a subroutine

order. In case any changes are made in the floating decimal accumulator while outside the floating decimal routine, control should be returned to the left hand side of word 19 rather than 29 so that this number may be standardized before re-entry.

Handling of Numbers. Each number is represented in the form $A \times 10^p$ where $1 > |A| \geq 1/10$, and $64 > p \geq -64$. In a single register of the memory, the number A is placed in the 33 most significant binary digits ($a_0, a_1, \dots, a_{32}$) in the same way as an ordinary fraction is placed in the entire register. An accuracy of between 8 and 9 decimal digits is therefore achieved. The exponent p is stored as the integer $p + 64$ in the 7 least significant digits of the same register. For convenience, the floating decimal accumulator uses two registers S3 and LS3 for holding the number $A \times 10^p$. The fraction $a/2$ is in S3 and the integer $p + 64$ is in LS3.

The only exception to the above rules is the number zero which cannot, of course, be represented as $A \times 10^p$ with $|A| \geq 10$. For this reason, zero is handled in a special way. It is represented as a number with $A = 0$ and $p = -64$. This representation happens to correspond exactly with the ordinary machine representation of zero.

After each arithmetic interpretive order is obeyed, the number in the floating decimal accumulator is standardized, i.e., the number in S3 representing $A/2$ is adjusted so $1 \leq |A| < 2$ and p is changed accordingly. To accomplish this, control is transferred to word 19 in the floating decimal routine after each arithmetic order.

If an interpretive store order is attempted when F has an exponent greater than 63, the machine will stop on the order 34 p at location p , where p is word 72 of the routine.

Important Words in the Routine. Word 2 in the floating decimal routine determines the location of the current interpretive order. When obeying the left hand interpretive order in location n , this word is 50 nF S3 20 F and when obeying the right hand interpretive order in location n , it is 15 nF 00 20 F . Other words of interest are the b-registers which start at word 158 (for g_0 and c_0) and go to 165 (g_7 and c_7 .) These registers hold g_b and c_b in the form 80 g_bF 00 (2048 $\neq c_b$) F .

Warning. When the same number is continually added to a sum, such as when an argument is being increased, the error can be quite large, because it is additive over a decade. For example, if we increase 10 to 100 by units, we can get a maximum error of 90×2^{-33} because the errors all have the

same sign. If we increase 10^3 to 10^4 , we can have a maximum error of 9000×2^{-33} . This can easily be prevented by writing an auxiliary subroutine to stabilize the fractional part of F , i.e., to replace it by the nearest multiple of say 10^{-7} .

NOMENCLATURE

D	Moles of overhead product
F	Moles of feed
H	Enthalpy of vapor stream
$\bar{H}$ or $\bar{h}$	Enthalpy of pure component as vapor or liquid
K	Equilibrium constant (y/x)
L	Moles of liquid
M	Plates above feed
N	Plates below feed
Q	Heat flux, enthalpy of vapor minus enthalpy of liquid in passing streams
R	Reflux ratio (L/D)
T	Temperature °F
V	Moles of vapor
W	Moles of bottom product
a,b,c,d	Constants
h	Enthalpy of liquid stream
p	Partial derivatives used in rectifying section
q	Partial derivatives used in stripping section
r	Ratio of composition of particular component on feed plate as calculated from opposite directions
x	Mole fraction in liquid
y	Mole fraction in vapor

SUBSCRIPTS

- a** Rectifying section
- c** Condenser
- D** Distillate
- f** Feed or feed plate
- h** Constant of enthalpy polynomial
- i** Particular component
- k** Constant of equilibrium constant polynomial
- m** Plate number in rectifying section, numbered in Arabic numerals from condenser to feed plate
- n** Plate number in stripping section, numbered in Roman numerals from reboiler to feed plate
- s** Reboiler
- r** Stripping section

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