NOTATION

D/Dt = material derivative operator
$\mathbf{d}$ = rate of strain tensor $[= \frac{1}{2} (\nabla \mathbf{v} + \nabla \mathbf{v}^t)]$
f = function defined by Equation (2)
g = function defined by Equation (4)
h = function defined by Equation (4)
k = parameter in Equation (7)
L = thickness of sample in Couette flow
P = material point P
p = pressure
R = tube radius
r, r' = radial coordinate
t = time
u = axial speed
$\mathbf{v}$ = velocity vector
z = axial coordinate

Greek Letters

$\dot{\gamma}$ = shear rate
∇ = gradient operator
λ = time constant in Equation (6)
ρ = density
$\boldsymbol{\tau}$ = deviator of the stress tensor
τ = shear stress
τ_c = critical shear stress
φ = fluidity
$\tilde{\varphi}$ = steady state fluidity
φ_0 = steady state fluidity at zero shear rate
φ_∞ = steady state fluidity at infinite shear rate

LITERATURE CITED

1. Bauer, W. H., and E. A. Collins, "Rheology," F. R. Eirich, ed., Vol. 4, Chapt. 8, pp. 423-459, Academic Press, New York (1967).
2. Bird, R. B., and B. D. Marsh, *Trans. Soc. Rheol.*, **12**, 479 (1968).
3. Bird, R. B., W. E. Stewart, and E. N. Lightfoot, "Transport Phenomena," pp. 81-82, Wiley, New York (1960).
4. Dierckes, A. C., Jr., and W. R. Schowalter, *Ind. Eng. Chem. Fundamentals*, **5**, 263 (1966).
5. Ericksen, J. L., *Arch. Rat. Mech. Anal.*, 4, 231 (1960); 8, 1 (1961).
6. Ferry, J. D., "Viscoelastic Properties of Polymers," pp. 88-93, Wiley, New York (1961).
7. Fredrickson, A. G., "Principles and Applications of Rheology," pp. 75-77, Prentice-Hall, Englewood Cliffs, N.J. (1964).
8. Kapoor, N. N., J. W. Kalb, E. A. Brumm, and A. G. Fredrickson, *Ind. Eng. Chem. Fundamentals*, **4**, 186 (1965).
9. Kim, H. T., and R. S. Brodkey, *AIChE J.*, 14, 61 (1968).
10. Merrill, E. W., "Modern Chemical Engineering," Andreas Acrivos, ed., Vol. 1, Chapt. 4, pp. 141-195, Reinhold, New York (1963).
11. Reiner, M., and G. W. Scott Blair, "Rheology," F. R. Eirich, ed., Vol. 4, Chapt. 9, pp. 461-488, Academic Press, New York (1967).
12. Weltmann, R. N., "Rheology," F. R. Eirich, ed., Vol. 3, Chapt. 6, pp. 189-248, Academic Press, New York (1960).

Manuscript received August 14, 1968; revision received October 10, 1968; paper accepted October 11, 1968.

On the Numerical Solution of Problems in Multicomponent Distillation at the Steady State II

D. S. BILLINGSLEY
IBM, Houston, Texas

A modification is presented of the K_b method described by Holland. This modified procedure exhibits substantially improved convergence characteristics when compared with the unmodified procedure or with the classical bubble point approach. Further, it provides by far the fastest algorithm known to the author. A second procedure for determining stage temperatures is also given. In this method, flow equations as well as equilibrium relations are satisfied by the temperature profile at each iteration. Next, an improved scheme for handling nonideal mixtures is given. Finally, it is shown that a positive solution to the convergence acceleration equations of Holland may not exist when this procedure is applied to a purity specification.

GENERAL PROCEDURE

In a previous paper (*4*), the author discussed certain aspects of the procedure recommended by Holland (*10*) for solving steady state multicomponent distillation problems. An improvement in this procedure is presented in this paper, and a comparison is made between this improved procedure and the method suggested by Boyum (*6*). Subsequently, certain theoretical results concerning the Holland correction procedure are obtained for the complex distillation column.

The problem under consideration is the computation of steady state values of liquid and vapor flows for each component on every stage of a perfectly insulated column having one or more feeds and perhaps side-draw product streams. Such a unit is termed a *complex distillation column* and is schematically illustrated in Figure 1. The scheme this author has found most effective for solving this type of problem is outlined below [compare with Amundson and Pontinen (*2*), Holland (*10*), Nartker et al. (*13*), Wang and Henke (*20*)]:

1. Initial estimates of the phase flow and temperature profiles are made. A standard initial estimate of the temperature profile is obtained by adding all feeds to the unit together component by component. The dew point and

bubble point of this sum of feeds are assigned as reboiler and condenser temperatures, respectively, and the temperature is assumed to vary linearly along the unit between these two values.

2. The procedure of Thiele and Geddes (*18*) for solving the equilibrium and component flow equations is employed. The equations are arranged as suggested by Ball (*3*). Details of this part of the solution have been given previously (*4*). Authors currently examining this problem appear to favor this procedure [see for instance Boyum (*6*), Wang and Henke (*20*) and Friday and Smith (*7*)].

3. The flow rates of individual components are corrected by the θ method of Holland (*10*). Holland has shown (*11*) that for a single stage, his θ factor is simply the quantity V/L. Thus, for this correction, the entire unit is treated as one compound stage. It has been this author's experience that this correction substantially accelerates convergence in those problems which would converge without it and brings about convergence in most problems which would not converge otherwise.

4. The stage temperature is determined in a manner explained subsequently. The temperature determination is the least satisfactory part of any published scheme for solving distillation problems. Although the method to be described has been found to be a substantial improvement over the use bubble or dew points and over the procedure recommended by Boyum (*6*), it remains the least satisfactory part of this scheme.

5. The phase rates are computed by the constant composition procedure stated by Holland (*10*). It should be noted that the constant composition equations are preferable not only because their denominators are unlikely to create numerical problems, but also because they satisfy the material balance for each component as well as the appropriate heat balance. This author has found it satisfactory and convenient to write all heat balance equations around the hot end of the unit and the stage under consideration, and solve at each stage for the smaller of the phase flows as determined by the algebraic difference of the total flows of external streams between the stage in question and one end of the unit. The larger of this value, or one-tenth of the value, last previously computed for this phase at the stage being calculated is then used, and the other phase flow at this stage is obtained by adding the known difference in phase flows.

6. Items 2 through 5 are repeated in that order until a solution is obtained. The term *iteration* will mean one execution of items 2 through 5 in that order. Thus, each such item is executed once per iteration. The term *solution* will mean $|1 - \Sigma\, K\, x| < 0.001$ for each stage.

No proof of convergence is available for solution schemes other than those of Greenstadt, Baird, and Morse (*8, 9*) and of Naphtali (*12*) which require a sufficiently good initial guess. Unfortunately, a sufficiently good initial guess is normally unavailable. Therefore, the number and variety of test problems which any proposed numerical method has successfully solved is important. The method outlined above has been tested on a set of over 220 problems selected over a period of several years. Many, if not most, of these problems were added to the set because some distillation program failed to solve them. The procedure just suggested has solved all of these problems. Testing on problems in which the dew and bubble points of feeds differ by more than 300°F., however, has not been extensive.

STAGE TEMPERATURES

Attention is now to be focused on the calculation of stage temperatures. This has often been accomplished by use of relative volatilities based upon one component denoted as the base component [see, for instance, Holland (*10*) the K_b method]. Nartker, Skrygley, and Holland (*13*) have shown that if the equilibrium ratio of the base component is represented by the Antoine equation

$$\ln (K_b) = c/T + c_1 \tag{1}$$

with c and c_1 being computed for a hypothetical component having K values about midway between the lightest and heaviest components of the mixture, the K_b method is superior to the bubble point method for determining stage temperatures. T is, of course, an absolute temperature. For computational purposes, the K_b method as described by Holland (*10*) and by Nartker et al. (*13*) can be substantially improved as follows. Let T_0 denote the bubble point of a mixture and T denote an estimate of T_0. Suppose that between T and T_0, $K_i/K_b = \alpha_i$ for each component i. Now, where $x_i = l_i/L$ and $L = \Sigma_i\, l_i$, the usual derivation is

$$l = \sum_i K_i\,(T_0)\,x_i$$

$$L = \sum_i K_i\,(T_0)\,l_i = K_b\,(T_0) \sum_i [K_i\,(T_0)/K_b\,(T_0)]\,l_i$$

$$\approx [K_b\,(T_0)/K_b\,(T)] \sum_i K_i\,(T)\,l_i$$

which with trivial changes is the relation normally employed in the K_b method.

The improvement previously mentioned is obtained by substituting Equation (1) into the last previous expression and by subsequently replacing the ln with another function:

$$\ln \left[L \Big/ \sum_i K_i\,(T)\,l_i \right] \approx (c/T_0) - (c/T) \tag{2}$$

Note that only the constant c is now involved. Equation (2) may be solved either for c or T_0 to yield

$$T_0 \approx c \Big/ \left\{ \ln \left[\mathrm{L} \Big/ \sum_i K_i\,(T)\,l_i \right] + (a/T) \right\} \tag{3}$$

and

$$c \approx [T_0\;T/(T - T_0)]\,\ln \left[\mathrm{L} \Big/ \sum_i K_i\,(T)\,l_i \right] \tag{4}$$

Since the entire derivation is based upon a fictitious component, one might as well replace the ln in Equation (3) by some function f easier to calculate and which retains certain salient properties of the ln. The properties f should possess in common with ln are:

$f(0) = -\infty$

$f(1) = 0.0$

$f \rightarrow \infty$ as the argument $\rightarrow \infty$

f is monotone increasing with respect to the argument

One such function is

$$f(q) = (q - 1)\,w + (1 - q^{-1}) \tag{5}$$

where w is an arbitrary positive number. For $w = 0.5$, Equation (3) becomes with

$$q = L \Big/ \sum_i K_i\,(T)\,l_i$$

$$T_0 \approx c/\{0.5q + 0.5 - q^{-1} + (c/T)\} \tag{6}$$

Equations (6) are to be employed once each time a stage temperature is to be computed.

The constant c may be initially determined by using the sum of feeds described previously and $T = T_0 + 50$, say, in Equation (4). One immediately suspects that it would be desirable to let c be a parameter and change it from iteration to iteration. This is the case indeed. The computation required to decide upon a new value for c should not

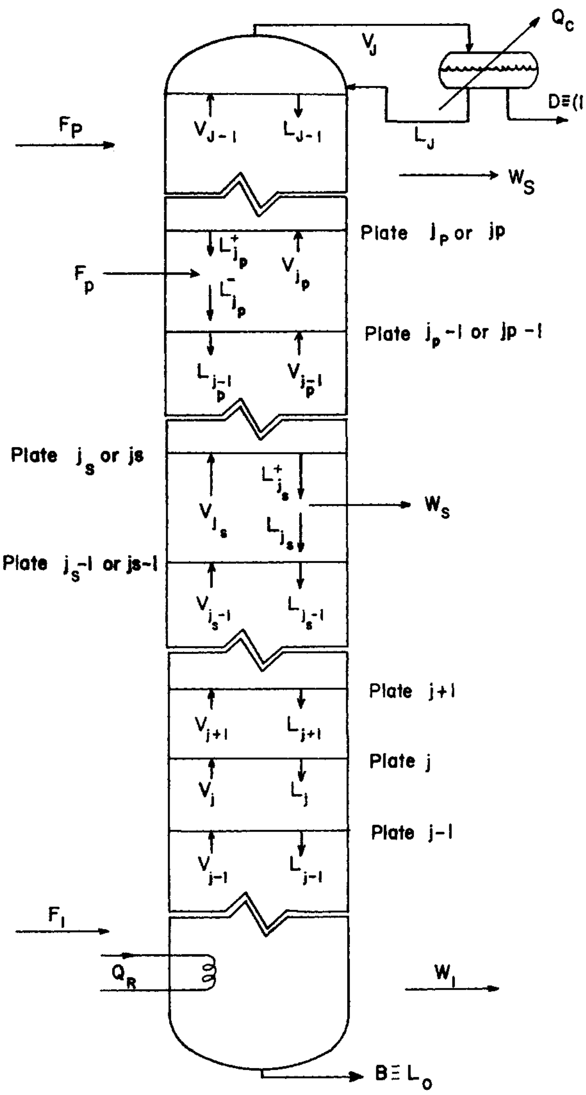

Fig. 1. Complex distillation column.

require a significant amount of time. Thus, the change in c should be made to depend upon a few easily obtained numbers which roughly indicate the success of the last two or three preceding iterations. It has been found sufficient to retain the multiplier θ_0 associated with the ratio d_i/b_i from step 3 above together with the temperature correction of largest magnitude from the last preceding iteration. The quantity θ_0 is retained from the last three preceding iterations. Any number of empirical formulas may be devised to relate a change in c to these four quantities. Even a somewhat crude formula will usually result in faster convergence than that obtained by using the same value for c in all iterations.

The procedure just described for determining stage temperatures has been effective in about 98% of the problems to which it has been applied. Its use as step 4 of the algorithm previously outlined results in by far the fastest algorithm known to the author; for instance, a 450 plate, five component problem obtained from another company required seventeen iterations and was solved in 2 min. on an IBM 360/50 machine. Problems with around forty stages and ten components usually require about ½ min. on the same machine. It is, therefore, feasible to perform case studies.

Friday and Smith (*7*) analyzed two types of algorithms and concluded that one could be expected to fail whenever more than about twenty stages were involved and that the other usually failed when the difference between the bubble and dew points of a feed exceeded approximately 150°F. The 2% of the cases not solved by the procedure described so far all involved feed streams for which the bubble and dew points differed by over 300°F., and all of these cases were brought to a condition in which $|1 - \Sigma\ K\ x| < 0.01$ for each stage.

When $|1 - \Sigma\ K\ x| < 0.01$ on each stage, the corresponding results are normally sufficiently accurate for engineering purposes; however, one cannot absolutely rule out the possibility of encountering a problem where the effects of small but appreciable changes in the temperature and phase flow profiles almost cancel each other in $\Sigma\ K x$. In such a situation, appreciable changes in these profiles might be required in order to reduce $|1 - \Sigma\ K\ x|$ from 0.01 to 0.001. Further, as Boyum (*6*) so succinctly explains, there are problems which one cannot expect to solve by any method in which the stage temperature is determined solely by the composition of the material on that stage. Sujata (*17*) developed a very appealing scheme for solving some of these problems, but Friday and Smith (*7*) show the severe limitations of that approach, in which stage temperatures were determined from heat balances.

A strategy which immediately suggests itself at this point is to assume that one now has a sufficiently good initial guess to permit Newton-Rapheson iteration on all unknown quantities as suggested by Greenstadt et al. (*8*, *9*) or by Naphtali (*12*). This approach is avoided for two reasons; the first, purely aesthetic, is the idea of requiring two programs to do the job of one. The second is that an inordinate number of partial derivatives would be required, considering that only the calculation of the temperature profile needs improvement.

The needed improvement can be obtained by manipulation of the tridiagonal equations expressing the equilibrium and flow relations for each individual component. When written as in reference *4*, these relations may be placed in the matrix-vector form

$$Z_i\ \Upsilon_i = \Omega_i \tag{7}$$

where

$$\Upsilon_i \equiv (v_{iJ},\ v_{iJ-1}\ \ldots,\ v_{i1})^T$$

$$\Omega_i \equiv (\omega_{iJ-1},\ \omega_{iJ-2},\ \ldots,\ \omega_{i0})^T$$

$$Z_i \equiv (z_{mn})_i$$

and

$$z_{mni} = \begin{cases} (A_i)_{J-n} + 1, & m = n \\ -\ 1, & m + 1 = n \\ (A_i)_{J-n}, & m - 1 = n \\ 0 & \text{otherwise} \end{cases}$$

$$(A_i)_{J-n} = L_{J-n}/[V_{J-n+1}\ K_i\ (T_{J-n})]$$

Note that ω_{ij} is zero except when stage j is a feed stage. If side draws are present, some of the z_{mni} have different forms as shown in (*4*). Equation (7) has been used by numerous authors (*2* to *4*, *7*, *10*, *19*) to determine the v_{ij}. It will now be used to determine the temperature profile. The resulting computational procedure is equivalent to that of Newman (*14*), but unlike Newman's, the relations obtained here do not depend explicitly on unknown compositions, and explicit expressions are obtained for all required partial derivatives. To this end define

$$\overline{V} \equiv (V_1, V_2, \ldots, V_J)^T$$

Then

$$\overline{V} = \sum_i\ \Upsilon_i = \sum_i\ Z_i^{-1}\ \Omega_i \tag{8}$$

Now, if the withdrawal rate of each product stream is fixed, specification of L_j/V_{j+1} for each stage j is tantamount to specifying $\overline{V}$. Hence, Equation (8) may be solved by

Newton's method to obtain the corresponding temperature profile. This solution will satisfy all the equilibrium relations as well as all the component flow (and hence phase flow) relations. In contrast to this, the temperature profile obtained by bubble or dew point evaluations does not satisfy the flow relationships. Equation (8) is the multidimensional (multistage) analogue of the well-known isothermal flash equation. Of course, by using the relation $l_{ij} = A_{ij} v_{ij+1}$ together with a specified set of L_j/V_{j+1} ratios, Equation (8) may be converted to a form in which only the liquid-phase flows appear, and this may be combined with Equation (8) to provide an expression in which phase flows appear only as L_j/V_{j+1} ratios.

What makes Equation (8) particularly useful is the manner in which the Newton-Rapheson iteration may be carried out. To this end define

$$\Lambda \equiv \overline{V} - \sum_i Z_i^{-1} \Omega_i \tag{9}$$

and

$$\overline{T} \equiv (T_{J-1}, T_{J-2}, \ldots, T_1, T_0)^T$$

$$\overline{T}^\circ \equiv (T^\circ_{J-1}, T^\circ_{J-2}, \ldots, T_1^\circ, T_j^\circ)^T$$

so that

$$\Lambda = \Lambda\,(\overline{T})$$

and

$$0 = \Lambda\,(\overline{T}^\circ) \approx \Lambda\,(\overline{T}) + [\Lambda'\,(\overline{T})]\,[\overline{T}^\circ - \overline{T}] \tag{10}$$

where

$$\Lambda' \equiv (\partial\Lambda/\partial T_{J-1},\ \partial\Lambda/\partial T_{J-2},\ \ldots,\ \partial\Lambda/\partial T_0)$$

From Equation (9)

$$\frac{\partial \Lambda}{\partial T_n} = \sum_i Z_i^{-1} \frac{\partial Z_i}{\partial T_n} Z_i^{-1} \Omega_i \tag{11}$$

[See, for instance, Pease (*16*) concerning the differentiation of negative powers of matrices.] Now the product $Z_i^{-1} \Omega_i$ is simply the solution to Equation (7) and may thus be obtained by the very fast and simple algorithm for Gaussian elimination in the case of a tridiagonal matrix. See in this regard Peaceman and Rachford (*15*), Ames (*1*), or the author's previous paper (*4*). Next, inspection shows that the matrix $\partial Z_i/\partial T_n$ contains at most two nonzero elements, and hence the product vector

$$\pi_{in} \equiv \frac{\partial Z_i}{\partial T_n} Z_i^{-1} \Omega_i$$

contains only two nonzero elements. Finally, we have $Z_i^{-1} \pi_{in}$ to evaluate, and this may, of course, be done in the same way as was $Z_i^{-1} \Omega_i$. Thus, the evaluation of the vectors $\partial\Lambda/\partial T_n$, $n = 0, 1, \ldots, J - 1$ may be very conveniently accomplished. Equations (10) and (11) are then solved alternately within step 4 above until $\Lambda(\overline{T}) = 0$.

The switch from Equations (6) to Equations (10) and (11) has been made when the multiplier θ_0 associated with the ratio d_i/b_i from step 3 above was such that $|\theta_0 - 1| < 0.01$. Under these conditions, Equation (10) has usually been solved two to eight times to obtain the next temperature profile in step 4, and in these cases two to six additional iterations (as defined in step 6 above) have been required to solve problems which were not solved by an additional fifty iterations by using Equations (6) in step 4. It is emphasized, however, that only a few problems requiring Equations (10) and (11) have been encountered.

It is informative to compare the use of Equations (10) and (11) with the procedure of Tirney and Bruno (*19*). For the case of constant molal overflow, they have derived equations for corrections to the temperature profile which include the effects of changes in composition on any and all stages. Their results show quadratic convergence close to the solution, and the same is true of Equations (10) and (11); however, these equations contain no explicit reference to the flow rates of individual components (for example, v_{ij}). Tirney's and Bruno's Equation (26), as pointed out by the authors, does require compositions which are unknown at the time the equation must be used. They employ a reasonable but arbitrary normalization to estimate the necessary values; Equations (10) and (11) obviate this drawback.

For purposes of comparison, Boyum's (*6*) cascade method was programmed and tested by using the data for his problem 4a. Boyum's suggested procedure was used because therein the temperature correction for each stage is obtained by solution of the adiabatic flash equations for that stage, thus making the correction depend upon the energy balance, among other things. This procedure did, indeed, converge for Boyum's problem 4a. It was then tested on a selection of five problems from the test set previously mentioned. These five were difficult in that they required between thirty-five and forty iterations to solve. Boyum's method did not solve any of these problems in sixty iterations, nor were the results close to a solution after sixty iterations. As a result, no further testing of this procedure was carried out.

NONIDEAL MIXTURES

Boyum (*6*) repeatedly returns to the point that various schemes for solving multicomponent distillation problems fail to allow the equilibrium values to depend upon composition. The experience of this author is that this shortcoming is more apparent than real. On the other hand, nonideal mixtures have often been handled by the brute force method of simply inserting a comparatively lengthy routine for computing a composition dependent equilibrium value and invoking this routine whenever such a value was needed. The following procedure requires much less computational effort than the brute force method and has been successfully employed:

1. Using the standard temperature profile previously described, perform an isothermal flash calculation of the sum of feeds at some or all of the temperatures in the profile. Use the full composition dependent equilibrium relations. This provides for each component a profile of equilibrium values between the bubble and dew points of the sum of feeds.
2. For each component, extrapolate this profile using the Antoine equation $\ln(K\pi) = [c/(T - c_0)] + c_1$. Rearrangement of this equation provides linear relations for evaluating c, c_0, and c_1 in terms of known pairs of corresponding values of K and T.
3. For each component, approximate the extended equilibrium profile by a power series in temperature alone. Note that an initial estimate of the composition dependence is now implicit in the coefficients of the power series. A useful form for this series is

$$\sqrt[4]{K_i\,\pi^p} = \sum_{n=0}^{4} \gamma_{in}\, T^n$$

where T is an absolute temperature and p is usually 1.0. The fourth root substantially reduces the required dynamic range of the series and also prohibits calculation of a negative value for K_i.

4. Use the power series just as if the equilibrium ratios were independent of temperature and carry out iterations on the distillation problem until the correction factor θ_0 associated with the ratio d_i/b_i is such that $|\theta_0 - 1| < 0.5$.
5. The first time $|\theta_0 - 1| < 0.5$ or after step 6 use the compositions of the liquid and vapor at some or all of the

stages to develop a new equilibrium profile for each component. Then repeat steps 2 and 3.

6. Resume iterations on the distillation problem using the new power series expressions for equilibrium values. Continue until the iterations converge and then repeat steps 5 and 6 once more.

The same strategy is obviously useful for including heats of mixing in the liquid enthalpy values and pressure effects in the vapor enthalpy values.

EXISTENCE OF HOLLAND CONVERGENCE FACTORS

The convergence acceleration procedure of Holland requires that a particular set of equations possess a vector solution each element of which is nonnegative. The equations can take one of several different forms depending upon the type of specification made. It can be shown (5) that if the total withdrawal rate of each product stream is specified, then a positive solution of the Holland equations will always exist at every iteration. It is perhaps not widely recognized however, that for other types of specifications, purity specifications, for instance, the Holland equations may fail to possess the required positive solution. Consider by way of example distillation of a binary mixture in a column having no side draws and where the mole fraction x_1 of one component is specified for the bottom product. The equation for the Holland correction factor at any iteration in this simple situation is readily developed as follows:

$$x_1 = b_1/(b_1 + b_2)$$

$$b_i = f_i/[1 + \theta(d_i/b_i)_c], \quad i = 1, 2$$

$$[(1 - x_1)(d_2/b_2)_c f_1 - x_1\,(d_1/b_1)_c f_2]\theta = (f_1 + f_2)x_1 - f_1 \tag{12}$$

Suppose for example

$$x_1 = 0.1$$
$$f_1 = 80.0$$
$$f_2 = 20.0$$

Then, from Equation (12)

$$\theta = 35\,[(d_1/b_1)_c - 36\,(d_2/b_2)_c]^{-1}$$

so that at any iteration in which $(d_1/b_1)_c < 36\,(d_2/b_2)_c$, $\theta < 0$. Note further that simply setting $\theta = 0$ is unsuitable, since then $b_i = f_i$ and there is no distillate. Obviously, if $(d_1/b_1) < 36\,(d_2/b_2)$ in the actual separation, another method is required. A similar argument may be applied to situations where a product temperature is specified.

NOTATION

A_{ij} = stripping factor, $A_{ij} = L_j/[V_{j+1} K_i (T_j)] = v_{ij+1}/l_{ij}$

b, b_i = flow rate of component i in the liquid product leaving the hot end (bottom) of the unit

B = total flow rate of the liquid stream leaving the hot end (bottom) of the unit, $B = \Sigma_i\, b_i$

c = constant in Equations (1) through (6)

c_0, c_1 = constants in the Antoine equation

d, d_i = flow rate of component i in the product leaving the cool end (top) of the unit

f_i = rate of feed of component i

K, K_i = equilibrium ratio for component i

l_i, l_{ij} = flow rate of component i in the liquid leaving stage j

L, L_j = total flow rate of liquid leaving stage j

p = power to which the total pressure is raised in the expression $K\,\pi^p = \phi\,(T)$

$T, T_j, T^\circ, T_j^\circ, T_0$ = absolute temperature

$\overline{T}, \overline{T}^\circ$ = vector of absolute temperatures defined after Equation (9)

v_i, v_{ij} = flow rate of component i in the vapor entering stage j

V, V_j = total flow rate of vapor entering stage j, $V = \Sigma\, v_i$

$\overline{V}$ = vector of total vapor flow rates defined prior to Equation (8)

w = weighting factor in Equation (5)

x_i = mole fraction of component i in a liquid mixture

z_{mni} = variable defined after Equation (7)

Z_i = matrix having as its m, n^{th} element z_{mni}

Greek Letters

γ_{in} = coefficient of T^n in power series expression for $\sqrt[t]{K_i\,\pi^p}$

θ_0 = factor defined in references *4* and *10* such that $d_i/b_i = (d_i/b_i)_c\,\theta_0$

Λ = vector function defined by Equation (9)

π = total pressure

π_{in} = matrix-vector product defined after Equation (11)

Υ_i = vector of flow rates of individual components in vapor streams, defined after Equation (7)

ω_{ij} = flow rate of external feed of component i to stage j

Ω_i = vector having ω_{ij} as its j^{th} element, defined after Equation (7)

Subscript

c = the last previously computed value of the quantity to which it applies

T = transposition

LITERATURE CITED

1. Ames, W. F., "Non-Linear Partial Differential Equations in Engineering," Academic Press, New York (1965).
2. Amundson, N. R., and A. J. Pontinen, *Ind. Eng. Chem.*, **50**, No. 5, 730-736 (1958).
3. Ball, W. E., paper presented at the 44th National Meeting, Am Inst. Chem. Engrs., New Orleans, La., (Feb. 27, 1961).
4. Billingsley, D. S., *AIChE J.*, **12**, No. 6, 1134-1141 (1966).
5. ———, *IBM J. Res. Develop.*, **14**, No. 1, 33-40 (1970).
6. Boyum, A. A., Ph.D. thesis, Polytechnic Institute of Brooklyn, New York (1966).
7. Friday, J. R., and B. D. Smith, *AIChE J.*, **10**, No. 5, 698-707 (1964).
8. Greenstadt, J. L., Y. Bard, and B. Morse, *Ind. Eng. Chem.*, **50**, No. 11, 1644-1647 (1958).
9. Greenstadt, J. L., and Y. Bard, *IBM Program IBDST2*, IBM, New York (1961).
10. Holland, C. D., "Multicomponent Distillation," Prentice-Hall, Englewood Cliffs, N.J. (1963).
11. ———, and J. D. Lindsay, "Encyclopedia of Chemical Technology," 2nd ed., Vol. 7, pp. 204-248, Interscience, N.Y. (1965).
12. Naphtali, L. M., paper presented at 56th National Meeting, Am. Inst. Chem. Engrs., San Francisco, Calif. (May 16-19, 1965).
13. Nartker, T. A., J. M. Skrygley, and C. D. Holland, *Can. J. Chem. Eng.*, **44**, No. 4, 217-226 (1966).
14. Newman, J. S., *Hydrocarbon Process.*, **42**, No. 4, 141-144 (1963).
15. Peaceman, D. W., and H. H. Rachford Jr., *SIAM J.*, **3**, No. 1, 28-65 (1955).
16. Pease, M. C., "Methods of Matrix Algebra," Academic Press, N.Y. (1965).
17. Sujata, A. D., *Petrol. Refiner*, **40**, No. 12, 137-140 (1961).
18. Thiele, E. W., and R. L. Geddes, *Ind. Eng. Chem.*, **25**, No. 3, 289-295 (1933).
19. Tierney, J. W., and J. A. Bruno, *AIChE J.*, **13**, No. 3, 556-563 (1967).
20. Wang, J. C., and G. E. Henke, *Hydrocarbon Process.*, **45**, No. 8, 155-163 (1966).

Manuscript received January 13, 1968; revision received October 17, 1968; paper accepted October 18, 1968.