Determination of Plate Efficiencies From Operational Data

D. L. TAYLOR, PARKE DAVIS, and C. D. HOLLAND

Texas A&M University, College Station, Texas

The objectives of this paper are to present and to demonstrate the use of extensions and improvements of the basic method (4, 5) for the determination of plate efficiencies from operational data (field tests). The basic method with extensions makes use of all known operational information, over and above that required to solve a problem for a fixed column, to determine a set of plate efficiencies. The information required to solve a problem for a fixed column consists of the complete definition of the feed stream, the number of plates in each section of the column, the type of condenser, the column pressure, and the distillate and reflux rates. The information over and above this, hereafter referred to as *additional information* or *additional specifications*, may be of the form of any combination of temperatures and product distributions.

In the original method (4, 5), it was supposed that the temperature of each plate was known. However, since each temperature of this collection is seldom known from field tests, an extension of the original method was developed whereby a set of efficiencies may be determined on the basis of any number of known temperatures and product distributions. As discussed herein, the efficiencies may be determined by use of the Newton-Raphson method in a manner analogous to that described in reference 5 for the original method. In this approach, a square array ($c + N + 2$, at most) of Newton-Raphson equations in ($c + N + 2$, at most) unknowns must be solved each trial. A significant improvement of this method with respect to speed is presented. In the improved version, the ($c + N + 2$) Newton-Raphson equations are reduced to c independent Newton equations, and the computer time required to determine a set of efficiencies is comparable to that required to solve a problem for a fixed column.

In addition to this extension, several other improvements of the original method (5) such as the treatment of separated components and the selection of relative values for the plate factors are presented. Also, since several field tests at total reflux (or total recycle) were available for analysis (2), the basic method for the determination of plate efficiencies was extended to include this case.

To demonstrate the type of results that may be expected, two numerical examples are presented, one at a finite operating reflux and one at total reflux. Actually, more than fifty field tests have been analyzed by Taylor (7) and others (3), and a further extension that makes use of any number of plate compositions has been developed (3).

Objectives of this method that appear within the realm of immediate possibility are twofold. First, on the basis of field tests such as acceptance tests, sets of efficiencies for a given unit may be determined for each of several operating conditions. From the sets of efficiencies so obtained, it appears possible to select a relatively accurate set of efficiencies of this particular unit at any intermediate set of operating conditions by use of either a suitable correlation or by interpolation. The second objective is concerned with the design of new units. On the basis of the several sets of efficiencies for a given unit, the selection of a suitable set for the design of similar units appears feasible.

After a review of the fundamentals involved in the determination of efficiencies, three particular types of problems are considered. The first of these deals with the case where some of the temperatures are unknown; the second consists of the treatment of separated components, and the third is concerned with the operational condition of total reflux (or recycle).

FUNDAMENTAL RELATIONSHIPS AND DEFINITIONS

The vaporization efficiency (5) is defined by

$$E^{\circ}_{ji} = \frac{y_{ji}}{Y_{ji}} \tag{1}$$

and

$$Y_{ji} = K_{ji} x_{ji} \tag{2}$$

where x_{ji} is the mole fraction of component i in the liquid leaving plate j. The equilibrium constant K_{ji} is evaluated at the temperature of the liquid leaving plate j and at the pressure of plate j. The customary assumption that the liquid leaving a plate is at its bubble point is not made. In the event that the liquid is at its bubble point, then the sum of the Y_{ji}'s is unity. For any given set of E°_{ji}'s and x_{ji}'s, the temperature of the liquid leaving plate j is that positive value of T_j which makes $f_j = 0$, where

$$f_j = \sum_{i=1}^{c} E^{\circ}_{ji} K_{ji} x_{ji} - 1 \tag{3}$$

In the statement of the material balance and equilibrium relationships, the use of vaporization efficiencies leads to a set of equations of the same form as those of the calculational procedure of Thiele and Geddes (8) for perfect plates, provided the customary absorption and stripping factors A_{ji} and S_{ji} are replaced by A°_{ji} and S°_{ji}, where

$$A^{\circ}_{ji} = \frac{L_j}{E^{\circ}_{ji} K_{ji} V_j} \text{ and } S^{\circ}_{ji} = \frac{E^{\circ}_{ji} K_{ji} V_j}{L_j} \tag{4}$$

When the plates are perfect, $E^{\circ}_{ji} = 1$, $A^{\circ}_{ji} = A_{ji}$, and $S^{\circ}_{ji} = S_{ji}$.

In general, methods for the determination of efficiencies make use of some form of the calculational procedure of Thiele and Geddes (8). For the case where all of the T_j's and b_i/d_i's are known, a brief review of this procedure follows. For any assumed set of E°_{ji}'s and L/V's the component-material balance equations of Thiele and Geddes may be applied to give a calculated set of values for the b_i/d_i's. Let the calculated values be denoted by the

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D. L. Taylor is at South Dakota School of Mines and Technology, Rapid City, South Dakota. Parke Davis is with the Dow Chemical Company, Freeport, Texas.

subscript *ca* and the specified values by the subscript *co*, and let

$$\theta_i = \frac{(b_i/d_i)_{co}}{(b_i/d_i)_{ca}} \tag{5}$$

When the correct set of E°_{ji}'s is assumed, $\theta_i = 1$ for all i, and $f_j = 0$ for all j. The x_{ji}'s that appear in the expression for f_j are computed by use of the following formula:

$$x_{ji} = \frac{(l_{ji}/b_i)_{ca}(b_i)_{ca}}{\sum_{i=1}^{c} (l_{ji}/b_i)_{ca}(b_i)_{ca}} \tag{6}$$

In addition, the set of the L/V's used to find the $(b_i/d_i)_{ca}$'s must be in agreement with those computed by use of enthalpy and material balances. The constant composition and Q methods (5) for making enthalpy balances were used. The liquid and vapor rates so obtained were used to make the next trial through the column. The remainder of the details of the calculational procedure for the determination of the plate efficiencies is best explained by consideration of particular cases or specifications.

I. ADDITIONAL SPECIFICATIONS: $(b_i/d_i)_{co}$ FOR EACH COMPONENT AND T_j FOR SOME BUT NOT ALL PLATES

In order to present a precise enumeration of the variables and the equations, consider the case of a column for which the usual operating conditions are known. A partial condenser is employed, and the reflux rate L_o or the overhead vapor rate V_1 is specified. In addition to the b_i/d_i's, the temperatures of the distillate and bottoms as well as the temperatures of the plates above and below the feed plate are known. These temperatures are denoted by T_0, T_{f-1}, T_{f+1}, and T_{N+1}, respectively. In the calculations, the temperature of the distillate or any vapor stream leaving a plate is taken to be the same as that of the liquid on and leaving a plate; that is the heat transfer efficiencies (5) are taken to be equal to unity.

Since the b_i/d_i's are known, D is fixed which determines B. The known value of V_1 (or L_o) is used to determine the condenser duty Q_c. Thus the problem reduces to the selection of $j \times i$ [or $c(N + 2)$] values of E°_{ji} such that $\theta_i = 1$ for all i and $f_j = 0$ for all j.

As described in reference 5, a relationship of the form

$$E^{\circ}_{ji} = \beta_j \bar{E}^{\circ}_i \tag{7}$$

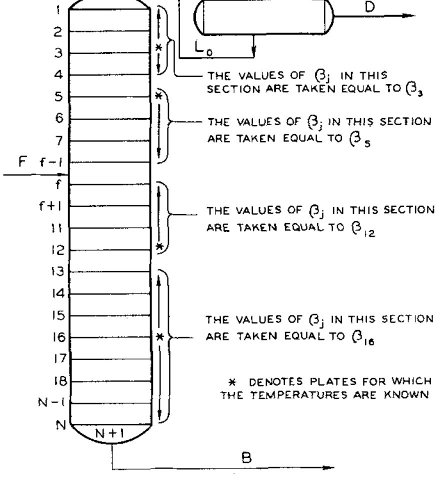

Fig. 1. Assignment of the β's.

may be used to generate $j \times i$ values of the vaporization efficiencies from j values of β and i values of $\bar{E}^{\circ}$. If the temperature for each plate were known, $(N + 2)$ values of β for a column (with partial condenser) could be determined as described by reference 5. However, for each plate for which the temperature is unknown, a β_j may be assigned arbitrarily and the function f_j for the given plate satisfied by finding a T_j such that $f_j = 0$. The assignment of the β_j's for the plates on which the temperatures were unknown was in accordance with the scheme shown in Figure 1.

Method I: Determination of Efficiencies by the Newton-Raphson Method

Except for differences that are described, the Newton-Raphson method may be applied in a manner analogous to that described in reference 5 for the case where all of the temperatures are known. The independent variables were taken to be the c values of $\bar{E}^{\circ}_i$, β_j, for all plates for which the temperatures are known, and T_j for all plates for which the temperatures are unknown; that is

$$\theta_i = \theta_i(\bar{E}^{\circ}_i, \beta_0, \beta_{f-1}, \beta_{f+1}, \beta_{N+1}, T_1, \ldots, T_{f-2}, T_f, T_{f+2}, \ldots, T_N), \; (1 \leqq i \leqq c) \tag{8}$$

$$f_j = f_j(\bar{E}^{\circ}_i, \ldots, \bar{E}^{\circ}_c, \beta_0, \beta_{f-1}, \beta_{f+1}, \beta_{N+1}, T_1, \ldots, T_{f-2}, T_f, T_{f+2}, \ldots, T_N), \; (0 \leqq j \leqq N + 1) \tag{9}$$

In the determination of efficiencies by means of the Newton-Raphson equations, it was found that the function log θ_i led to a more rapid rate of convergence for all problems considered than did the function θ_i, which was suggested by reference 5. Also, problems which could not be solved by use of the function θ_i were solved when the function log θ_i was used. The Newton-Raphson equations are of the general form

$$0 = \log_e \theta_i + \left(\frac{\partial \log_e \theta_i}{\partial \bar{E}_i^{\circ}}\right) \Delta \bar{E}_i^{\circ} + \left(\frac{\partial \log_e \theta_i}{\partial \beta_0}\right) \Delta\beta_0 + \ldots + \left(\frac{\partial \log_e \theta_i}{\partial \beta_{N+1}}\right) \Delta\beta_{N+1} + \left(\frac{\partial \log_e \theta_i}{\partial T_1}\right) \Delta T_1 + \ldots + \left(\frac{\partial \log_e \theta_i}{\partial T_N}\right) \Delta T_N, \; (1 \leqq i \leqq c) \tag{10}$$

and

$$0 = f_j + \left(\frac{\partial f_j}{\partial \bar{E}_1^{\circ}}\right) \Delta \bar{E}_1^{\circ} + \ldots + \left(\frac{\partial f_j}{\partial \bar{E}_c^{\circ}}\right) \Delta \bar{E}_c^{\circ} + \left(\frac{\partial f_j}{\partial \beta_o}\right) \Delta\beta_o + \ldots + \left(\frac{\partial f_j}{\partial \beta_{N+1}}\right) \Delta\beta_{N+1} + \left(\frac{\partial f_j}{\partial T_1}\right) \Delta T_1 + \ldots + \left(\frac{\partial f_j}{\partial T_N}\right) \Delta T_N, \; (0 \leqq j \leqq N + 1) \tag{11}$$

where

$$\Delta \bar{E}_i^{\circ} = \bar{E}^{\circ}{}_{i,n+1} - \bar{E}^{\circ}{}_{i,n}; \; \Delta\beta_j = \beta_{j,n+1} - \beta_{j,n};$$

and

$$\Delta T_j = T_{j,n+1} - T_{j,n}.$$

The values of the functions ($\log_e \theta_i$ and f_j) appearing in the Newton-Raphson equations were evaluated at the last set of values for the variables $(\bar{E}^{\circ}{}_{i,n}, \beta_{j,n}, T_{j,n})$. After the derivatives had been evaluated by the same procedure as that described for $\partial \log_e \theta_k/\partial \bar{E}_k^{\circ}$, the Newton-Raphson equations were solved for the $\Delta \bar{E}_i^{\circ}$'s, ΔT_j's, and the $\Delta\beta_j$'s from which the next set of values for the variables was computed. Let all of the T_j's, β_j's, and the E_i°'s be held fixed at their values for the n'th trial except for $\overline{E}_k^{\circ}$, and for this variable use the value $\overline{E}^{\circ}_{k,p}$ given by

$$\overline{E}^{\circ}_{k,p} = \overline{E}^{\circ}_{k,n} + p \qquad (12)$$

On the basis of this set of values, compute $(b_k/d_k)_{ca}$ by use of the material balance expressions. Then compute the corresponding value of θ_k, denoted by θ_{kp}. This value of θ_k and the one found for the n'th trial, θ_{kn}, were used to compute the desired derivative as follows:

$$\frac{\partial \log_e \theta_k}{\partial \overline{E}_k^{\circ}} = \frac{\log_e \theta_{k,p}/\theta_{k,n}}{p} \qquad (13)$$

In the application of this method for the determination of the efficiencies, it was found that the rate of convergence to the desired set of values for T_j, β_j, and $\overline{E}_i^{\circ}$ depended strongly upon the choice of the value for p. For all examples considered, the following scheme for the selection of p has given very satisfactory results. This scheme seeks to choose a value of p that is proportional to a mean value of all the functions. The following procedure was used:

1. For the first two trials, the value $p = 0.1$ was used in the calculation of all of the partial derivatives that appear in the Newton-Raphson equations.
2. For the third and all successive trials, the value of p calculated by the formula

$$p = \sum_{j=0}^{N+1} \frac{\log_e (f_j + 1)}{N + 2} + \sum_{i=1}^{c} X_i \log_e \theta_i \qquad (14)$$

was employed, provided $10^{-3} \leqq p \leqq 0.1$. If a value of p greater than 0.1 was calculated, p was taken equal to 0.1. A value of $p = 10^{-3}$ indicated that convergence had been obtained.

The β_j's and $\overline{E}_i^{\circ}$'s determined by the Newton-Raphson equations were accepted provided they were no greater than 1.3 and no less than 1/1.3 times the values used to make the given trial; otherwise the limiting values were used. In the evaluation of the partial derivatives with respect to temperatures, a change in temperature equal to one hundred times the value of p computed by Equation (14) was employed.

After an improved set of values for the unknown T_j's, β_j's, and $\overline{E}_i^{\circ}$'s had been computed by the Newton-Raphson equations, the β_j's were normalized as described in a subsequent section. The improved set of values of the variables were used to determine a new set of L/V's by enthalpy balance, and then the corresponding set of θ_i's and f_j's were found. Except for the fact that numerical evaluations of the partial derivatives were time consuming, this method was satisfactory. The following method reduced the time required to solve a problem several fold.

Method II: Newton's Method

Instead of taking the unknown T_j's, β_j's, and $\overline{E}_i^{\circ}$'s as independent variables, the $\overline{E}_i^{\circ}$'s may be taken as the independent variables and the unknown T_j's and β_j's as dependent variables. For this choice of independent and dependent variables, Equations (10) and (11) reduce to at most c independent Newton equations of the form

$$0 = \log_e \theta_i + \left(\frac{\partial \log_e \theta_i}{\partial \overline{E}_i^{\circ}}\right) \Delta \overline{E}_i^{\circ}, \ (1 \leqq i \leqq c) \qquad (15)$$

On the basis of the last set of L/V's, T_j's, and β_j's used to make a calculation through the column, the following sequence of calculations were performed. First the $\overline{E}_i^{\circ}$ for each component was computed by use of Equation (15). Next these $\overline{E}_i^{\circ}$'s were used to compute a set of compositions. For all plates for which the temperatures are known, a better set of β_j's is found by setting $f_j = 0$ and solving for β_j to obtain

$$\beta_j = \frac{1}{\sum_{i=1}^{c} \overline{E}_i^{\circ} K_{ji} x_{ji}} \qquad (16)$$

For all plates j for which the temperatures are unknown, f_j is again set equal to zero and the resulting expression solved for K of the base component to give

$$K_{jb} \Big|_{T_{j,n+1}} = \frac{1}{\sum_{i=1}^{c} \beta_j \overline{E}_i^{\circ} \alpha_{ji} \Big|_{T_{j,n}} x_{ji}} \qquad (17)$$

In making this calculation, the most recent values for β_j, $\overline{E}_i^{\circ}$, and x_{ji} were employed. For the case of perfect plates, this method for the calculation of temperature has been described (5). As suggested in the reference, the base component was selected as one that approximated the mid-boiling component of the mixture. Actually, in order to make the calculation of temperature direct, a hypothetical component with a K given by

$$\log_e K = \frac{a}{T} + b$$

was used. The constants a and b were selected on the basis of the K values for the mid-boiling component at the upper and lower limits of curve fits.

Although a larger number of complete trials through the column was required by this method than by the previous one, the computer time required to solve a problem by this method was only a fraction of that required by the Newton-Raphson method.

Normalization of the β_j's and $\overline{E}_i^{\circ}$'s

Since β_j and $\overline{E}_i^{\circ}$ appear as the product $\beta_j \cdot \overline{E}_i^{\circ}$ in the equations that describe the column, only the product $\beta_j \cdot \overline{E}_i^{\circ} = E^{\circ}_{ji}$ may be determined uniquely. If the β_j's and $\overline{E}_i^{\circ}$'s are normalized with respect to any given plate, there exists only one set of β_j's and $\overline{E}_i^{\circ}$'s that correspond to the computed set of E°_{ji}'s. Harris and others (4, 5) normalized the β_j's and the E°_{ji}'s with respect to $\beta_j = 1$ for the top plate. However, in the determination of the efficiencies at total reflux, it was found particularly advantageous to use a normalization procedure whereby the product of all of the normalized values of the β_j's had the value of unity. Because of the existence of this advantage, this procedure was adopted for columns at all refluxes. To illustrate this procedure, let the calculated values of β_j's and $\overline{E}_i^{\circ}$'s be identified by the subscript ca. Let the normalized value of β_j be defined by

$$\beta_j = \frac{(\beta_j)_{ca}}{\sqrt[N+2]{\prod_{j=0}^{N+1} (\beta_j)_{ca}}} \qquad (18)$$

Then, it is evident that

$$\prod_{j=0}^{N+1} \beta_j = 1$$

The values of E^{o}_{ji} are unchanged by the normalization procedure; that is

$$E^{o}_{ji} = (\beta_j)_{ca}\,(\overline{E}_i{}^{o})_{ca} = \beta_j\,\overline{E}_i{}^{o}$$

By use of this relationship and Equation (18), it is readily shown that the formula for the normalized value of $\overline{E}_i{}^{o}$ is given by

$$\overline{E}_i{}^{o} = (\overline{E}_i{}^{o})_{ca} \sqrt[N+2]{\prod_{j=0}^{N+1} (\beta_j)_{ca}} \tag{19}$$

II. ADDITIONAL SPECIFICATIONS: $(b_i/d_i)_{co}$ FOR SOME BUT NOT ALL COMPONENTS AND T_j FOR SOME BUT NOT ALL PLATES

The following procedure consists of an extension of the one presented in reference 5. Generally the b_i/d_i's are not known for all components from test results. This limitation led to the development of the following calculational procedure for the determination of efficiencies.

The heaviest component for which b_i/d_i is known is called the *heavy key,* which is identified by the subscript h. The lightest component for which b_i/d_i is known is called the *light key,* which is identified by the subscript l. The components for which the b_i/d_i's are unknown are called *separated components* and referred to as a group by the letter s. In the procedure proposed (5), values for the separated components were selected that satisfied the specified value of D in the following manner. For any separated component $(i = s)$

$$(b_i/d_i)_{co} = \overline{\theta}\,(b_i/d_i)_{ca},\ (i = s) \tag{20}$$

and in view of the definition of θ_i [Equation (5)], it follows that

$$\theta_i = \overline{\theta},\ (i = s) \tag{21}$$

where $\overline{\theta}$ is that positive number that makes $g(\overline{\theta}) = 0$. Since $g(\overline{\theta})$ is defined by

$$g(\overline{\theta}) = \sum_{s} \frac{FX_i}{1 + \overline{\theta}(b_i/d_i)_{ca}} + \sum_{\substack{i=l \\ i \neq s}}^{h} \frac{FX_i}{1 + (b_i/d_i)_{co}} - D \tag{22}$$

it is seen that when a $\overline{\theta}$ is found that makes $g(\overline{\theta}) = 0$, all of the (b_i/d_i)'s are in agreement with the specified value of D. The quantity $\overline{\theta}$ is used to determine one $\overline{E^{o}}$ (denoted by $\overline{E}_s{}^{o}$) for all of the separated components such that the specification D is satisfied. If prior knowledge of the relative values of the $\overline{E}_i{}^{o}$'s for the separated components exists, this information may be included by the assignment of a multiplier η_i for each separated component:

$$\overline{E}_i{}^{o} = \eta_i\,\overline{E}_s{}^{o} \tag{23}$$

The number of θ_i functions is equal to the number of distributed components [those for which the (b_i/d_i)'s are known], and there is one $\overline{\theta}$ function. Again an f_j function exists for each plate j.

This scheme applies when there are both separated lights and separated heavies. If all of the separated components are lights, or if all of the separated components are heavies, then the $\overline{\theta}$ function is not used, and the value of $\overline{E}_s{}^{o} = 1$ is used for the first trial. For the second and all subsequent trials, the assumed value for $\overline{E}_s{}^{o}$ is obtained by multiplying the previous one by the normalization factor of Equation (19).

The calculational procedure follows closely that described for the first type of specification. The β_j's and the unknown T_j's may be found by either of the two methods described.

SPECIFICATIONS: TOTAL REFLUX (OR RECYCLE), x_{Bi}/X_{Di} FOR SOME OR ALL COMPONENTS, AND T_j FOR SOME OR ALL PLATES

Because of the availability of several field tests at the operating condition of total reflux, the following calculational procedure was developed. In the available tests, the temperature of each plate was known as well as the product distribution for each component. For this case, the $\overline{E}_i{}^{o}$'s and the β_j's may be found by direct solution in the following manner. A component-material balance enclosing a condenser or partial condenser yields

$$y_{1i} = x_{oi} \tag{24}$$

$$E^{o}_{oi} = \frac{y_{oi}}{K_{oi}\,x_{oi}} = \frac{X_{Di}}{K_{oi}\,x_{oi}} \tag{25}$$

and

$$E^{o}_{1i} = \frac{y_{1i}}{K_{1i}\,x_{1i}} \tag{26}$$

It follows that

$$\frac{x_{1i}}{X_{Di}} = \frac{1}{K_{oi}K_{1i}E^{o}_{oi}E^{o}_{1i}}$$

Continuation of this procedure yields the following expression for plate $j = N + 1$:

$$\frac{x_{N+1,i}}{X_{Di}} = \frac{x_{Bi}}{X_{Di}} = \frac{1}{K_{oi}K_{1i}\ldots K_{N+1,i}\,E^{o}_{oi}E^{o}_{1i}\ldots E^{o}_{N+1,i}} \tag{27}$$

Since the product of the β_j's over all j has the value of unity by virtue of the normalization procedure, it follows that Equation (27) reduces to

$$\frac{x_{Bi}}{X_{Di}} = \frac{1}{\left(\prod_{j=0}^{N+1} K_{ji}\right)(\overline{E}_i{}^{o})^{N+2}} \tag{28}$$

For this unique choice of a normalization procedure, the distribution ratios x_{Bi}/X_{Di} are independent of the β_j's, and Equation (28) may be solved explicitly for $\overline{E}_i{}^{o}$ to give

$$\overline{E}_i{}^{o} = \frac{1}{\sqrt[N+2]{\left[\prod_{j=0}^{N+1} K_{ji}\right](x_{Bi}/X_{Di})}} \tag{29}$$

If the temperatures are all known as well as the x_{Bi}/X_{Di}'s and the X_{Di}'s, each component efficiency $\overline{E}_i{}^{o}$ is uniquely determined by Equation (29), and the β_j's may be computed directly by a step-by-step procedure that may be initiated at either the top or at the bottom of the column. When the calculations are commenced at the top of the column, Equation (25) is rearranged to give

$$x_{oi} = \frac{y_{oi}}{\beta_o \overline{E}_i{}^{o} K_{oi}} \tag{30}$$

Summation of both sides of this equation over all components followed by rearrangement yields the formula for the calculation of β_o, namely

$$\beta_o = \sum_{i=1}^{c} \frac{y_{oi}}{\overline{E}_i{}^{o}\,K_{oi}},\ \text{or}\ \beta_o = \sum_{i=1}^{c} \frac{X_{Di}}{\overline{E}_i{}^{o}\,K_{oi}} \tag{31}$$

This value of β_o is used to compute x_{oi} by Equation (29), and hence a value will have been found for y_{1i}, since $y_{1i} = x_{oi}$. Then, from Equation (26), the formula

TABLE 1. STATEMENT OF EXAMPLE 1

Component	Component No.	FX_i	$(b_i/d_i)_{co}$	Plate No.	Temp., °F.
C_2H_6	1	2.16	—	0 (condenser)	116·0
C_3H_8	2	25.19	0.0241	1	125.0
i-C_4H_{10}	3	16.86	29.93	18	202.0
n-C_4H_{10}	4	54.33	—	28	219.0
i-C_5H_{12}	5	1.46	—	29	219.0
				31 (reboiler)	220.0

Other specifications

$V_1 = 160.8$; $D = 27.3$, column pressure = 271 lb./sq. in. abs.; thermal condition of feed: superheated liquid at 207°F. ($L_F = 87.95$, $V_F = 12.05$, flash temperature is 189.1°F.). A partial condenser is employed. Limiting vapor rates: $V_{min} = 119 \leqq V_j \leqq 198 = V_{max}$, $2 \leqq j \leqq 30$. $\eta_i = 1.0$ for $i = s$ (components 1, 4, 5). The feed enters on Plate 15. Use the enthalpy data given in Table A-8 of reference 5 and the K data given in reference 7.

TABLE 3. STATEMENT OF EXAMPLE 2

Component	Component No.	$x_{oi}(=X_{Di})$	$x_{N+1,i}(=x_{Bi})$	Plate No.	Temp., °F.
C_3H_8	1	0.202	0.0001	1	155.4
i-C_4H_8	2	0.655	0.316	2	162.5
n-C_4H_8	3	0.143	0.683	3	166.6
				4	168.9
				5	171.0
				6	172.8
				7	174.3
				8	176.4
				9	177.3
				10	179.5

Other specifications

Total reflux (or total recycle), total condenser, column pressure = 165 lb./sq. in. abs. Use the K data given in equilibrium data in reference 7.

$$B_1 = \sum_{i=1}^{c} \frac{y_{1i}}{\overline{E}_i^{\circ} K_{1i}}$$

is obtained in the same manner as that shown for β_o. After β_1 has been computed by use of this expression, x_{1i} is found by use of Equation (26). Continuation of this process throughout the remainder of the column yields all of the β_j's.

When some of the temperatures are unknown, the efficiencies may be determined by use of either Method I or II of Specification I. In the application of Methods I and II, the calculated values of b_i/d_i are needed. On the basis of an assumed set of values for the unknown temperatures and the $\overline{E}_i^{\circ}$'s, the calculated distribution ratios x_{Bi}/X_{Di} are given by Equation (28), from which the calculated values of b_i/d_i are found by multiplication of each distribution ratio by B/D. The corresponding calculated values of the component-distillate rates are found by overall material balance

$$(d_i)_{ca} = \frac{FX_i}{1 + (b_i/d_i)_{ca}} \tag{32}$$

and the corresponding compositions are given by

$$x_{ji} = \frac{(x_{ji}/X_{Di})_{ca}(X_{Di})_{ca}}{\sum_{i=1}^{c} (x_{ji}/X_{Di})_{ca}(X_{Di})_{ca}} \tag{33}$$

Usually the data are collected at the operating conditions $F = D = B = 0$ with V_j and L_j finite. In order to use these data for the determination of efficiencies, a value of $D < F$ is selected arbitrarily, and F is for convenience taken to be 100 moles/hr. Then, the feed rates for each component are found by means of the overall material balance. This value of FX_i is used in Equation (32).

The remainder of the calculational procedures are analogous to those described under Specification I except that it is not necessary to make enthalpy balances.

ILLUSTRATIVE EXAMPLES

To demonstrate the use of the proposed calculational procedures and the type of results which may be obtained, two examples were selected, one at a finite operating reflux and one at total reflux.

Example 1 (see Table 1) is based on the results of a test by the Esso Research and Engineering Company (*1*). This example represents the case where in addition to the usual operating variables, only part of the temperatures

TABLE 2. SOLUTION OF EXAMPLE 1

Component efficiencies, $\overline{E}_i^{\circ}$

$\overline{E}_2^{\circ} = 1.03$, $\overline{E}_3^{\circ} = 1.13$

$\overline{E}_s^{\circ} = \overline{E}_1^{\circ} = \overline{E}_4^{\circ} = \overline{E}_5^{\circ} = 0.83$

Calculated β_j's, temperatures, and vapor rates

Plate No.	β_j	Temp., °F.	V_j	Plate No.	β_j	Temp., °F.	V_j
0 (condenser)	1.02	116.0*	—	16	0.97	197.2	140.0
1	0.98	125.0*	160.8*	17	0.97	199.6	140.7
2	0.98	127.2	164.6	18	0.97	202.0*	141.4
3	0.98	129.4	163.4	19	1.02	196.2	146.7
4	0.98	131.8	162.0	20	1.02	198.5	135.5
5	0.98	134.7	160.4	21	1.02	200.9	136.3
6	0.98	138.1	158.6	22	1.02	203.3	137.2
7	0.98	141.8	156.7	23	1.02	205.7	138.1
8	0.98	145.9	154.8	24	1.02	208.0	139.0
9	0.98	150.4	152.9	25	1.02	210.3	140.0
10	0.98	155.4	151.2	26	1.02	212.9	140.9
11	0.98	161.0	149.5	27	1.02	215.7	141.9
12	0.98	167.7	147.6	28	1.02	219.0*	143.0
13	0.98	175.6	145.9	29	1.05	219.0*	146.7
14	0.98	184.6	144.3	30	1.13	224.1	142.2
15 (feed)	0.97	194.9	130.9	31 (reboiler)	1.13	220.0*	150.7

* Specified values.

TABLE 4. COMPARISON OF MEASURED AND CALCULATED VALUES OF LIQUID COMPOSITIONS FOR EXAMPLE 2

	Component No. 1		Component No. 2		Component No. 3	
Plate No.	x_{ji} observed	x_{ji} calculated	x_{ji} observed	x_{ji} calculated	x_{ji} observed	x_{ji} calculated
0 (reflux)	0.202	0.202	0.655	0.655	0.143	0.143
1	0.111	0.106	0.701	0.700	0.188	0.194
3	0.0263	0.025	0.696	0.676	0.278	0.298
5	0.0056	0.0056	0.618	0.585	0.376	0.409
7	0.0014	0.0011	0.523	0.476	0.476	0.523
9	0.0005	0.0002	0.382	0.367	0.617	0.633
10 (reboiler)	0.0001	0.0001	0.317	0.317	0.683	0.683

and part of the b_i/d_i's are known for a column operating at a finite reflux. The solution of Example 1 appears in Table 2. The η's for the separated components were taken equal to unity. When additional problems are solved, it is anticipated that it will be possible to assign a better set of η's than those employed. In this example so few temperatures were known that minor inverses in the temperature profile were produced on Plates 18 and 30 where the assignment of the β's was made in accordance with Figure 1.

Example 2 (see Table 3) was selected to demonstrate the method presented for the determination of the plate efficiencies for columns operating at total reflux (or recycle). This example is based on results obtained by Fractionation Research, Inc. (2). The component efficiencies and plate factors obtained were as follows: $\overline{E}_1^{o} = 1.048$, $\overline{E}_2^{o} = 0.981$, $\overline{E}_3^{o} = 0.974$, $\beta_1 = 0.993$, $\beta_2 = 0.993$, $\beta_3 = 0.997$, $\beta_4 = 1.002$, $\beta_5 = 1.003$, $\beta_6 = 1.004$, $\beta_7 = 1.005$, $\beta_8 = 1.000$, $\beta_9 = 1.005$, and $\beta_{10} = 0.998$. A comparison of the calculated and the observed compositions appears in Table 4. Although the calculated and measured compositions are not identical, the agreement is good. This is particularly gratifying since the method used to determine the efficiencies did not make use of the fact that the compositions on one or more plates were known.

Present results indicate that the vaporization efficiencies are far more useful both for the description of existing columns and the design of new columns than are the modified Murphree efficiencies (5).

It should be observed that the vaporization efficiencies as multipliers of the K_{ji}'s may be used to include the activity coefficients. Thus, the determination of the vaporization efficiencies represents a method for the determination of the combined activity and plate efficiency corrections for columns used to separate highly nonideal solutions such as those commonly encountered in the chemical industry.

Values of the E^{o}_{ji}'s close to unity suggest that the plates are nearly perfect and that the K data and the enthalpy data used to make the calculations are representative of the mixture. Although significant statistical deviations of the efficiencies have been observed by Taylor (7) for hydrocarbon systems, the efficiencies for these systems are usually close to unity.

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NOTATION

A^{o}_{ji} = absorption factor with the modified vaporization efficiency included, defined by Equation (4)
b_i = molal withdrawal rate of component i in the bottoms
B = total molal withdrawal rate of the bottoms
d_i = molal withdrawal rate of component i in the distillate
D = total molal withdrawal rate of the distillate
e = base for natural (or Naperian) logarithms
E^{o}_{ji} = vaporization efficiency, defined by Equation (1)
$\overline{E}_i^{o}$ = component efficiency; depends upon component i as defined by Equation (7); $\Delta\overline{E}_i^{o}$ is the difference between two values of $\overline{E}_i^{o}$ as defined after Equation (11)
f_j = temperature function for plate j, defined by Equation (3)
F = total molal flow rate of the feed
$g(\overline{\theta})$ = function of $\overline{\theta}$, defined by Equation (22)
K_{ji} = equilibrium constant for component i and plate j, evaluated at the temperature of the liquid leaving plate j
L_j = total molal flow rate of the liquid leaving plate j
p = change in the value of an independent variable used to find the numerical values of the derivatives
S^{o}_{ji} = stripping factor with the modified vaporization efficiency included; defined by Equation (4)
V_j = total molal flow rate of the vapor leaving plate j
x_{ji} = mole fraction of component i in the liquid leaving plate j
x_{Bi} = mole fraction of component i in the bottoms
X_{Di} = total mole fraction of component i in the distillate, regardless of state
X_i = total mole fraction of component i in the feed, regardless of state
y_{ji} = mole fraction of component i in the vapor leaving plate j
Y_{ji} = function defined by Equation (2)
β_j = plate factor, depends upon plate j alone as defined by Equation (7); $\Delta\beta_j$ is the difference between two values of β_j as defined after Equation (11)
η = multiplier defined by Equation (23)
$\theta_i, \overline{\theta}$ = multipliers defined by Equations (5) and (20), respectively

Subscripts

c = total number of components
ca = calculated value
co = corrected value
h = heaviest component for which b/d is known
i = any component of the mixture, numbered in the order of decreasing volatility, $1 \leqq i \leqq c$
j = plate number. The plates are numbered down from the top. The condenser has the number zero, the top plate the number 1, the feed plate the number f, the bottom plate number N, and the reboiler the number $N + 1$
l = lightest component for which b/d is known
s = separated component, any component for which b/d is unknown

LITERATURE CITED

1. Esso Research and Engineering Co., Personal communication.
2. Fractionation Research, Inc., Taken from data released to Fritz W. Glitsch & Sons, Inc., and published in their *Bulletin No. 160*.

3. Davis, Parke, D. L. Taylor, and C. D. Holland, Paper to be presented at the 55th National Meeting of the A.I.Ch.E. in Houston, Texas, February 7-11, 1965.
4. Harris, T. R., M.S. thesis, Texas A&M University, College Station, Texas (1962).
5. Holland, C. D., "Multicomponent Distillation," Prentice-Hall, Englewood Cliffs, New Jersey (1963).
6. Lenoir, J. M., and G. A. White, *Hydrocarbon Processing and Petroleum Refiner*, 37, No. 3, p. 173 (1958).
7. Taylor, D. L., dissertation, Texas A&M University, College Station, Texas (1964).
8. Thiele, E. W., and R. L. Geddes, *Ind. Eng. Chem.*, **25**, 289 (1933).

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The Isotropic Turbulent Mixer: Part II. Arbitrary Schmidt Number

STANLEY CORRSIN

The Johns Hopkins University, Baltimore, Maryland

One of the useful effects of turbulent fluid motion is its tendency to hasten the approach toward uniformity of a nonuniform fluid mixture. The stirring of cream into coffee is a familiar illustration. The simplest statistical measure of the departure from mixture uniformity at an instant is $\overline{c^2}(t)$, the mean-square fluctuation in contaminant concentration. To get a differential equation for $\overline{c^2}$, one begins with the mass transfer equation

$$\frac{\partial C}{\partial t} + u_i \frac{\partial C}{\partial x_i} = D_v \nabla^2 C \tag{1}$$

The diffusivity is taken constant, under restriction to low concentrations.

For a Newtonian fluid at very small Mach number with zero body forces, the corresponding momentum conservation statement is the Navier-Stokes equation

$$\frac{\partial u_i}{\partial t} + u_K \frac{\partial u_i}{\partial x_K} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \nabla^2 u_i \tag{2}$$

Total mass conservation with $\rho =$ constant is given by

$$\frac{\partial u_j}{\partial x_j} = 0 \tag{3}$$

If one writes the concentration as the sum of mean and fluctuating parts, $C(\underline{\underline{x}}, t) = \overline{C} + c(\underline{\underline{x}}, t)$, then $\overline{c} \equiv 0$ by definition. Restricting to statistical homogeneity in space, $\overline{C} = \overline{C}(t)$ only, one sees that since there is no chemical reaction term in (1), $\overline{C} =$ constant. Therefore (1) reduces to an equation for c:

$$\frac{\partial c}{\partial t} + u_i \frac{\partial c}{\partial x_i} = D_v \nabla^2 c \tag{4}$$

Multiplying (4) by c, averaging, using mass conservation to get u_i inside the derivative, and invoking homogeneity, one converts (4) to (*1*)

$$\frac{d}{dt}\overline{c^2} = -2 D_v \overline{\left(\frac{\partial c}{\partial x_j}\right)\left(\frac{\partial c}{\partial x_j}\right)} \tag{5}$$

The corresponding decay equation for a typical velocity component in isotropic turbulence was given by Taylor (*2*):

$$\frac{d}{dt}\overline{u_1^2} = -2 \nu \overline{\left(\frac{\partial u_1}{\partial x_K}\right)\left(\frac{\partial u_1}{\partial x_K}\right)} \tag{6}$$

Although the turbulent velocity does not appear explicitly in (5), its mixing action is of course felt through the concentration gradients; the random convection tends to steepen the gradients, thereby tending to increase the mean-square derivatives. This in turn accelerates molecular transport.

It is convenient, following Taylor, to replace the derivative products by defining characteristic lengths, the microscales, such that (5) and (6) are written as

$$\frac{d\overline{c^2}}{dt} = -12 D_v \frac{\overline{c^2}}{l^2} \tag{7}$$

$$\frac{d\overline{u_1^2}}{dt} = -20 \nu \frac{\overline{u_1^2}}{\lambda_f^2} \tag{8}$$