

Multicomponent Distillation Calculations on a Large Digital Computer

Solution of the multicomponent rectification problem, in which equations for the whole column are solved simultaneously component by component, involves simultaneous solution of a large number of equations by an iterative procedure which needs only assumption of a column temperature distribution for light hydrocarbon rectifications. The successive iterations then correct the temperature distribution. The number of iterations depends on the precision required, but generally four or five are adequate

THE use of large digital computers for distillation calculations has not been investigated to date, although the high speed of computation seems to offer economies and present the opportunity of making calculations not otherwise possible. Methods and techniques become feasible which by their very nature are precluded from use on small digital machines or by desk calculation.

The number of articles each year devoted to the computational methods in multicomponent distillation is perhaps larger than the importance of the topic justifies. The system of equations describing the process has certain intriguing features. Essentially, it is necessary to solve a system of simultaneous algebraic equations in the compositions in which a set of parameters, the temperatures, must be fixed, in order that the over-all material and heat balances will not be violated. For hydrocarbon rectifications, at least those of low molecular weight, the set of equations may be considered linear in the compositions with coefficients that are nonlinear in the parameters. For general multicomponent mixtures the coefficients depend in a highly nonlinear fashion on the compositions also. The solution of the equations is difficult, as

a thermodynamic analysis of the column limits in a very restrictive way the number of quantities that may be specified *a priori*.

Because of the high degree of nonlinearity of the system, approximate and short-cut methods have been proposed in almost a continuous stream, with graphical techniques and empirical correlations. Plate by plate methods have been used to obtain semirigorous solutions. There is always some question as to what is meant by a solution to the multicomponent rectification problem. Most of the methods proposed do not give rigorous answers and cannot be made rigorous. However, each has its particular area of application and their use is justified, as the data for the system at hand are not known with precision and factors of safety may be incorporated in the design. Nevertheless, the general solution should be available for comparison purposes and a method is needed which could be made as accurate as one pleased. The advent of the large high speed digital machine has made this possible.

This is a preliminary report on a technique developed and programmed for the Remington Rand Univac Scientific Computer Model 1103 of the St. Paul Service Bureau. The mass balances on each component and the heat balance on each tray will give a set of algebraic equations which may be expressed in matrix form (7). If the number of components is m and the number of plates is N , including the reboiler but not the partial condenser, the equations for the system will reduce to m matrix equations of order $N + 1$ and one matrix equation of order N , the heat balance. The m matrix equations will contain as unknowns the compositions, while the unknowns in the heat balance matrix will be the vapor rates throughout the column. All the matrices contain as a parameter the temperatures that must be fixed on each tray. To be specific, a light hydrocarbon rectification is used as illustration with equilibrium established on each tray and the numbers of plates above and below the feed plate location are specified. Under ordinary circumstances

two further quantities may be specified; these are taken as the drawoff rate of the vapor overhead and the boil-up heat absorbed in the reboiler, although other conditions such as draw-off and reflux may be specified.

Equations for a Single Feed and No Drawoff

Suppose the plates are numbered from the top to the bottom, the zeroth being the partial condenser and the N th the reboiler. An arbitrary number of feeds may be introduced and an arbitrary number of side streams withdrawn. The number of components and number of plates are left open. In this first analysis a single feed column without side stream drawoff is discussed. The feed composition and condition are supposed known and the pressure has been arbitrarily fixed in advance. The overhead vapor drawoff will be fixed and the amount of heat to the reboiler is known. The unknowns are then the vapor rates and compositions and temperatures on every tray.

The usual over-all material balances are

$$L_{j-1} + D = V_j \quad 1 \leq j \leq$$

$$L_j = V_{j+1} + W \quad f \leq j \leq N - 1$$

where f is the feed plate number. The material balance equations around each tray are easily written, if one assumes the equilibrium relation around each tray to be of the form

$$y_{ji} = K_{ji} x_{ji}$$

The first subscript indicates the plate number and the second is a component-designating variable. The function K_{ji} depends on total pressure, temperature, and composition. Thus

$$\begin{aligned} &= [V_1 + (K_{01} - 1)D]x_{01} + V_1 K_{11} x_{11} = 0 \\ &(V_1 - D)x_{01} - (V_2 - D + V_1 K_{11})x_{11} + V_2 K_{21} x_{21} = 0 \end{aligned}$$

¹ Present address, Department of Chemical Engineering, University of Minnesota, Minneapolis 14, Minn.

$$\begin{aligned}
(V_2 - D) x_{1i} - (V_3 - D + V_2 K_{2i}) x_{2i} + \\
\vdots \\
(V_f - D) x_{f-1,i} - \\
\vdots \\
(V_{f+1} + W + V_f K_{fi}) x_{fi} + \\
\vdots \\
V_{f+1} K_{f+1,i} x_{f+1,i} = -F x_{Fi} \\
(V_{N-1} + W) x_{N-2,i} - \\
(V_N + W + V_{N-1} K_{N-1,i}) x_{N-1,i} + \\
V_N K_{Ni} x_{Ni} = 0 \\
(V_N + W) x_{N-1,i} - \\
(W + V_N K_{Ni}) x_{Ni} = 0
\end{aligned}$$

If a total condenser is used on the overhead, the first equation is modified by setting $K_{0i} = 1$.

This set of equations may be formally written as a matrix equation

$$\bar{M}_i \bar{X}_i = \bar{F}_i \quad (1)$$

where \bar{X}_i is a composition column vector and \bar{F} is a feed column vector, each having $N + 1$ elements,

$$\bar{X}_i = \begin{pmatrix} x_{0i} \\ x_{1i} \\ x_{2i} \\ \vdots \\ x_{fi} \\ \vdots \\ x_{Ni} \end{pmatrix} \quad \bar{F}_i = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ -F x_{Fi} \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

the only nonzero elements in \bar{F}_i being the $f + 1$ st from the top. The matrix, \bar{M}_i , is a square matrix of order $N + 1$ having nonzero elements only on the main diagonal and each adjacent diagonal. If the rows and columns of \bar{M}_i are numbered each from 0 to N to correspond to plate numbers, and if a_{pq} is an element in the p th row and q th column, then

$$\begin{aligned}
a_{00} &= -V_1 - (K_{0i} - 1) D \\
a_{pp} &= -(V_{p+1} - D + V_p K_{pi}), \quad 1 \leq p \leq f - 1 \\
&= -(V_{p+1} + W + V_p K_{pi}), \quad f \leq p \leq N - 1 \\
&= -(W + V_p K_{pi}), \quad p = N \\
a_{p-1,p} &= V_p K_{pi}, \quad 1 \leq p \leq N \\
a_{p,p-1} &= V_p - D, \quad 1 \leq p \leq f \\
&= V_p + W, \quad f + 1 \leq p \leq N
\end{aligned}$$

Consider now the heat balance equations, writing the heat balance around each tray, omitting the partial condenser. These may be written after some manipulation

$$(h_0 - H_1) V_1 + (H_2 - h_1) V_2 = D(h_0 - h_1)$$

$$\begin{aligned}
(h_1 - H_2) V_2 + (H_3 - h_2) V_3 = \\
D(h_1 - h_2) \\
\vdots \\
(h_{f-1} - H_f) V_f + (H_{f+1} - h_f) V_{f+1} = \\
D h_{f-1} + W h_f - F H_F \\
(h_{N-2} - H_{N-1}) V_{N-1} + (H_N - h_{N-1}) V_N \\
= W(h_{N-1} - h_{N-2})
\end{aligned}$$

If V_j 's are treated as unknowns in a set of linear simultaneous algebraic equations, the above may be written formally in matrix notation

$$\bar{H} \bar{V} = \bar{G} \quad (2)$$

in which the enthalpy matrix is of N th order and square, while \bar{V} and \bar{G} are vapor rate column vectors and product enthalpy vectors, respectively, each having N elements. If b_{pq} is an element of the p th row and q th column of \bar{H} and rows and columns are measured from 1 to N , then

$$\begin{aligned}
b_{pp} &= h_{p-1} - H_p, \quad 1 \leq p \leq N \\
b_{p,p+1} &= H_{p+1} - h_p, \quad 1 \leq p \leq N - 1 \\
\bar{V} &\text{ has vertical column elements } V_1, V_2, \dots, V_N. \text{ If } c_p \text{ is the element in the } p\text{th} \\
&\text{ row of } \bar{G}, \text{ then} \\
c_p &= D(h_{p-1} - h_p), \quad 1 \leq p \leq f - 1 \\
&= D h_{p-1} + W h_p - F H_F, \quad p = f \\
&= W(h_p - h_{p-1}), \quad f + 1 \leq p \leq N - 1 \\
&= W(h_p - h_{p-1}) - Q_w, \quad p = N
\end{aligned}$$

Thus the general multicomponent rectification problem is characterized by $m + 1$ matrices, m of which are determined by the equilibrium properties of the mixture and the other by the enthalpy of the mixture. To these equations must be appended the condition that the temperature on each plate must be chosen such that

$$\sum_i x_{ji} = 1 = \sum_i K_{ji} x_{ji}$$

Method of Computation

Consider now the method by which the computation would be carried through in general. Suppose that partial molar enthalpies of mixtures of the components under consideration are available as functions of the temperature, so that

$$\begin{aligned}
h_j &= \sum_i h_{ji} x_{ji} \\
H_j &= \sum_i H_{ji} y_{ji}
\end{aligned}$$

where h_{ji} and H_{ji} are the partial molar enthalpies and summations are taken over all components; h_{ji} and H_{ji} are taken as polynomial functions of the temperature, although other more rigorous forms may be used.

To be specific, let us discuss the prob-

lem of light hydrocarbon rectification in which the vapor-liquid equilibrium relation is expressed as a conventional equilibrium constant which is a function of the temperature alone (and, of course, the total pressure). Suppose also that the problem with constant molar overflow is taken first. If a set of temperatures are estimated throughout the column, a complete set of equilibrium constants may be calculated. With a machine calculation this can be accomplished by fitting the equilibrium data to a polynomial (or other) function for each component in the form

$$K_{ji} = \alpha_i + \beta_i t_j + \gamma_i t_j^2 + \delta_i t_j^3 + \dots + \omega_i t_j^n$$

where the $\alpha_i, \beta_i, \gamma_i, \delta_i, \dots, \omega_i$ are characteristic of the component and the total pressure. If the total pressure is fixed as well as the cooling water temperature, a rough calculation of the top and bottom temperature as well as the feed plate temperature is possible. The intermediate plate temperatures may then be made a linear function of the plate number. With constant molal overflow the vapor rates may be estimated from a simple heat balance and it is not necessary to use Equation 2.

As matrix \bar{M}_i contains only K_{ji} and V_j , compositions \bar{X}_i may be obtained from Equation 1. If a matrix inversion technique is available for the machine, as it is for the Model 1103, these compositions are available after multiplication of \bar{M}_i^{-1} by \bar{F}_i , since

$$\bar{X}_i = \bar{M}_i^{-1} \bar{F}_i \quad (3)$$

$$\bar{V} = \bar{H}^{-1} \bar{G} \quad (4)$$

Now \bar{M}_i contains only information about the i th component. Thus if the assumed temperature distribution is not correct, the sum of the mole fractions on a particular plate need not be 1; in fact, some of the mole fractions of a plate may be negative and some may be greater than 1. If a mole fraction is negative, it is made zero. Therefore a procedure is needed for making a new estimation of the temperature. This causes some difficulty. Consider the function

$$\phi_j = \sum_i K_{ji} x_{ji}$$

where ϕ depends upon temperature alone. If one expands ϕ_j in a Taylor series taking only the linear terms,

$$\phi_j(t_j) = \phi_j(t_j') + \left(\frac{\partial \phi_j}{\partial t_j} \right)_{t_j'} (t_j - t_j')$$

If t_j is the temperature which $\phi_j = 1$, then

$$t_j = t_j' + [1 - \phi_j(t_j')] \left[\frac{\partial \phi_j}{\partial t_j} \right]_{t_j'}^{-1} \quad (5)$$

and this is recognized as the Newton approximation for the corrected temperature. Now

Table I. Coefficients in Quadratic Expression for Enthalpy

| | $a_i \times 10^{-8}$ | b_i | $c_i \times 10^2$ | $A_i \times 10^{-3}$ | B_i | $C_i \times 10^2$ |
|-------|----------------------|-------|-------------------|----------------------|-------|-------------------|
| C_2 | 6.12 | 9.35 | 1.5 | 8.31 | 13.2 | 0.602 |
| C_3 | 3.62 | 40.5 | -1.32 | 1.195 | 12.35 | 2.21 |
| C_4 | 6.28 | 25.0 | 4.65 | 1.655 | 9.01 | 3.78 |
| C_5 | 6.84 | 38.5 | 2.52 | 1.920 | 29.5 | 0.72 |
| C_6 | 7.92 | 43.5 | 3.02 | 2.20 | 37.0 | 0 |

Table II. Coefficients in Cubic Approximation to Equilibrium Constants

| | α_i | $\beta_i \times 10^4$ | $\gamma_i \times 10^6$ | $\delta_i \times 10^8$ |
|-------|------------|-----------------------|------------------------|------------------------|
| C_2 | 1.665 | -1.50 | 73.5 | -3.00 |
| C_3 | 0.840 | -46.6 | 49.4 | -3.033 |
| C_4 | -0.177 | 49.5 | -4.15 | 2.22 |
| C_5 | -0.0879 | 17.70 | 0.2031 | 1.310 |
| C_6 | 0.0930 | -15.39 | 10.37 | -0.1590 |

$$\left(\frac{\partial \phi_j}{\partial t_j}\right)_{t_j'} = \sum_i x_{ji} (\beta_i + 2\gamma_i t_j' + 3\delta_i t_j'^2 + \dots + n\omega_i t_j'^{n-1})$$

$$\sum_i K_{ji} x_{ji} = 1$$

$$\text{and } \sum_i x_{ji} = 1$$

and a direct machine calculation enables one to calculate a new temperature for the j th plate from Equation 5. If this procedure is used directly and the whole process repeated in an iterative manner, the process diverges in general.

A second scheme was to try to drive $\sum_i x_{ji}$ toward 1 by making a calculation on the column for two different temperature distributions differing on each plate by a small amount. Thus on each plate two values of $\sum_i x_{ji}$ were available, one for each temperature. A temperature could then be obtained by linear interpolation or extrapolation which would give $\sum_i x_{ji} = 1$. These new temperatures could then be used and the whole procedure repeated. This process also diverged in general. This simple interpolation procedure could be generalized to interpolations of higher order by making calculations at additional temperatures, but this was not pursued further.

A third technique which produced fairly rapid convergence was a modification of the first method. Suppose that after an initial temperature distribution has been assumed and compositions calculated, $\sum_i x_{ji} \neq 1$. Let the compositions on each plate be normalized by dividing each composition by the composition sum on that plate. With these normalized compositions Equation 5 is used. If this procedure is to converge, it follows that at the convergence point

$$\sum_i K_{ji} x_{ji} = \sum_i x_{ji} \quad (6)$$

It may be shown from Equation 1 that if $\sum_i x_{ji} = 1$, $\sum_i K_{ji} x_{ji} = 1$; the converse is also true. However, if Equation 6 is to be valid and the procedure is to give the correct answer, Equation 6 must imply that

Naturally if one of these is true, the other is. It may be shown that Equation 6 implies that

$$\sum_i x_{ji} = 1 = \sum_i K_{ji} x_{ji}$$

For constant molal overflow the steps in the process are:

A. From rough calculations and a heat balance estimate the temperatures and vapor flow rates through the column.

B. With these temperatures and vapor flow rates compute K_{ji} and then the compositions, using Equation 3.

C. Normalize the compositions obtained in B.

D. Using Equation 5 calculate a corrected set of temperatures.

E. Repeat starting with B.

F. Stop when the desired degree of accuracy in x_{ji} , $\sum_i x_{ji}$, or $\sum_i K_{ji} x_{ji}$ has been reached.

If the variation in molal overflow is to be reckoned with, only a slight modification is needed. It is perhaps better to solve the problem first as if it were one of constant molal overflow. This will serve as a good first approximation to the present problem and produce a complete set of compositions as well as temperatures. With these compositions and temperatures a complete set of liquid and vapor enthalpies may be computed from the appropriate equations. By substituting these in Equation 4, a set of V_j throughout the column is obtained. These V_j and the K_{ji} obtained from the assumed temperature distribution then allow one to calculate a complete new set of compositions. The temperature corrections may then be obtained from these compositions and now the whole process repeated.

First Numerical Example

As a first example consider the distillation of a feed with the composition

| | | |
|-------|----------|------|
| C_2 | x_{F1} | 0.03 |
| C_3 | x_{F2} | 0.20 |
| C_4 | x_{F3} | 0.37 |
| C_5 | x_{F4} | 0.35 |
| C_6 | x_{F5} | 0.05 |

The column is to operate at 250 pounds per square inch. There will be 15 trays, including the reboiler, and a partial condenser. The basis for the calculation will be a feed of 100 moles per hour ($F = 100$). The vapor overhead will be 22.6 moles per hour ($D = 22.6$) and the bottoms 77.4 moles per hour ($W = 77.4$). Of the 100 moles of feed preheated to 225° F., 16.4 moles are vapor and this should be the difference between the vapor rates in the top and bottom sections of the column. A reflux of 5 is assumed ($L_0/D = 5.0$). This would indicate the vapor rate in the top of the column to be 135.6 and in the bottom section 119.2. Calculations (3) on a problem after which this one was modeled indicate that for constant molal overflow it is probably more accurate to assume

$$V_j = 135.6, \quad 1 \leq j \leq f$$

$$= 125.10, \quad f+1 \leq j \leq N$$

The feed is to be admitted to the seventh tray from the top. The enthalpy data are to be approximated as a quadratic function of the temperature.

$$h_{ji} = a_i + b_i t_i + c_i t_i^2$$

$$H_{ji} = A_i + B_i t_i + C_i t_i^2$$

Values of a_i , b_i , and c_i have been obtained by fitting the data of Maxwell (2) (Table I).

The equilibrium constants at 250 pounds per square inch have been fitted to a cubic polynomial in the temperature

$$K_{ji} = \alpha_i + \beta_i t + \gamma_i t^2 + \delta_i t^3$$

These constants are shown in Table II, the original data having been taken from Robinson and Gilliland (4).

Constant Molal Overflow. The calculation for constant molal overflow will be carried out, as it illustrates the technique and its solution serves as a good approximation to the more general problem. The details of the programming of the problem for the computer are not presented here. A set of temperatures throughout the column must be assumed. For the problem at hand a temperature at the vapor outlet of the partial condenser of 110° F. was taken, while the bottom temperature was set initially at 305° F. These temperatures were obtained by making a rough estimate of top and bottom compositions and with a pressure of 250 p.s.i., estimating the temperature of the dew point and bubble point. The coefficients in the cubic polynomial having been previously stored in the machine, the equilibrium constants for each component on each plate could be calculated and stored in the memory. Vapor rates, D , W , F , and feed compositions can be

stored in the memory for use and substitution in matrices \bar{M}_i . The matrix inversion scheme is programmed and the computation of the inverse carried out, followed by multiplication of the inverse by \bar{F}_i . This gives the composition column vectors, \bar{X}_i , which are stored in the appropriate places ready for further computation.

At this point it is necessary to compute $\sum_i x_{ji}$ and $\sum_i K_{ji}x_{ji}$ and the program for calculation of the corrected temperature distribution is instituted. The first iteration has now been completed and the new temperatures are available in the memory for the second iteration. Successive iterations are carried out until a preassigned accuracy in individual compositions, $\sum_i x_{ji}$ or $\sum_i K_{ji}x_{ji}$, is obtained. In general, in the calculations described here $\sum_i K_{ji}x_{ji}$ was used as an indicator for a stopping procedure.

In Table III are given the results of a calculation made using the temperatures in the second column as an initial temperature distribution. $\sum_i x_{ji}$ is in general not equal to 1. Further iterations do not change the normalized compositions; in fact, all normalized compositions at the fourth iteration are within 3% of the compositions at the eighth iteration. Agreement is in general considerably better in the lower part of the column than at the top—that is, convergence seems to be considerably more rapid in the bottom section than at the very top of the column, although the disagreement between assumed temperatures and final temperatures at the bottom is greater. Each iteration in this calculation requires about 8 seconds or less; thus, answers of sufficient accuracy are obtained in $3\frac{1}{2}$ to 4 minutes, including complete punchout on each tray of temperature, composition, and $\sum_i K_{ji}x_{ji}$ at the end of each iteration. If punchout is made at the end of the final iteration only, the total time is reduced to less than a minute.

To determine the speed of convergence, four additional runs were made, using different initial temperature distributions:

- 25° above final temperatures.
- 25° below final temperatures.
- 25° above originally assumed initial temperatures.
- 25° below originally assumed temperatures.

In all these cases the convergence was almost as good as and in some cases better than the 110° to 305° assumption. Although the values in Table III show three significant figures, calculations were performed at the full accuracy of the computer.

Complete Heat Balancing. The complete heat balancing over each tray was carried out with enthalpies of each component expressed as quadratic functions

Table III. Temperatures and Compositions

(Constant molal overflow, 15-plate column)

| Plate No. | Temp., ° F. | C_2 | C_3 | C_4 | C_5 | C_6 | $\sum_i x_{ji}$ |
|-------------|-------------|-------|-------|-------|-------|-------|-----------------|
| Iteration 1 | | | | | | | |
| 0 | 110 | 0.053 | 0.983 | 0.072 | 0.000 | 0.000 | 01.108 |
| 1 | 126 | 0.024 | 0.987 | 0.151 | 0.000 | 0.000 | 01.162 |
| 2 | 140 | 0.014 | 0.902 | 0.263 | 0.002 | 0.000 | 01.181 |
| 3 | 154 | 0.010 | 0.758 | 0.393 | 0.007 | 0.000 | 01.168 |
| 4 | 168 | 0.009 | 0.594 | 0.516 | 0.021 | 0.000 | 01.140 |
| 5 | 182 | 0.008 | 0.443 | 0.603 | 0.054 | 0.002 | 01.111 |
| 6 | 196 | 0.007 | 0.322 | 0.633 | 0.124 | 0.007 | 01.093 |
| 7 | 210 | 0.006 | 0.235 | 0.600 | 0.249 | 0.029 | 01.119 |
| 8 | 225 | 0.002 | 0.194 | 0.695 | 0.262 | 0.030 | 01.183 |
| 9 | 237 | 0.001 | 0.148 | 0.787 | 0.277 | 0.031 | 01.244 |
| 10 | 250 | 0.000 | 0.103 | 0.856 | 0.296 | 0.032 | 01.287 |
| 11 | 262 | 0.000 | 0.067 | 0.887 | 0.318 | 0.034 | 01.306 |
| 12 | 274 | 0.000 | 0.040 | 0.864 | 0.345 | 0.036 | 01.285 |
| 13 | 285 | 0.000 | 0.022 | 0.785 | 0.379 | 0.040 | 01.226 |
| 14 | 300 | 0.000 | 0.011 | 0.638 | 0.408 | 0.046 | 01.103 |
| 15 | 305 | 0.000 | 0.005 | 0.471 | 0.452 | 0.065 | 00.993 |
| Iteration 4 | | | | | | | |
| 0 | 122.07 | 0.049 | 0.895 | 0.066 | 0.000 | 0.000 | 1.010 |
| 1 | 134.48 | 0.022 | 0.859 | 0.126 | 0.000 | 0.000 | 1.007 |
| 2 | 144.02 | 0.013 | 0.778 | 0.213 | 0.002 | 0.000 | 1.006 |
| 3 | 154.18 | 0.010 | 0.667 | 0.319 | 0.007 | 0.000 | 1.003 |
| 4 | 165.75 | 0.009 | 0.543 | 0.429 | 0.021 | 0.000 | 1.002 |
| 5 | 178.94 | 0.008 | 0.420 | 0.514 | 0.055 | 0.002 | 0.999 |
| 6 | 194.80 | 0.007 | 0.311 | 0.545 | 0.127 | 0.008 | 0.998 |
| 7 | 215.43 | 0.006 | 0.220 | 0.500 | 0.245 | 0.029 | 1.000 |
| 8 | 223.21 | 0.002 | 0.182 | 0.535 | 0.250 | 0.030 | 0.999 |
| 9 | 230.02 | 0.001 | 0.143 | 0.568 | 0.257 | 0.030 | 0.999 |
| 10 | 236.27 | 0.000 | 0.108 | 0.596 | 0.263 | 0.031 | 0.998 |
| 11 | 242.04 | 0.000 | 0.077 | 0.617 | 0.273 | 0.031 | 0.998 |
| 12 | 247.57 | 0.000 | 0.053 | 0.625 | 0.287 | 0.032 | 0.997 |
| 13 | 253.71 | 0.000 | 0.034 | 0.614 | 0.315 | 0.034 | 0.997 |
| 14 | 262.21 | 0.000 | 0.020 | 0.569 | 0.366 | 0.042 | 0.997 |
| 15 | 276.12 | 0.000 | 0.010 | 0.470 | 0.452 | 0.065 | 0.997 |
| Iteration 7 | | | | | | | |
| 0 | 121.49 | 0.050 | 0.896 | 0.061 | 0.000 | 0.000 | 1.007 |
| 1 | 133.63 | 0.022 | 0.865 | 0.118 | 0.000 | 0.000 | 1.005 |
| 2 | 142.85 | 0.013 | 0.789 | 0.200 | 0.002 | 0.000 | 1.004 |
| 3 | 152.75 | 0.010 | 0.681 | 0.305 | 0.006 | 0.000 | 1.002 |
| 4 | 164.20 | 0.009 | 0.558 | 0.415 | 0.020 | 0.000 | 1.003 |
| 5 | 177.46 | 0.008 | 0.433 | 0.503 | 0.054 | 0.002 | 1.000 |
| 6 | 193.56 | 0.007 | 0.321 | 0.538 | 0.126 | 0.008 | 1.000 |
| 7 | 214.57 | 0.006 | 0.225 | 0.496 | 0.244 | 0.029 | 1.000 |
| 8 | 222.31 | 0.002 | 0.187 | 0.531 | 0.250 | 0.030 | 1.000 |
| 9 | 229.15 | 0.001 | 0.148 | 0.564 | 0.256 | 0.030 | 0.999 |
| 10 | 235.48 | 0.000 | 0.112 | 0.593 | 0.263 | 0.030 | 0.998 |
| 11 | 241.37 | 0.000 | 0.081 | 0.615 | 0.272 | 0.030 | 0.999 |
| 12 | 247.04 | 0.000 | 0.055 | 0.624 | 0.287 | 0.032 | 0.998 |
| 13 | 253.30 | 0.000 | 0.036 | 0.614 | 0.314 | 0.034 | 0.998 |
| 14 | 261.91 | 0.000 | 0.021 | 0.570 | 0.366 | 0.042 | 0.999 |
| 15 | 275.93 | 0.000 | 0.010 | 0.471 | 0.452 | 0.065 | 0.998 |

of the temperature for both the liquid and the vapor. The degree of the polynomial used is immaterial. Two courses of action are possible. The above solution may be used as a first approximation in starting the problem, or assuming a temperature distribution, calculate a set of x_{ji} , assuming a fixed set of V_j as in constant molal overflow, compute the h_{ji} , calculate from Equation 4 \bar{V} and thus a new set of V_j , and these in Equation 3 to compute a new set of x_{ji} , having corrected the temperature. How often V_j should be recalculated and the procedure for making the calculations so that the time of computation is to be minimized, are open questions.

In these calculations after the first approximation Equations 3 and 4 were used alternately, so that a new set of vapor flow rates were used in each iteration.

Each iteration required somewhat less than 10 seconds. The punchout of temperature, composition, vapor flow rate, and $\sum_i K_{ji}x_{ji}$ on each tray after each iteration requires more time. Complete punchout may require 30 seconds, depending upon the number of significant figures.

To specify Q_w a heat balance was made around the bottom of the column for the constant molal overflow case, using the enthalpy data cited above. H_F was calculated using the same data, giving

$$H_F = 15,600 \text{ B.t.u./mole}$$

$$Q_w = 1.03 \times 10^8 \text{ B.t.u./100 moles of feed}$$

In Table IV are found the results of four of the 15 iterations on this problem. The compositions are not appreciably

Table IV. Temperatures, Compositions, and Vapor Rates

(Nonconstant molal overflow, 15-plate column)

| Plate No. | Temp., ° F. | C_2 | C_3 | C_4 | C_5 | C_6 | V_j | Σx_{ji} |
|----------------|-------------|-------|-------|-------|-------|-------|--------|-----------------|
| 1st Iteration | | | | | | | | |
| 0 | 121.39 | 0.050 | 0.896 | 0.060 | 0.000 | 0.000 | ... | 1.006 |
| 1 | 133.48 | 0.022 | 0.866 | 0.116 | 0.000 | 0.000 | 135.60 | 1.004 |
| 2 | 142.64 | 0.013 | 0.791 | 0.198 | 0.002 | 0.000 | 135.60 | 1.004 |
| 3 | 152.50 | 0.010 | 0.684 | 0.302 | 0.006 | 0.000 | 135.60 | 1.002 |
| 4 | 163.92 | 0.009 | 0.560 | 0.412 | 0.020 | 0.000 | 135.60 | 1.001 |
| 5 | 177.18 | 0.008 | 0.436 | 0.501 | 0.054 | 0.002 | 135.60 | 1.001 |
| 6 | 193.33 | 0.007 | 0.322 | 0.537 | 0.126 | 0.008 | 135.60 | 1.000 |
| 7 | 214.41 | 0.006 | 0.226 | 0.495 | 0.244 | 0.029 | 135.60 | 1.000 |
| 8 | 222.13 | 0.002 | 0.189 | 0.530 | 0.252 | 0.030 | 125.10 | 1.001 |
| 9 | 228.97 | 0.001 | 0.149 | 0.564 | 0.256 | 0.030 | 125.10 | 1.000 |
| 10 | 235.32 | 0.000 | 0.113 | 0.593 | 0.263 | 0.030 | 125.10 | 0.999 |
| 11 | 241.23 | 0.000 | 0.082 | 0.614 | 0.272 | 0.031 | 125.10 | 0.999 |
| 12 | 246.93 | 0.000 | 0.056 | 0.624 | 0.287 | 0.032 | 125.10 | 0.999 |
| 13 | 253.21 | 0.000 | 0.036 | 0.614 | 0.314 | 0.034 | 125.10 | 0.998 |
| 14 | 261.85 | 0.000 | 0.021 | 0.570 | 0.366 | 0.042 | 125.10 | 0.999 |
| 15 | 275.89 | 0.000 | 0.010 | 0.471 | 0.452 | 0.065 | 125.10 | 0.998 |
| 5th Iteration | | | | | | | | |
| 0 | 120.20 | 0.050 | 0.909 | 0.047 | 0.000 | 0.000 | ... | 1.006 |
| 1 | 131.93 | 0.021 | 0.889 | 0.095 | 0.000 | 0.000 | 176.04 | 1.005 |
| 2 | 140.76 | 0.012 | 0.821 | 0.170 | 0.001 | 0.000 | 176.56 | 1.004 |
| 3 | 150.52 | 0.009 | 0.715 | 0.274 | 0.005 | 0.000 | 172.98 | 1.003 |
| 4 | 162.28 | 0.007 | 0.585 | 0.391 | 0.018 | 0.000 | 167.26 | 1.001 |
| 5 | 176.22 | 0.007 | 0.449 | 0.492 | 0.051 | 0.002 | 160.26 | 1.001 |
| 6 | 193.00 | 0.006 | 0.326 | 0.538 | 0.122 | 0.008 | 152.11 | 1.000 |
| 7 | 214.16 | 0.006 | 0.227 | 0.501 | 0.239 | 0.029 | 142.74 | 1.002 |
| 8 | 221.72 | 0.002 | 0.188 | 0.540 | 0.242 | 0.029 | 129.06 | 1.001 |
| 9 | 228.60 | 0.001 | 0.147 | 0.577 | 0.247 | 0.029 | 132.06 | 1.001 |
| 10 | 235.02 | 0.000 | 0.109 | 0.610 | 0.252 | 0.029 | 134.71 | 1.000 |
| 11 | 240.98 | 0.000 | 0.076 | 0.633 | 0.260 | 0.029 | 137.43 | 0.998 |
| 12 | 246.75 | 0.000 | 0.051 | 0.642 | 0.276 | 0.030 | 139.92 | 0.999 |
| 13 | 253.20 | 0.000 | 0.032 | 0.627 | 0.307 | 0.033 | 141.44 | 0.999 |
| 14 | 262.10 | 0.000 | 0.018 | 0.576 | 0.363 | 0.041 | 141.06 | 0.998 |
| 15 | 276.27 | 0.000 | 0.009 | 0.473 | 0.452 | 0.065 | 138.24 | 0.999 |
| 10th Iteration | | | | | | | | |
| 0 | 119.89 | 0.050 | 0.910 | 0.044 | 0.000 | 0.000 | ... | 1.004 |
| 1 | 131.45 | 0.021 | 0.892 | 0.090 | 0.000 | 0.000 | 176.58 | 1.003 |
| 2 | 140.04 | 0.012 | 0.827 | 0.163 | 0.001 | 0.000 | 177.24 | 1.003 |
| 3 | 149.58 | 0.009 | 0.725 | 0.264 | 0.005 | 0.000 | 173.69 | 1.003 |
| 4 | 161.21 | 0.007 | 0.596 | 0.380 | 0.017 | 0.000 | 167.91 | 1.000 |
| 5 | 175.15 | 0.007 | 0.459 | 0.483 | 0.050 | 0.001 | 160.90 | 1.000 |
| 6 | 192.09 | 0.006 | 0.334 | 0.532 | 0.121 | 0.007 | 152.85 | 1.000 |
| 7 | 213.54 | 0.006 | 0.231 | 0.497 | 0.238 | 0.028 | 143.29 | 1.000 |
| 8 | 221.04 | 0.002 | 0.192 | 0.536 | 0.241 | 0.029 | 129.56 | 1.000 |
| 9 | 227.91 | 0.001 | 0.150 | 0.574 | 0.246 | 0.029 | 132.47 | 1.000 |
| 10 | 234.27 | 0.000 | 0.112 | 0.607 | 0.251 | 0.029 | 134.98 | 0.999 |
| 11 | 240.42 | 0.000 | 0.079 | 0.631 | 0.260 | 0.029 | 137.48 | 0.999 |
| 12 | 246.31 | 0.000 | 0.053 | 0.640 | 0.276 | 0.030 | 139.74 | 0.999 |
| 13 | 252.88 | 0.000 | 0.033 | 0.627 | 0.307 | 0.033 | 141.17 | 1.000 |
| 14 | 261.89 | 0.000 | 0.019 | 0.576 | 0.363 | 0.041 | 140.94 | 0.999 |
| 15 | 276.14 | 0.000 | 0.009 | 0.473 | 0.452 | 0.065 | 138.28 | 0.999 |
| 15th Iteration | | | | | | | | |
| 0 | 119.70 | 0.050 | 0.910 | 0.042 | 0.000 | 0.000 | ... | 1.002 |
| 1 | 131.16 | 0.021 | 0.894 | 0.087 | 0.000 | 0.000 | 176.89 | 1.002 |
| 2 | 139.60 | 0.012 | 0.831 | 0.158 | 0.001 | 0.000 | 177.70 | 1.002 |
| 3 | 149.00 | 0.009 | 0.730 | 0.257 | 0.005 | 0.000 | 174.29 | 1.001 |
| 4 | 160.53 | 0.007 | 0.603 | 0.373 | 0.017 | 0.000 | 168.57 | 1.000 |
| 5 | 174.46 | 0.007 | 0.466 | 0.477 | 0.049 | 0.001 | 161.52 | 1.000 |
| 6 | 191.49 | 0.006 | 0.338 | 0.528 | 0.120 | 0.007 | 153.31 | 0.999 |
| 7 | 213.11 | 0.006 | 0.233 | 0.495 | 0.238 | 0.028 | 143.52 | 1.000 |
| 8 | 220.57 | 0.002 | 0.194 | 0.534 | 0.241 | 0.029 | 129.57 | 1.000 |
| 9 | 227.46 | 0.001 | 0.153 | 0.572 | 0.246 | 0.029 | 132.38 | 1.001 |
| 10 | 233.97 | 0.000 | 0.114 | 0.605 | 0.251 | 0.029 | 134.84 | 0.999 |
| 11 | 240.09 | 0.000 | 0.081 | 0.630 | 0.260 | 0.029 | 137.34 | 1.000 |
| 12 | 246.06 | 0.000 | 0.053 | 0.640 | 0.276 | 0.030 | 139.64 | 1.000 |
| 13 | 252.70 | 0.000 | 0.034 | 0.626 | 0.307 | 0.033 | 141.11 | 1.000 |
| 14 | 261.77 | 0.000 | 0.019 | 0.576 | 0.363 | 0.041 | 140.91 | 0.999 |
| 15 | 276.06 | 0.000 | 0.009 | 0.473 | 0.452 | 0.065 | 138.27 | 0.999 |

different for any of the iterations shown. The second iteration is considerably poorer than the first and the third and fourth get progressively better, until the fifth may be considered satisfactory. Five iterations on this problem amount to about 50 seconds of computing time.

Multiple Feeds and Side Stream Drawoffs

The method of solution outlined is applicable to multiple feeds and drawoffs. For illustration only, the case of two feeds and a single side stream is con-

sidered. The equations of the mass and heat balances are written and a numerical problem is discussed. The numbering system used previously is used here also, with additional nomenclature. The over-all material balances are:

$$L_j + D_1 = V_{j+1}, \quad 0 \leq j \leq d-1$$

$$L_j + D_1 + D_2 = V_{j+1}, \quad d \leq j \leq f_1 - 1 \quad (7)$$

$$L_j + D_1 + D_2 - F_1 = V_{j+1}, \quad f_1 \leq j \leq f_2 - 1$$

$$L_j - W = V_{j+1}, \quad f_2 \leq j \leq N-1$$

where all envelopes are taken around the top except the last one, which is around the bottom. Mass balances around single trays are:

$$L_0 x_{0i} + D_1 y_{0i} = V_1 y_{1i}, \quad 1 \leq j \leq d-1$$

$$L_{j-1} x_{j-1,i} - L_j x_{ji} - V_j y_{ji} + V_{j+1} y_{j+1,i} = 0, \quad d+1 \leq j \leq f_1 - 1$$

$$f_1 + 1 \leq j \leq f_2 - 1$$

$$f_2 + 1 \leq j \leq N - 1$$

$$L_{j-1} x_{j-1,i} - (L_j + D_2) x_{ji} - V_j y_{ji} + V_{j+1} y_{j+1,i} = 0, \quad j = d$$

$$L_{j-1} x_{j-1,i} - L_j x_{ji} - V_j y_{ji} + V_{j+1} y_{j+1,i} = -F_1 x_{F1,i}, \quad j = f_1$$

$$L_{j-1} x_{j-1,i} - L_j x_{ji} - V_j y_{ji} + V_{j+1} y_{j+1,i} = -F_2 x_{F2,i}, \quad j = f_2$$

$$L_{j-1} x_{j-1,i} - W x_{ji} - V_j y_{ji} = 0, \quad j = N$$

Equations 7 and 8 may be used to eliminate L_j throughout to give mass balances involving only V_j , D_1 , D_2 , F_1 , F_2 , W , and x_{ji} . These equations may then be written in terms of m matrix equations of the form of Equation 1.

If the elements of \bar{M}_i are a_{pq} , then

$$a_{00} = -V_1 - (K_{0i} - 1) D_1$$

$$a_{pp} = -(V_{p+1} - D_1 + V_p K_{pi}), \quad 1 \leq p \leq d$$

$$= -(V_{p+1} - D_1 - D_2 + V_p K_{pi}), \quad d+1 \leq p \leq f_1 - 1$$

$$= -(V_{p+1} - D_1 - D_2 + F_1 + V_p K_{pi}), \quad f_1 \leq p \leq f_2 - 1$$

$$= -(V_{p+1} + W + V_p K_{pi}), \quad f_2 \leq p \leq N - 1$$

$$a_{p-1,p} = V_p K_{pi}, \quad 1 \leq p \leq N$$

$$a_{p,p-1} = V_p - D_1, \quad 1 \leq p \leq d$$

$$= V_p - D_1 - D_2, \quad d+1 \leq p \leq f_1$$

$$= V_p - D_1 - D_2 + F_1, \quad f_1 + 1 \leq p \leq f_2$$

$$= V_p + W, \quad f_2 + 1 \leq p \leq N$$

All other a_{pq} are zero and again there are nonzero elements only on the main diagonal and two adjacent diagonals in matrix \bar{M}_i . If d_p is a typical element of \bar{F}_i , then

$$d_p = 0, \quad 0 \leq p \leq f_1 - 1$$

$$f_1 + 1 \leq p \leq f_2 - 1$$

$$f_2 + 1 \leq p \leq N$$

$$d_p = -F_1 x_{F_1 i}, \quad p = f_1$$

$$= -F_2 x_{F_2 i}, \quad p = f_2$$

The composition column vector, \bar{X}_i , has as elements

$$x_{pi}, \quad 0 \leq p \leq N$$

The enthalpy matrix, H , may be written as before

$$b_{pp} = h_{p-1} - H_p, \quad 1 \leq p \leq n$$

$$b_{p,p+1} = H_{p+1} - h_p, \quad 1 \leq p \leq N-1$$

The vapor flow column vector, \bar{V} , has as elements

$$V_p, \quad 1 \leq p \leq N$$

The product enthalpy vector, \bar{G} , whose elements are c_p is

$$c_p = D(h_{p-1} - h_p), \quad 1 \leq p \leq d$$

$$= (D_1 + D_2)(h_{p-1} - h_p), \quad d+1 \leq p \leq f_1 - 1$$

$$= (D_1 + D_2)(h_{p-1} - h_p) + F_1(h_p - H_{F_1}), \quad p = f_1$$

$$= (D_1 + D_2 - F_1)(h_{p-1} - h_p), \quad f_1 + 1 \leq p \leq f_2 - 1$$

$$= (D_1 + D_2 - F_1)(h_{p-1} - h_p) + F_2(h_p - H_{F_2}), \quad p = f_2$$

$$= W(h_p - h_{p-1}), \quad f_2 + 1 \leq p \leq N - 1$$

$$= W(h_p - h_{p-1}) - Q_w, \quad p = N$$

With these definitions for the matrices Equations 1, 2, 3, and 4 are still valid. The use of multiple feeds and side stream drawoffs does not complicate the overall problem, although it makes the individual matrices more complicated.

Second Numerical Example

To test the program on a larger problem, a column consisting of 50 plates plus a reboiler and a partial condenser with two feeds and a side stream drawoff was considered. The case for constant molal overflow is shown. Two feeds at their boiling points and 250 pounds per square inch were admitted, F_1 on plate 25 and F_2 on plate 40. The side stream drawoff, D_2 , was the liquid from plate 15. The vapor rates throughout the column were taken as 130 moles per 100 moles of feed.

| | $x_{F_1 i}$ | $x_{F_2 i}$ |
|-------|-------------|-------------|
| C_2 | 0.03 | 0.01 |
| C_3 | 0.48 | 0.20 |
| C_4 | 0.33 | 0.44 |
| C_5 | 0.15 | 0.29 |
| C_6 | 0.01 | 0.06 |

$$D_1 = 28 \text{ moles (vapor O.H.)}$$

$$D_2 = 8 \text{ moles (tray 15)}$$

$$W = 64 \text{ moles (bottoms)}$$

$$F_1 = 50 \text{ moles (tray 25)}$$

$$F_2 = 50 \text{ moles (tray 40)}$$

$$V_j = 130 \text{ moles, } 1 \leq j \leq 51$$

$$N = 51$$

$$m = 5$$

Table V. Plate Temperatures on Successive Iterations, 51-Plate Column

| Plate No. | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|-----------|-----|--------|--------|--------|--------|--------|--------|--------|--------|
| 0 | 110 | 124.63 | 123.05 | 122.86 | 122.78 | 122.76 | 122.72 | 122.70 | 122.69 |
| 1 | 113 | 127.91 | 126.39 | 126.30 | 126.25 | 126.24 | 126.22 | 126.22 | 126.21 |
| 2 | 116 | 128.54 | 127.34 | 127.29 | 127.26 | 127.25 | 127.24 | 127.24 | 127.23 |
| 3 | 120 | 128.38 | 127.62 | 127.58 | 127.55 | 127.54 | 127.53 | 127.53 | 127.53 |
| 4 | 123 | 128.29 | 127.71 | 127.67 | 127.64 | 127.63 | 127.62 | 127.61 | 127.61 |
| 5 | 126 | 128.27 | 127.76 | 127.70 | 127.67 | 127.66 | 127.65 | 127.64 | 127.64 |
| 6 | 129 | 128.38 | 127.82 | 127.74 | 127.70 | 127.68 | 127.67 | 127.66 | 127.66 |
| 7 | 133 | 128.71 | 127.91 | 127.78 | 127.73 | 127.71 | 127.69 | 127.68 | 127.68 |
| 8 | 136 | 129.25 | 128.07 | 128.87 | 127.79 | 127.75 | 127.73 | 127.72 | 127.71 |
| 9 | 139 | 130.10 | 128.35 | 128.01 | 127.89 | 127.83 | 127.80 | 127.78 | 127.76 |
| 10 | 142 | 131.37 | 128.84 | 128.28 | 128.07 | 127.98 | 127.92 | 128.89 | 127.86 |
| 11 | 146 | 133.28 | 129.67 | 128.74 | 128.40 | 128.24 | 128.15 | 128.09 | 128.04 |
| 12 | 149 | 135.72 | 131.01 | 129.54 | 128.97 | 128.70 | 128.54 | 128.44 | 128.36 |
| 13 | 152 | 138.91 | 133.08 | 130.87 | 129.96 | 129.50 | 129.23 | 129.05 | 128.92 |
| 14 | 155 | 142.88 | 136.09 | 132.99 | 131.59 | 130.86 | 130.42 | 130.12 | 129.89 |
| 15 | 159 | 147.65 | 140.19 | 136.18 | 134.16 | 133.05 | 132.36 | 131.88 | 131.52 |
| 16 | 162 | 152.85 | 145.32 | 140.59 | 137.95 | 136.40 | 135.39 | 134.67 | 134.12 |
| 17 | 165 | 157.94 | 150.82 | 145.78 | 142.68 | 140.75 | 139.43 | 138.46 | 137.71 |
| 18 | 168 | 162.70 | 156.28 | 151.38 | 148.13 | 145.96 | 144.41 | 143.23 | 142.29 |
| 19 | 172 | 166.97 | 161.36 | 156.98 | 153.90 | 151.80 | 150.06 | 148.76 | 147.69 |
| 20 | 175 | 170.60 | 165.87 | 162.23 | 159.56 | 157.54 | 155.95 | 154.65 | 153.55 |
| 21 | 178 | 173.67 | 169.75 | 166.93 | 164.80 | 163.10 | 161.69 | 160.49 | 159.45 |
| 22 | 181 | 176.34 | 173.16 | 171.10 | 169.51 | 168.17 | 167.01 | 165.99 | 165.08 |
| 23 | 185 | 178.94 | 176.42 | 175.00 | 173.88 | 172.87 | 171.97 | 171.15 | 170.41 |
| 24 | 188 | 181.98 | 180.22 | 179.29 | 178.51 | 177.78 | 177.11 | 176.48 | 175.91 |
| 25 | 191 | 186.85 | 185.86 | 185.27 | 184.73 | 184.21 | 183.73 | 183.27 | 182.85 |
| 26 | 194 | 193.87 | 193.38 | 192.85 | 192.32 | 191.80 | 191.30 | 190.84 | 190.41 |
| 27 | 198 | 199.77 | 199.80 | 199.41 | 198.93 | 198.45 | 197.99 | 197.56 | 197.16 |
| 28 | 201 | 204.79 | 205.24 | 204.96 | 204.56 | 204.16 | 203.77 | 203.41 | 203.06 |
| 29 | 204 | 208.99 | 209.62 | 209.43 | 209.11 | 208.79 | 208.48 | 208.20 | 207.93 |
| 30 | 207 | 212.45 | 213.00 | 212.84 | 212.58 | 212.33 | 212.11 | 211.90 | 211.70 |
| 31 | 211 | 215.23 | 215.51 | 215.32 | 215.10 | 214.92 | 214.76 | 214.61 | 214.47 |
| 32 | 214 | 217.43 | 217.33 | 217.07 | 216.88 | 216.74 | 216.63 | 216.53 | 216.44 |
| 33 | 217 | 219.15 | 218.63 | 218.29 | 218.11 | 218.00 | 217.93 | 217.87 | 217.81 |
| 34 | 220 | 220.55 | 219.56 | 219.14 | 218.96 | 218.88 | 218.83 | 218.74 | 218.75 |
| 35 | 224 | 221.73 | 220.27 | 219.77 | 219.59 | 219.52 | 219.48 | 219.46 | 219.44 |
| 36 | 227 | 222.76 | 220.89 | 220.32 | 220.13 | 220.07 | 220.05 | 220.03 | 220.02 |
| 37 | 230 | 223.81 | 221.59 | 220.98 | 220.79 | 220.74 | 220.72 | 220.71 | 220.71 |
| 38 | 233 | 225.17 | 222.74 | 222.12 | 221.94 | 221.89 | 221.87 | 221.86 | 221.86 |
| 39 | 237 | 227.50 | 225.14 | 224.56 | 224.40 | 224.34 | 224.33 | 224.32 | 224.32 |
| 40 | 240 | 232.20 | 230.70 | 230.24 | 230.10 | 230.05 | 230.03 | 230.03 | 230.02 |
| 41 | 243 | 236.10 | 235.28 | 234.85 | 234.70 | 234.65 | 234.63 | 234.62 | 234.61 |
| 42 | 246 | 238.74 | 238.61 | 238.25 | 238.11 | 238.06 | 238.04 | 238.03 | 238.02 |
| 43 | 250 | 240.60 | 241.02 | 240.73 | 240.61 | 240.57 | 240.54 | 240.53 | 240.52 |
| 44 | 253 | 241.92 | 242.74 | 242.53 | 242.42 | 242.38 | 242.36 | 242.34 | 242.33 |
| 45 | 256 | 243.01 | 243.98 | 243.83 | 243.74 | 243.70 | 243.68 | 243.67 | 243.66 |
| 46 | 259 | 244.09 | 244.94 | 244.85 | 244.77 | 244.73 | 244.71 | 244.69 | 244.68 |
| 47 | 263 | 245.49 | 245.87 | 245.81 | 245.73 | 245.70 | 245.67 | 245.66 | 245.65 |
| 48 | 266 | 247.37 | 247.18 | 247.10 | 247.03 | 246.99 | 246.97 | 246.95 | 246.94 |
| 49 | 269 | 250.37 | 249.63 | 249.51 | 249.43 | 249.39 | 249.36 | 249.34 | 249.33 |
| 50 | 272 | 255.80 | 254.87 | 254.70 | 254.60 | 254.55 | 254.51 | 254.49 | 254.47 |
| 51 | 275 | 266.64 | 266.09 | 265.89 | 265.77 | 265.71 | 265.66 | 265.63 | 265.61 |

Equations 3 and 4 are used with the revised definitions of the elements given in the previous section. The same constants were used in the cubic expression for the equilibrium constants for each of the five components. As an initial assumption on the temperatures, values from 110° F. from the partial condenser outlet to 275° F. for the reboiler were used, the range of 165° F. giving a change of 3° or 4° F. per plate. On the first iteration these temperatures give some individual mole fractions in the top portion of the column which are greater than 1 and some other components negative mole fractions. In the computation of the temperature corrections negative mole fractions were changed to zeros throughout. The initial temperature distribution gave

values of Σx_{ji} from 1.363 on tray 3 to 0.806 on tray 15. The calculation was carried through 9 iterations. Again the compositions after three or four iterations, especially when normalized, appear to be almost as good as after the ninth iteration. The convergence in the bottom of the column is very fast, while the poorest plates seem to be in the vicinity of the top feed and continuing up to the side stream drawoff.

Temperatures used in successive iterations are given in Table V. It is apparent that better estimates on the first approximation will give more rapid convergence. For example, on the sixteenth plate the initial estimate was incorrect by almost 30°. A little experience with the system and the method should enable better estimates before

the first iteration. The compositions are not shown, but these are almost identical at the top and bottom of the fourth and eighth iterations. This problem requires about 30 seconds per iteration for computing time.

Further Comments on Method

In general, the problem of multicomponent distillation as it occurs in practice is stated in one of two forms. One is interested either in calculating the number of plates required for a given feed composition and separation or in calculating the required reflux ratio and feed location for a fixed number of plates. Although neither problem is presented here, it is assumed that the technique described would be a part of a larger program which would solve either problem.

Thus far use has been made of the equilibrium constants, K_{ji} , assumed to be a function only of temperature, pressure, and the single component designated as i . In the general case K_{ji} would also depend on all the other components. As long as there is a feasible method for obtaining K_{ji} , no serious difficulty should present itself. If the equilibrium data are available from more fundamental thermodynamic considerations such as the Benedict-Webb-Rubin equation of state, or from empirical correlations, the appropriate machine program may be arranged. The tower calculations are complicated, however, by the fact that before the elements in matrix \bar{M}_i may be computed, the compositions throughout the column must be estimated. Although this appears to be a serious disadvantage, in the few cases treated to date with light hydrocarbon rectifications better first temperatures could be obtained by assuming composition distributions and temperature distributions and calculating a corrected temperature distribution for the first trial. Computation of K_{ji} 's from fundamental thermodynamic data is now being considered.

A machine routine is needed for inversion of matrices \bar{M}_i and \bar{H} . Usual matrix routines make the system triangular, which results in a system in which back substitution is possible. As \bar{H} is already triangular, such a process is not necessary. However, \bar{M}_i requires some treatment, although a matrix of this form is simple to invert, because it contains a large number of zero elements. The use of matrices is not essential, as none of the more basic properties of matrices have been used and the only real application of matrix methods has been notational. The equations presented have been algebraic and simultaneous and the method has presented these equations as linear as well as simultaneous and algebraic. Hence any method of solving linear

simultaneous algebraic equations should be applicable to the solution of the distillation problem. The plate by plate method does exactly this by grouping the equations in a different manner. It would be interesting to make a detailed composition of the rapidity of convergence of the two methods of solution.

Other Methods of Stating the Problem. Suppose that two compositions are to be specified—one in the overhead and one in the bottoms. Let these be specified as x_p and x_w , where in general x_p is a heavy component and x_w is a lighter one. Perhaps a direct method could be developed, but the specification of these two compositions would ruin the symmetry of the previous computations and probably increase computing time appreciably. A suggested technique is the following. Everything else being fixed, x_p and x_w are functions of D and Q_w , so that

$$x_p = x_p(D, Q_w)$$

$$x_w = x_w(D, Q_w)$$

or taking differentials

$$dx_p = \frac{\partial x_p}{\partial D} dD + \frac{\partial x_p}{\partial Q_w} dQ_w = a_{11} dD + a_{12} dQ_w$$

$$dx_w = \frac{\partial x_w}{\partial D} dD + \frac{\partial x_w}{\partial Q_w} dQ_w = a_{21} dD + a_{22} dQ_w$$

and solving for dD and dQ_w

$$dD = \frac{a_{22} dx_p - a_{12} dx_w}{a_{11} a_{22} - a_{21} a_{12}}$$

$$dQ_w = \frac{a_{11} dx_w - a_{21} dx_p}{a_{11} a_{22} - a_{21} a_{12}}$$

Suppose that x_p and x_w are calculated at two different values of D , say D_1 and D_2 , at a fixed Q_w , followed by x_p and x_w calculated at two different values of Q_w , say Q_{w1} and Q_{w2} , at a fixed D_1 . This requires three calculations, and by replacing the partial derivatives, a_{ij} , by their difference quotients, their values may be computed. If in addition differentials dx_p and dx_w are replaced by Δx_p and Δx_w , where these are now the differences between the desired values and previously calculated values, the corrections to D and Q_w , ΔD and ΔQ_w may be computed. The whole process may then be repeated until the required composition requirements are met.

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Nomenclature

a_{pq} = element of matrix \bar{M}_i
 b_{pq} = element of matrix \bar{H}

c_p = element of matrix \bar{G}
 d_p = element of matrix \bar{F}_i
 d = side stream drawoff plate number
 D = vapor drawoff rate, without side stream drawoff
 D_1 = vapor drawoff rate in general
 D_2 = side stream drawoff rate
 f = feed plate number (f_1 and f_2 similarly)
 F = feed rate, single feed case (taken as 100 moles per hour)
 F_1 = feed rate, two feed case, upper feed
 F_2 = feed rate, two feed case, lower feed
 \bar{F}_i = feed column vector
 \bar{G} = product enthalpy matrix defined by Equation 2
 h_i = liquid enthalpy, j th plate
 H_i = vapor enthalpy, from j th plate
 h_{ji} = partial molar enthalpy of i th component on j th plate (liquid)
 H_{ji} = partial molar enthalpy of i th component on j th plate (vapor)
 H_F = enthalpy of feed per mole (H_{F1} and H_{F2} similarly)
 \bar{H} = enthalpy matrix defined by Equation 2
 i = component designating variable
 j = plate designating variable
 K_{ji} = equilibrium constant for i th component on j th plate
 L_j = liquid from j th plate (moles per 100 moles of feed)
 \bar{M}_i = characteristic column matrix defined by Equation 1
 Q_w = boiling heat to reboiler, B.t.u./100 moles feed
 t_j = plate temperature
 V_j = vapor flow rate from j th plate (per 100 moles feed)
 W = bottoms drawoff rate
 x_{ji} = mole fraction of i th component on j th plate (liquid)
 y_{ji} = mole fraction of i th component in vapor from j th plate
 x_{Fi} = mole fraction of i th component in the feed (similarly x_{F1i} and x_{F2i})
 x_p = specified mole fraction in overhead
 x_w = specified mole fraction in bottoms

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