Multicomponent Distillation on a Large Digital Computer

II. Generalization With Side-Stream Stripping

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The problem of multicomponent distillation is considered for a column with an arbitrary number of feed streams and an arbitrary number of side-stream withdrawals. The overheads from the side-stream strippers are admitted to the column, introducing the inert stripping medium into the main column. Provisions are made in the calculations for complete heat balancing, inert injection, and internal reflux cooling. The method of computation is that of a previous paper involving the component-by-component technique. Calculations are made on the main column and give first approximations to the side-stream compositions; stripper calculations are then initiated. An alternating procedure is instituted between the main column and the strippers, the successive iterations continuing until a preassigned accuracy in the desired quantities is reached. An extensive numerical problem is worked.

In a previous paper (*1*) a technique for multicomponent distillation calculations was developed. If the equations of conservation of mass and energy are written around each plate, there are $(m + 1)$ equations, m equations arising from the conservation of each of the m components and one from the heat balance. With $N + 1$ stages in the column it was shown that there are a total of $(N + 1)\, m + N$ equations which must be solved simultaneously under the condition of restraint that temperatures are so chosen that the vapor and liquid mole fractions in each stage total one. It was assumed that the number of plates, feed-plate location, condition of feed, etc., were fixed in advance so that the composition profile through the column might be computed, reflux rate and overhead vapor draw off having been fixed. Design problems such as optimum feed-plate location or number of plates for a given separation were not discussed, since such problems could be solved by the successive application of the above technique with a resultant bracketing of the desired values. In this paper the equations will be written in a more general form to include the effects of side-stream strippers, inert injection, and internal-reflux cooling. A method will be described which should be useful for hydrocarbon distillations in which side streams must be stripped of light components and the overhead from the stripper returned to the column. An extensive numerical example will be discussed.

DEVELOPMENT OF EQUATIONS—MAIN COLUMN

The column shown in Figure 1 is considered with N theoretical stages and a partial condenser, the latter denoted as the zeroth stage and the reboiler the Nth stage. It is assumed that the inert is noncondensible in the column and insoluble in the liquid phase. The inert part of the feed to the jth stage will be treated as an s_j with the remainder F_j. The vapor flow from the jth stage U_j is

$$U_j = V_j + I_j \qquad (1)$$

$$Y_j = \sum_{k=0}^{j} (F_k - S_k) \qquad (2)$$

must also be defined, and then

$$L_j = Y_j + V_{j+1}$$

The usual mass balance on the ith component is

$$\begin{aligned} L_{j-1}x_{j-1,i} + U_{j+1}y_{j+1,i} + F_j x_{Fji} \\ - L_j x_{ji} - U_j y_{ji} - S_j x_{ji} = 0 \end{aligned} \qquad (3)$$

where this equation does not apply to the inert component. With the equilibrium relation $y_{ji} = K_{ji}x_{ji}$, this reduces to

$$\begin{aligned} (Y_{j-1} + V_j)x_{j-1,i} - (Y_{j-1} \\ + F_j + V_{j+1} + U_jK_{ji})x_{ji} \\ + U_{j+1}K_{j+1,i}x_{j+1,i} \\ = -F_j x_{Fji} \end{aligned} \qquad (4)$$

This equation holds for all stages including the partial condenser and the reboiler provided one chooses

$$x_{ji} = 0, \quad j < 0, \quad j > N$$

$$U_j = 0, \quad j > N$$

$$Y_{-1} = -V_0$$

$$Y_0 = -V_0$$

Equation (4) is a set of equations which may be written in matrix form:

$$\overline{\overline{M}}_i \bar{X}_i = -\bar{F}_i, \quad i = 1, 2, \cdots, m$$

or, when one inverts $\overline{\overline{M}}_i$,

$$\bar{X}_i = -\overline{\overline{M}}_i^{-1}\bar{F}_i, \qquad i = 1, 2, \cdots, m \qquad (5)$$

If a_{pq} is an element of $\overline{\overline{M}}_i$, then

$$a_{jj} = -(Y_{j-1} + F_j + V_{j+1} + U_jK_{ji}), \quad 0 \le j \le N$$

$$a_{j,j+1} = U_{j+1}K_{j+1,i} \qquad 0 \le j \le N - 1$$

$$a_{j,j-1} = V_j + Y_{j-1}, \qquad 1 \le j \le N$$

all other elements being zero. The elements of $\bar{x}_i$ are x_{ji}, $j = 0$ to N; $\bar{F}_i$ has components $F_j x_{Fji}$, $j = 0$ to N.

The heat balance around the jth stage gives

$$\begin{aligned} Q_j + (L_{j-1}h_{j-1} + V_{j+1}H_{j+1} \\ + I_{j+1}H_{s,j+1}) \\ - (L_jh_j + V_jH_j + I_jH_{sj}) \\ + F_jH_{Fj} - S_jh_j + s_j\tilde{H}_{sj} = 0 \end{aligned}$$

From

$$I_j - I_{j+1} = s_j$$

and

$$Y_j - Y_{j-1} = F_j - S_j$$

it follows that

$$\begin{aligned} V_j(h_{j-1} - H_j) + V_{j+1}(H_{j+1} - h_j) \\ = -Q_j + Y_{j-1}(h_j - h_{j-1}) \\ + F_j(h_j - H_{Fj}) \\ + I_j(H_{sj} - H_{s,j+1}) \\ + s_j(H_{s,j+1} - \tilde{H}_{sj}) \end{aligned}$$

or

$$\begin{aligned} V_j(h_{j-1} - H_j) + V_{j+1}(H_{j+1} - h_j) \\ = -Q_j + Y_{j-1}(h_j - h_{j-1}) \\ + F_j(h_j - H_{Fj}) \\ + I_{j+1}(H_{sj} - H_{s,j+1}) \\ + s_j(H_{sj} - \tilde{H}_{sj}) \end{aligned}$$

This equation is a set of equations which may be written in matrix form

$$\overline{\overline{H}}\bar{V} = \bar{G}, \qquad \bar{V} = \overline{\overline{H}}^{-1}\bar{G} \qquad (6)$$

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Table 1. Data for Illustrative Problem

Component	Equilibrium constant				Vapor enthalpy			Liquid enthalpy		Mole Fraction in feed
	α_i	$\beta_i \times 10$	$\gamma_i \times 10^4$	$\Delta_i \times 10^6$	A_i	$B_i \times 10^2$	$C_i \times 10^4$	a_i	b_i	
C_6	− 22.93	27.42	− 9.64	1.290	9,259	3,125	232	−4,940	45.1	0.11
C_8	− 29.72	37.34	− 4.22	1.761	12,390	4,000	312	−4,800	57.5	0.06
C_9	− 2.631	3.702	− 1.681	0.2828	13,000	4,900	300	−4,250	64.5	0.04
C_{10}	− 1.380	2.125	− 1.040	0.1812	14,400	5,350	350	−3,380	71.4	0.03
C_{11}	− 2.115	2.896	−11.252	0.1841	15,890	5,700	412	−2,660	78.1	0.06
C_{12}	− 1.363	1.864	− 0.811	0.1193	17,650	6,100	450	−1,250	85.0	0.30
C_{13}	− 2.872	3.680	− 1.446	0.1825	18,860	6,650	488	360	91.9	0.07
C_{14}	− 0.950	1.260	− 0.528	0.0723	20,310	7,050	538	2,350	98.8	0.13
C_{15}	− 0.738	0.987	− 0.398	0.0550	22,920	6,250	625	4,700	105.5	0.12
C_{16}	− 0.538	0.722	− 0.300	0.0400	22,800	8,350	550	7,600	112.0	0.08

Number of plates including reboiler = 20 + partial condenser
Side-stream draw off from plate 9
Overhead from side-stream stripper to plate 5
Number of plates in stripper = 6
Feed on plate 15 at 100 moles/unit time
Moles steam in stripper = 5
Side-stream draw-off rate = 35
Overhead vapor rate = 25 (hydrocarbon only)
Reflux ratio = 4
Feed − saturated liquid at 300°F., H_F = 24,769 B.t.u./lb. mole
Steam to stripper superheated to 400°F., H_s = 22,324 B.t.u./lb. mole
$H_s = 18{,}918 + 8.514\ T$ (T in °F.)

where $\bar{V}$ has as elements V_j, $j = 1$ to N. The elements of $\bar{G}$ are

$$c_j = -Q_j + Y_{j-1}(h_j - h_{j-1}) + F_j(h_j - H_{Fj}) + I_{j+1}(H_{sj} - H_{s,j+1}) + s_j(H_{sj} - \tilde{H}_{sj}), \qquad j = 1 \text{ to } N$$

and the elements of $\bar{H}$ are b_{pq}, where

$$b_{jj} = h_{j-1} - H_j, \qquad 1 \le j \le N$$

$$b_{j,j+1} = H_{j+1} - h_j, \qquad 1 \le j \le N - 1$$

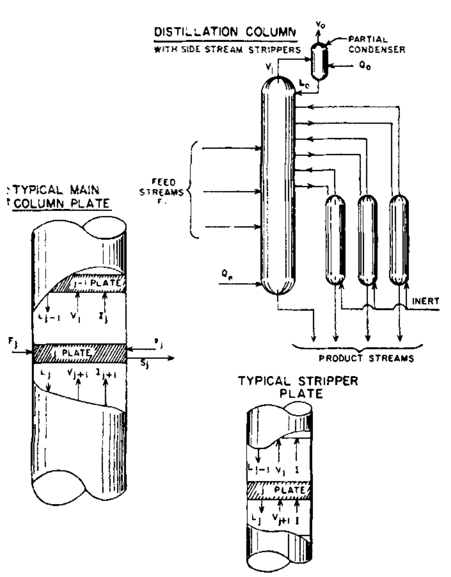

Fig. 1. Diagrammatic sketch of distillation column with side-stream strippers.

all other elements being zero. $\bar{\bar{H}}$ is already in triangular form.

A complete heat balance around the column but excluding the partial condenser gives

$$\begin{aligned} Q_N &= V_1H_1 + I_1H_{s1} - \sum_1^N F_jH_{Fj} + \sum_1^N S_jh_j - \sum_1^N s_j\tilde{H}_{sj} - L_0h_0 - \sum_1^{N-1} Q_j \\ &= (R + 1)V_0H_1 - RV_0h_0 + I_1H_{s1} - \sum_1^N F_jH_{Fj} + \sum_1^N S_jh_j - \sum_1^N s_j\tilde{H}_{sj} - \sum_1^{N-1} Q_j \end{aligned} \tag{7}$$

and Q_N may be eliminated from the enthalpy matrix. Ordinarily all other Q_j's are zero. The heat balance around the partial condenser gives

$$Q_0 = V_0[H_0 - H_1 + R(h_0 - H_1)] \tag{8}$$

Before the method of solution is described, the temperature-correction procedure must be considered. Since V_j represents the noninert vapor and I_j the inert vapor, while y_{ji} is the mole fraction of the ith component in the total vapor U_j, it follows that

$$U_j \sum_i y_{ji} = (V_j + I_j) \sum_i y_{ji} = V_j$$

$$\sum_i y_{ji} = \frac{V_j}{U_j} = g_j$$

where g_j is a number less than 1. In the main column I_j is generally not large compared with V_j, and so g_j is only slightly less than 1. In a side-stream stripper however, where the liquid vaporization is usually not large, g_j may be small, say of the order of one tenth. Thus

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

on each plate. When one uses the first two terms of the Taylor series in the expansion of $\sum_i K_{ji}x_{ji}$ in the temperature,

$$\left(\sum_i K_{ji}x_{ji}\right)_{T_j} = \left(\sum_i K_{ji}x_{ji}\right)_{T_j'} + \left[\frac{\partial \sum_i K_{ji}x_{ji}}{\partial T}\right]_{T_j'} (T_j - T_j')$$

If T_j' is a temperature at which $\sum_i K_{ji}x_{ji}$ is known, then T_j is the temperature at which this same quantity may be approximately computed. If it is assumed that the only necessity for correcting the temperature is that the K_{ji}'s are incorrect, the x_{ji} should be normalized on each tray by division by $\sum_i x_{ji}$. Thus the temperature correction necessary to produce $\sum_i K_{ji}x_{ji} = g_j$ will be

$$T_j - T_j' = \left[g_j \sum_i x_{ji} - \sum_i K_{ji}x_{ji}\right]_{T_j'} \cdot \left[\sum_i x_{ji} \frac{\partial K_{ji}}{\partial T_k}\right]_{T_j'}^{-1} \tag{9}$$

In the computations described in this paper the equilibrium constants used are the ideal-solution constants and hence are independent of composition but dependent upon pressure and temperature. Although there are other rational expressions, it will be assumed here that K_{ji} is a cubic polynomial in T_j with the

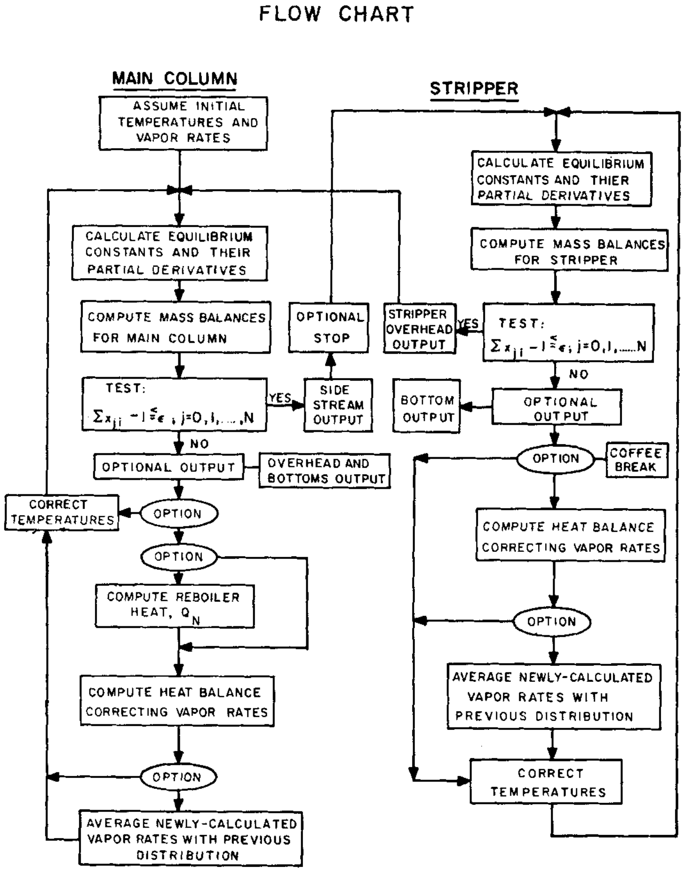

Fig. 2. Simplified flow chart for computer program.

coefficients functions of the pressure. Thus

$$K_{ji} = \alpha_i + \beta_i T_j + \gamma_i T_j^2 + \Delta_i T_j^3$$

$$\frac{\partial K_{ji}}{\partial T_j} = \beta_i + 2\gamma_i T_j + 3\ \Delta_i T_j^2$$

More sophisiticated expressions for the equilibrium constants may be used, such as the one derived from the Benedict-Webb-Rubin equation of state. In this case one may perform the temperature correction as above using the values of the composition from a previous iteration.

SIDE-STREAM STRIPPER ANALYSIS

The equations for the strippers may be obtained from the equations already developed. It will be assumed that the only feeds to the strippers are the side streams from the main column into the top and the inert stripping medium into the bottom. The stripped side stream is the effluent from the bottom, and the vapor overhead, including inert, enters the main column.

If I is the inert rate into the stripper bottom, L_0 is the side stream rate to the top, V_j is the noninert vapor rate from the jth stage, then Equation (4) may be written

$$\begin{aligned}(L_0 - V_1 + V_j)x_{j-1,i} \\ - (L_0 - V_1 + V_{j+1} + U_jK_{ji})x_{ji} \\ + U_{j+1}K_{j+1,i}x_{j+1,i} = 0\end{aligned}$$

for the jth stage. This formula also holds for the top and bottom stages, as x_{0i} is known and $x_{N+1,i} = 0$. It can be written as a set of equations in matrix form:

$$\bar{\bar{S}}_i\bar{X}_i = -\bar{S}_i, \quad \bar{X}_i = -\bar{\bar{S}}_i^{-1}\bar{S}_i \quad (10)$$

where the elements d_{pq} of $\bar{\bar{S}}_i$ are

$$\begin{aligned}d_{jj} &= -(L_0 + V_{j+1} - V_1 \\ &\quad + U_jK_{ji}), \qquad 1 \leq j \leq N \\ d_{j,j+1} &= U_{j+1}K_{j+1,i}, \\ &\qquad 1 \leq j \leq N - 1 \\ d_{j,j-1} &= L_0 + V_j - V_1, \\ &\qquad 2 \leq j \leq N\end{aligned}$$

The vector $\bar{S}_i$ has L_0x_{0i} as its first element and zeros elsewhere.

The heat balance around the stripper may be obtained as

$$\begin{aligned}V_j(h_{j-1} - H_j) + V_{j+1}(H_{j+1} - h_j) \\ = (L_0 - V_1)(h_j - h_{j-1}) \\ + I(H_{sj} - H_{s,j+1}) - Q_j\end{aligned}$$

TABLE 2. MAIN-COLUMN CALCULATIONS—SUMMARIZED*

	Initial assumption Temperature, °F.	Vapor	Problem 1 Temperature, °F.	Vapor	Problem 2 Temperature, °F.	Vapor	Problem 3 Temperature, °F.	Vapor	Problem 5 Temperature, °F.	Vapor
P.C.†	200	25	287	25	288	25	263	25	251	25
1	212	125	351	125	351	124.8	347	139.1	333	139.2
2	225	125	368	125	369	137.6	366	163.0	357	164.7
3	237	125	376	125	379	138.9	376	164.8	369	166.8
4	250	125	384	125	386	139.0	383	165.2	376	167.3
5	262	125	389	125	391	139.0	389	165.3	383	167.2
6	275	125	393	125	395	139.1	395	164.0	389	156.9
7	287	125	397	125	398	139.3	399	165.4	393	157.7
8	300	125	400	125	402	139.4	403	165.6	396	157.4
9	312	125	404	125	405	139.3	406	165.5	400	157.1
10	325	125	408	125	409	138.9	410	165.1	403	156.9
11	337	125	412	125	412	138.3	413	164.4	406	156.7
12	350	125	416	125	415	137.7	416	163.7	408	156.3
13	362	125	419	125	419	137.2	420	162.9	410	155.7
14	375	125	423	125	422	136.5	424	161.9	414	154.6
15	387	125	428	125	426	135.4	429	160.4	420	152.7
16	400	125	444	125	442	184.8	443	210.4	432	202.2
17	412	125	451	125	450	197.1	451	222.2	438	212.9
18	425	125	458	125	458	200.7	458	225	444	214.7
19	437	125	467	125	467	203.4	468	226.8	452	215.2
20	450	125	479	125	480	205.4	480	226.9	466	215.0

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*Vapor rates are in pound moles per hundred moles of feed of hydrocarbon only.
†Partial condenser.

TABLE 3. FINAL RESULTS, COLUMN AND STRIPPER

Composition of Liquid In Each Stage - hydrocarbon mole fraction

	Partial Condenser Vapor	0	1	2	3	4	5	6
C_6	0.36666	0.06579	0.01362	0.00703	0.00593	0.00550	0.00522	0.00536
C_8	0.19857	0.08868	0.05584	0.03313	0.02164	0.01621	0.01345	0.01225
C_9	0.13104	0.24009	0.13615	0.06636	0.03316	0.01950	0.01407	0.01215
C_{10}	0.09223	0.33986	0.31281	0.22684	0.14478	0.08718	0.05238	0.03471
C_{11}	0.04411	0.24982	0.43508	0.56820	0.62164	0.60328	0.53511	0.46021
C_{12}	0.00151	0.01579	0.04543	0.09663	0.17083	0.26634	0.37762	0.47300
C_{13}	0.00000	0.00000	0.00000	0.00001	0.00004	0.00016	0.00050	0.00085
C_{14}	0.00000	0.00000	0.00000	0.00000	0.00000	0.00001	0.00002	0.00003
C_{15}	0.00000	0.00000	0.00000	0.00000	0.00002	0.00007	0.00019	0.00029
C_{16}	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
T_j	-	251.4	337.9	357.3	368.6	376.5	382.6	388.6
V_j	-	25	139.3	164.7	166.8	167.3	167.2	156.9
		7	8	9 Side Stream	10	11	12	13
C_6		0.00518	0.00502	0.00488	0.00475	0.00466	0.00458	0.00450
C_8		0.01114	0.01025	0.00950	0.00887	0.00845	0.00810	0.00773
C_9		0.01100	0.01022	0.00963	0.00914	0.00881	0.00855	0.00829
C_{10}		0.02460	0.01892	0.01569	0.01376	0.01279	0.01218	0.01167
C_{11}		0.37240	0.28396	0.20445	0.13891	0.10041	0.07810	0.06462
C_{12}		0.57238	0.66555	0.74327	0.79776	0.81546	0.80393	0.76537
C_{13}		0.00174	0.00380	0.00829	0.01739	0.03047	0.04820	0.07005
C_{14}		0.00008	0.00023	0.00072	0.00223	0.00553	0.01248	0.02628
C_{15}		0.00056	0.00122	0.00282	0.00650	0.01273	0.02293	0.03890
C_{16}		0.00000	0.00000	0.00000	0.00002	0.00010	0.00048	0.00227
T_j		392.6	396.4	399.9	403.1	405.5	407.8	410.3
V_j		157.7	157.4	157.1	156.9	156.7	156.3	155.7
		14	15	16	17	18	19	20

or

$$V_1(h_j - h_{j-1}) + V_j(h_{j-1} - H_j) + V_{j+1}(H_{j+1} - h_j) = L_0(h_j - h_{j-1}) + I(H_{sj} - H_{s,j+1}) - Q_j$$

for any stage. For the bottom stage $V_{N+1} = 0$. In matrix form

$$\bar{\bar{h}}\bar{v} = \bar{g}, \qquad \bar{v} = \bar{\bar{h}}^{-1}\bar{g} \tag{11}$$

If e_{pq} is an element of $\bar{\bar{h}}$,

$$e_{11} = h_1 - H_1$$

$$e_{jj} = h_{j-1} - H_j, \qquad 2 \le j \le N$$

$$e_{j,j+1} = H_{j+1} - h_j, \qquad 1 \le j \le N - 1$$

$$e_{j1} = h_j - h_{j-1}, \qquad 2 \le j \le N$$

The elements of $\bar{v}$ are V_j, $j = 1$ to N; $\bar{g}$ has elements f_p

$$f_j = L_0(h_j - h_{j-1}) + I(H_{sj} - H_{s,j+1}) - Q_j \qquad 1 \le j \le N - 1$$

$$f_N = L_0(h_N - h_{N-1}) + I(H_{sN} - H_{sN}) - Q_N, \qquad j = N$$

As in the main column, enthalpies are written as a sum of partial-molar enthalpies and each partial-molar enthalpy may be taken as a cubic in the temperature

$$H_{ji} = A_i + B_iT_j + C_iT_j^2 + D_iT_j^3$$

$$h_{ji} = a_i + b_iT_j + c_iT_j^2 + d_iT_j^3$$

The enthalpy of the inert may usually be calculated when one assumes a constant heat capacity; thus where a difference in enthalpy occurs, the heat capacity is multiplied by the temperature difference.

METHOD OF COMPUTATION

The general method of computation, not including the stripper analysis, was described in the previous paper. The problem to be discussed here is a light-hydrocarbon distillation in which the total number of plates in the main column and the strippers, the feed-stage locations and side-stream draw-off locations and their respective amounts, inert injection in the main column and strippers, pressure, and reflux ratio are specified in advance, and it is desired to obtain the compositions of the top, bottom, and side-stream stripper effluent. Instead of fixing the reflux ratio, one may specify the boil-up heat into the reboiler. It was found that better convergence usually resulted when the reflux ratio was specified. This problem is the analysis problem of distillation as opposed to the synthesis problem. To solve the synthesis problem by this technique it would be necessary to bracket the desired separation by an iterative procedure.

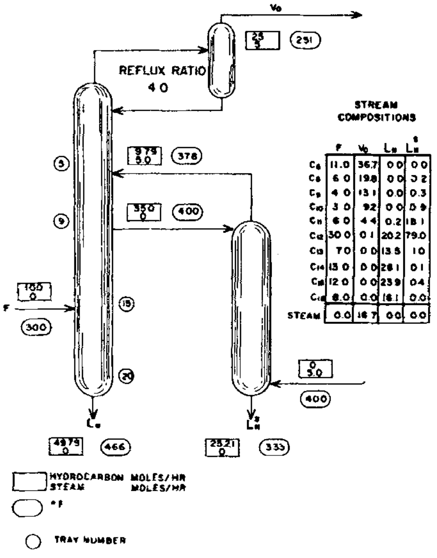
If a temperature distribution is assumed, equilibrium constants may be computed. For the nonheat-balancing problem the vapor rates may be computed directly, and Equations (5) and (9) may be used alternately to obtain the composition of liquid and vapor on each tray. Since the side-stream-stripper over-

TABLE 3. FINAL RESULTS, COLUMN AND STRIPPER (*Continued*)

		Feed Plate					Bottoms
C_6	0.00439	0.00423	0.00027	0.00002	0.00000	0.00000	0.00000
C_8	0.00727	0.00662	0.00101	0.00014	0.00002	0.00000	0.00000
C_9	0.00795	0.00748	0.00194	0.00047	0.00011	0.00002	0.00000
C_{10}	0.01109	0.01030	0.00425	0.00164	0.00059	0.00019	0.00005
C_{11}	0.05536	0.04746	0.03127	0.01899	0.01060	0.00523	0.00211
C_{12}	0.69795	0.59760	0.58804	0.53549	0.44842	0.33169	0.20183
C_{13}	0.09261	0.10729	0.13290	0.15874	0.17704	0.17316	0.13537
C_{14}	0.05123	0.08948	0.10025	0.12210	0.15987	0.21313	0.26061
C_{15}	0.06204	0.09103	0.10163	0.12150	0.15384	0.19806	0.23927
C_{16}	0.00989	0.03837	0.03827	0.04071	0.04933	0.07839	0.16066
T_j	414.0	419.9	432.2	437.6	443.6	452.4	466.0
V_j	154.6	152.7	202.2	212.9	214.7	215.2	215.0

	Vapor Overhead-Stripper	1-S	2-S	3-S	4-S	5-S	6-S Stripper Bottoms
C_6	0.01152	0.00091	0.00022	0.00006	0.00002	0.00001	0.00000
C_8	0.01958	0.00592	0.00449	0.00364	0.00300	0.00240	0.00168
C_9	0.01815	0.00693	0.00572	0.00492	0.00424	0.00356	0.00270
C_{10}	0.02155	0.01360	0.01262	0.01192	0.01126	0.01045	0.00911
C_{11}	0.17466	0.19791	0.19486	0.19259	0.19035	0.18736	0.18072
C_{12}	0.41298	0.76088	0.76784	0.77235	0.77635	0.78107	0.78980
C_{13}	0.00207	0.00887	0.00912	0.00930	0.00948	0.00972	0.01031
C_{14}	0.00014	0.00078	0.00081	0.00083	0.00084	0.00087	0.00092
C_{15}	0.00084	0.00302	0.00311	0.00317	0.00322	0.00330	0.00342
C_{16}	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
T_j	-	377.9	368.2	361.4	355.0	347.3	333.4
V_j	-	9.793	7.225	4.849	3.948	3.142	2.186

head composition is not known at this time, it is assumed to be pure inert. The solution to this problem may then be used as a first approximation for the heat balancing. The order of the iterations here is somewhat arbitrary, but it has been found that a new heat balance need not be made to obtain new vapor rates each time Equations (5) and (9) are iterated. Generally it has been found that the convergence to the final solution is most rapid if Equations (5) and (9) are iterated about three times before new vapor rates are computed from Equation (6).



STREAM COMPOSITIONS

	F	Vo	L20	L_6^S
C_6	11.0	36.7	0.0	0.0
C_8	6.0	19.8	0.0	0.2
C_9	4.0	13.1	0.0	0.3
C_{10}	3.0	9.2	0.0	0.9
C_{11}	6.0	4.4	0.2	18.1
C_{12}	30.0	0.1	20.2	79.0
C_{13}	7.0	0.0	13.5	1.0
C_{14}	13.0	0.0	28.1	0.1
C_{15}	12.0	0.0	23.9	0.4
C_{16}	8.0	0.0	16.1	0.0
STEAM	0.0	16.7	0.0	0.0

Fig. 3. Schematic diagram showing equilibrium flow rates, temperatures, and compositions for terminal streams in the sample problem.

At this point in the calculation one has a fair idea concerning the side-stream composition from the main column, and the stripper computation may now be instituted. For the strippers vapor rates must be assumed throughout the column. Iterations are then made by the use of Equations (9), (10), and (11). The number of mass-balance iterations between calculations of new vapor rates may be varied to improve the convergence. When the convergence point is reached on the strippers, the main column calculations are reinstituted since the stripper overhead may perturb the previous calculations. It is apparent that the computations are then repeated in an obvious way, iterating between the column and the stripper. Calculations are repeated until the desired degree of accuracy in the pertinent variables is reached. Figure 2 gives a schematic flow chart for the computation.

In an iterative procedure, such as that described here, certain tricks may make the technique converge when otherwise it may converge slowly or not al all. For example the vapor rates calculated from the heat balance may tend to oscillate and thus cause the successive mass-balance iterations to diverge. This may be overcome by using the average of the last two calculated vapor rates as vapor rates. Similar techniques may be used at other points in the computation such as on compositions and temperatures. The convergence of the iterations in these distillation calculations is indeed a delicate and difficult question, for although the methods of this paper have proved satisfactory in the problems considered to date, what seemed like more elegent methods diverged rather badly.

DISCUSSION OF NUMERICAL PROBLEM

A series of numerical problems will now be considered by means of a main column of twenty stages with a side stream drawn from the ninth stage. The overhead from the stream stripper is admitted to the main column in the fifth stage. The final solution is obtained as the result of the solution of a series of five problems. The data are summarized in Table 1.

Problem 1: Main Column Only With Side-Stream Draw Off (No Heat Balancing)

In this problem the vapor rates through the column were held constant at 125 moles with a side-stream draw-off rate at 35 moles. An initial temperature distribution of 200°F. in the partial condenser and 450°F. in the bottom was assumed with a linear distribution throughout the column. With this assumption the $\sum_i x_{ji}$ varied from a minimum of 0.1112 to a maximum of 1.765 throughout, and $\sum_i K_{ji}x_{ji}$ varied from 0.2112 to 1.772. After five iterations results of sufficient accuracy were obtained. The final temperature and vapor rates are summarized in Table 2.

Problem 2: Main Column Only With Side-Stream Draw Off (Heat Balancing Included)

Complete heat balancing was carried out in this problem. The reflux ratio was held fixed, and Q_N was computed from Equation (7) for insertion into $\bar{G}$. To initiate the solution the results of the previous calculation were used as a first approximation. The mass balancing and heat balancing were alternated, and Q_N was recalculated at each iteration. The average of the last two calculated vapor rates were used in $\overline{\overline{M}}_i$. Temperatures on the plates were not significantly different from those in problem 1, but vapor rates changed substantially below the feed. This is attributed to the fact that the feed was introduced at an unfortunate position, for the feed temperature is at 300°F., which corresponds to a slight subcooling, but the feed tray temperature is 426°F. A rough heat balance at the feed tray indicated that the vapor rates in Table 2 were correct.

Problem 3: Main Column Only With Side-Stream Draw Off and Steam Injection

This problem was no different from problem 2 save that 5 moles of steam was admitted to the column at stage 5. The effects were insignificant except for some changes in composition and temperature at the tower top.

Problem 4: Side-Stream Stripper

By use of the composition of the side stream from problem 3 the stripper computations were initiated. As a first guess the stripper top temperature was taken to be the same as the side-stream plate temperature in the main column. The bottom temperature was assumed to be 450°F., although it was realized that this could not be correct. Vapor rates were assumed to be 6 moles at the bottom and 11 at the top, where these are the total vapor rates. These rates were held fixed for a few iterations on the mass balance. Vapor rates were then calculated after about every third mass-balance calculation. It was essential in these calculations to use the average of the last two calculated vapor rates in the mass balance to ensure convergence. With the latter it was found that the initial guess on vapor rates could be varied quite widely. It is obvious that the lower part of the stripper contains vapor which is mostly inert, and so the compositions may vary appreciably.

Problem 5: Final Solution To Main Column Plus Side-Stream Stripper

With the result of problem 4 the main-column calculations may now be corrected for the effect of the introduction of the stripper overhead to the column. These calculations are repeated to determine what the effect will be on the side-stream composition. If the latter is significantly different, the stripper calculations must be repeated as in problem 4 and successive alterations are made until preassigned accuracy on pertinent variables is obtained. Various modifications of the program may be made here, since it is clear that some variables will not be affected. Table 3 shows the final compositions, temperatures, and vapor rates for both the column and stripper. Vapor rates shown are for the hydrocarbon only. Complete mass balances on each component check. The equilibrium constants were programed as cubics, vapor enthalpies as quadratics, and liquid enthalpies as linear functions of the temperature. The complete program is in floating-point arithmetic. The final mass balance on the system is

Feed to column
= 100 moles hydrocarbon
Vapor overhead
= 25 moles hydrocarbon
Side stream from column
= 35 moles hydrocarbon
Bottom from stripper
= 25.21 moles hydrocarbon
Overhead from stripper
= 9.79 moles hydrocarbon
Bottoms from column
= 49.79 moles hydrocarbon

and the results are shown graphically in Figure 3.

Finally a word should be given on the times required for computation. Problem 1 requires approximately 25 sec. iteration; Problem 2 requires about 5 sec. in addition for each vapor-rate calculation. A full punch out of x_{ji}, $\sum_i x_{ji}$, $\sum_i K_{ji}x_{ji}$, T_j, and V_j for each plate requires 90 sec. for the whole column and 30 sec. on the stripper. In the stripper each cycle requires about 8 sec., 6 sec. on the mass-balance iteration and 2 sec. on the vapor-rate calculation. The total running time for a complete problem, problem 1 through problem 5, involving some 75 cycles on the main column and 26 on the stripper, required about $\frac{1}{2}$ hr. For engineering purposes the total number of iterations may be reduced considerably with a resultant running time of about 10 min. The criterion used in this paper was the sum of the liquid mole fractions on each stage. A 1% check at each stage will be obtained in four or five iterations. An increase in the desired accuracy requires more than a proportional increase in the number of iterations. One tenth of one per cent in the total mole fractions requires of the order of ten iterations.

CONCLUSIONS

A general method of setting up the equations for multicomponent distillation has been presented. A complete machine program has been prepared, and the whole has been applied to a sample problem, with use of side-stream strippers and multiple feeds to the column illustrated. Complete heat and mass balancing is carried out on both the column and strippers, and the technique can be made as accurate as one pleases.

NOTATION

a_{pq} = matrix element of $\overline{\overline{M}}_i$
b_{pq} = matrix element of $\overline{\overline{H}}$
c_p = matrix element of $\bar{G}$
d_{pq} = matrix element of $\overline{\overline{S}}_i$
e_{pq} = matrix element of $\overline{\overline{h}}$
f_p = matrix element of $\bar{g}$
a_i, b_i, c_i, d_i = coefficients in cubic in temperature for h_{ji}
A_i, B_i, C_i, D_i = coefficients in cubic in temperature for H_{ji}
$\alpha_i, \beta_i, \gamma_i, \Delta_i$ = coefficients in cubic in temperature for K_{ji}
F_j = feed rate to the jth stage
$\bar{F}_i$ = feed vector
$\bar{G}$ = feed-enthalpy vector
g_j = ratio of noninert to total vapor rate $- V_jU_j - 1$
h_j = liquid enthalpy in jth stage
h_{ji} = partial molar enthalpy of ith component in jth-stage liquid
H_j = vapor enthalpy in jth stage
H_{ji} = partial molar enthalpy of ith component in the vapor in the jth stage
H_{sj} = partial molar enthalpy of inert in jth-stage vapor
$\tilde{H}_{sj}$ = enthalpy of inert injected into jth tage
$\overline{\overline{H}}$ = enthalpy matrix for vapor-rate computations
I_j = inert vapor rate from jth stage (I for stripper)
K_{ji} = equilibrium constant of ith component in jth stage
$\underline{L_j}$ = liquid overflow from jth stage
$\overline{\overline{M}}_i$ = mass-balance matrix
N = number of stages counting partial condenser as zeroth and reboiler as Nth
Q_j = heat absorbed in the jth stage
Q_N = reboiler heat
R = reflux ratio at top
s_j = inert injection to the jth stage
S_j = side stream draw off from jth stage
T_j = temperature of jth stage
U_j = vapor rate from jth stage
$\bar{v}$ = vector
V_j = noninert vapor rate from jth stage
x_{ji} = mole fraction of ith component in liquid in jth stage
x_{Fji} = mole fraction of ith component in feed to jth stage
$\bar{X}_i$ = composition vector ith component
y_{ji} = mole fraction of ith component in vapor in jth stage
Y_j = sum of feeds minus sum of draw offs from top to jth stage, inclusive

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