Separation Science and Technology
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713708471

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To cite this Article Kim, Jeung Kun and Ju, Dong Pyo(2000) 'Simulation of a Multicomponent Batch Distillation Column with Total Reflux through the Distillate Receiver', Separation Science and Technology, 35: 10, 1517 — 1537
To link to this Article: DOI: 10.1081/SS-100100239
URL: http://dx.doi.org/10.1081/SS-100100239

SEPARATION SCIENCE AND TECHNOLOGY, **35**(10), pp. 1517–1537, 2000

Simulation of a Multicomponent Batch Distillation Column with Total Reflux through the Distillate Receiver

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ABSTRACT

A shortcut procedure applicable to a multicomponent distillation in a batch column with a distillate receiver under total reflux condition was developed. It is based on the assumptions of constant molar overflow, constant vapor boilup rate, and constant relative volatilities. The effect of liquid holdup in each stage and condenser is taken into consideration in modeling the dynamic behavior of the batch column. Estimates of the volume of the distillate receiver, changes in compositions in the receiver and still, concentration profiles of the column, and total distillation time required to complete the separation can be made in the proposed model. Illustrative calculations were performed for the separation of a quaternary system for two cases: an initially empty distillate receiver and an initially filled-up distillate receiver.

Key Words. Shortcut procedure; Multicomponent batch distillation; Distillate receiver; Total reflux; Batch distillation time; Effect of holdup

1. INTRODUCTION

Batch distillation is becoming more important as a result of the recent increase in the production of high added value, low volume specialty chemicals and biochemicals. The flexibility in operation and the lower costs for the sep-

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aration of relatively pure components are the advantages of batch distillation over continuous distillation. The two basic modes of operation of a batch distillation column are (i) constant reflux and variable product composition and (ii) variable reflux and constant product composition. The transient or dynamic behavior of these columns can be analyzed either by rigorous stage-by-stage calculation methods (1–4) or by shortcut methods (5–12) which assume negligible vapor and liquid holdups and constant molar overflows.

Meadows (1) developed the first rigorous multicomponent batch distillation model, based on the assumptions of adiabatic equilibrium stages and constant molar liquid holdups for each stage and condenser. Distefano (2) extended the model and developed a computer-based method for solving a set of differential mass and energy balance equations. Seader (8) presented an excellent review of modeling of batch distillation columns. Recently Diwekar and Madhavan (9) presented shortcut methods for multicomponent batch distillation operation for two cases of constant reflux and constant distillate composition. Sundaram and Evans (10) also performed a simulation of the multicomponent batch distillation operations at constant reflux, under the same assumptions of constant molal overflow and negligible vapor and liquid holdups.

Another mode of operation of batch distillation columns was proposed by Treybal (11) for the separation of a binary mixture, and a detailed analysis of the dynamics has been reported. A conventional apparatus with a distillate receiver as depicted in Fig. 1 was used. The equipment setup has provision for total reflux. The batch charge is introduced into the still, and the level of the overflow reflux line is adjusted for the distillate receiver to hold a correct amount of distillate. Heat is then supplied, and distillation proceeds until the liquid in the distillate receiver, which becomes progressively richer in the light component, reaches the desired composition. The operation can be performed with the distillate receiver either initially empty or filled with the original batch charge. The advantages of this operating mode are (i) simplified equipment set-up because of no reflux control and (ii) no influence by the variation in the heating rate on either the yield or the quality of the products. Moreover, since the column operates under the total reflux condition, it operates at its maximum distillation capacity and less stages are required in comparison to the other mode of operation under a finite reflux ratio. Sørensen and Skogestad (12) found that total reflux operation was advantageous for separations with a small amount of light component.

For the purpose of extending Treybal's mode of operation for a binary mixture to a multicomponent system, Kim and Ju (13) proposed a shortcut calculation procedure based on the assumptions of constant molar overflow, constant relative volatilities, and negligible liquid and vapor holdups. The authors compared the simulation results with the experimental data obtained in the separation of a ternary mixture of benzene, toluene, and *o*-xylene. The agree-

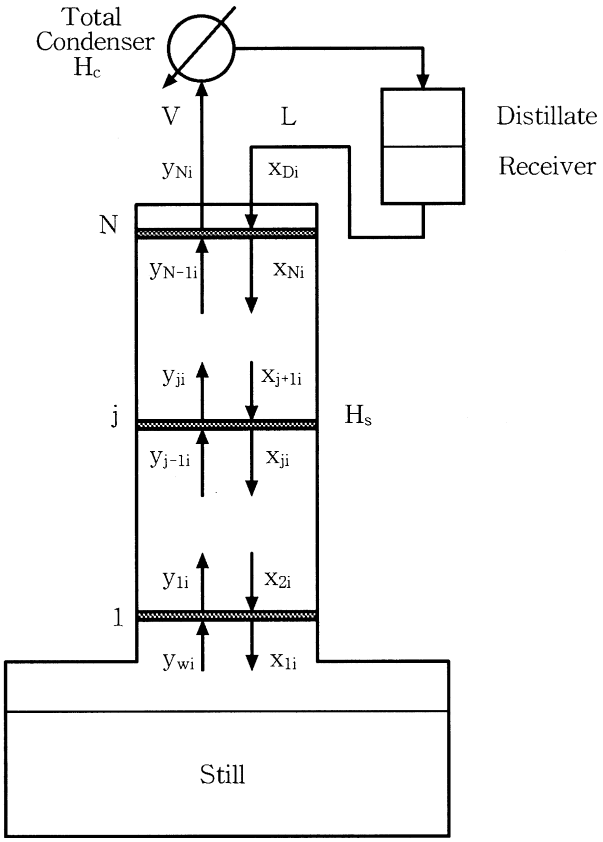

FIG. 1 Batch column with a distillate receiver.

ment between the theoretical and experimental results was considered satisfactory.

The objective of this study is to further develop a calculation procedure for a multicomponent batch distillation operation with a distillate receiver. In this model, liquid holdups in the column and the condenser were taken into consideration in simulating the dynamics of the column. With the desired product concentration of the lightest component in the distillate receiver specified, the calculation procedure for determining the characteristics of the operation, such as the volume of the distillate receiver, the variation of compositions in the distillate receiver and the still, the stagewise concentration profiles, and the distillation time necessary to complete the separation, will be presented for both cases of startup policies of the distillate receiver. In order to demonstrate the advantage of the mode of operation with distillate receiver over conventional constant reflux and variable reflux operations, the batch distillation times to obtain same amount and purity of distillate were compared.

2. ANALYSIS OF THE SYSTEM

2-1. Assumptions

In the analysis of dynamic behavior of a batch distillation column consisting of $N + 1$ theoretical stages including a still and a distillate receiver and operating under the total reflux mode, the following assumptions were made;

- Constant molal overflows
- Constant relative volatilities of the mixture:

$$\alpha_{in} = \text{constant}, \qquad i = 1, 2, \ldots, n \tag{1}$$

- Constant molar liquid holdups
- Negligible vapor holdups in the column and the condenser
- Constant vapor boilup rate
- Negligible heat loss from the column wall

2-2. Maximum Possible Distillate Concentration of the Lightest Component, $x_{\mathrm{D1}}^{\max}$

By the definition of the relative volatility between component i and n, the relations for the still and for the bottom plate are

$$\frac{x_{1i}}{x_{\mathrm{W}i}} = \alpha_{in} \frac{x_{1n}}{x_{\mathrm{W}n}} \tag{2}$$

$$\frac{x_{2i}}{x_{1i}} = \alpha_{in} \frac{x_{2n}}{x_{1n}} \tag{3}$$

The two relations lead to

$$\frac{x_{2i}}{x_{\mathrm{W}i}} = \alpha_{in}^{2} \frac{x_{2n}}{x_{\mathrm{W}n}} \tag{4}$$

and can be generalized for any stage as

$$\frac{x_{ji}}{x_{\mathrm{W}i}} = \alpha_{in}^{j} \frac{x_{jn}}{x_{\mathrm{W}n}}, \qquad i = 1, 2, \ldots, n-1; \qquad j = 1, 2, \ldots, N+1 \tag{5}$$

which is the Fenske equation for a multicomponent system when $j = N + 1$.

The material balances for the column are

$$\begin{aligned} &Dx_{\mathrm{D}i} + (W_0 - D - N \times H_{\mathrm{S}} - H_{\mathrm{C}})x_{\mathrm{W}i} \\ &\quad + H_{\mathrm{S}} \sum_{j=1}^{N} x_{ji} + H_{\mathrm{C}} x_{\mathrm{D}i} = W_0 x_{\mathrm{W}i}^{0}, \qquad i = 1, 2, \ldots, n-1 \end{aligned} \tag{6}$$

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The constraints imposed for the still, the receiver, and the plates are

$$\sum_{i=1}^{n} x_{\mathrm{W}i} = 1 \tag{7}$$

$$\sum_{i=1}^{n} x_{\mathrm{D}i} = 1 \tag{8}$$

and

$$\sum_{i=1}^{n} x_{ji} = 1, \qquad j = 1, 2, \ldots, N \tag{9}$$

The total number of equations in Eqs. (5) to (9) are $n(N + 2)$ with an equal number of variables ($x_{\mathrm{D}i}$, $x_{\mathrm{W}i}$, x_{ji}, $i = 1, \ldots, n$; $j = 1, \ldots, N$). Hence the maximum possible concentration of the lightest component in the distillate receiver, $x_{\mathrm{D}1}^{\max}$ can be calculated by solving the system of equations simultaneously under the restriction of

$$D = 0 \tag{10}$$

since the purity of the lightest component increases as the volume of the receiver decreases. In actual operation, the desired product concentration, $x_{\mathrm{D}1}^{\mathrm{F}}$ should be specified somewhat lower than $x_{\mathrm{D}1}^{\max}$ since a definite volume of the distillate product is taken in the receiver. The value of $x_{\mathrm{D}1}^{\max}$ is influenced by the amount of holdups in the column and the condenser as shown in Section 3.

2-3. Minimum Possible Still Concentration of the Lightest Component, $x_{\mathrm{W}1}^{\min}$

As distillation continues, the concentration of the lightest component in the still, $x_{\mathrm{W}1}$, decreases continuously. However, under given operating conditions, a lower limit of $x_{\mathrm{W}1}^{\min}$ always exists which differs according to the given $x_{\mathrm{D}1}^{\mathrm{F}}$ and holdup characteristics of the apparatus. The lower limit can be estimated by solving Eqs. (5) to (9) simultaneously over again, but in this case under the condition of

$$x_{\mathrm{D}1} = x_{\mathrm{D}1}^{\mathrm{F}} \tag{11}$$

2-4. Scaling of the Volume of the Distillate Receiver

This procedure also gives the volume of the distillate receiver, $D^{\max}$, corresponding to the product compositions $x_{\mathrm{D}1}^{\mathrm{F}}$ and $x_{\mathrm{W}1}^{\min}$. However, if these compositions are used as product purities, the distillation time will be theoretically infinite since the rate of change of compositions of the system slows down with time. Two alternative strategies may be possible in order to surmount the circumstance: (i) specification of the product purity for the still, x_{W1}^{F}, as somewhat higher value than x_{W1}^{min}, or (ii) specification of the actual volume of the receiver, D, somewhat lower than D^{max}. The selection is optional, and the latter strategy is used in this article. The actual volume of the receiver is specified by the relation

$$D = f_D \times D^{max} \tag{12}$$

where f_D is a scaling factor whose value is defined arbitrarily between 0 and 1. The variation of the distillation time due to the adjustment of the receiver volume is demonstrated in Section 3.

2-5. Operation with an Initially Empty Distillate Receiver

2-5-1. Analysis of the Regime of Rayleigh Distillation

Suppose the distillate receiver is initially empty. Then a time θ_1 will be required to condense D moles of vapor to fill the receiver:

$$\theta_1 = D/V \tag{13}$$

During this time period there will be no reflux and the contents of the still will undergo a Rayleigh distillation. The compositions of the distillate receiver and the still vary continuously during this period. Since the theoretical stages in the column play no role during Rayleigh distillation, the composition of the first drop of distillate deposited in the distillate receiver is in equilibrium with the composition of the initial charge. Hence the initial composition is estimated by the relation

$$x_{Di}^{0} = \frac{\alpha_{in}\, x_{Wi}^{0}}{\sum_{i=1}^{n} \alpha_{in}\, x_{Wi}^{0}} \tag{14}$$

The procedure for the estimation of the compositions of the receiver and the still when the receiver is first filled up with the condensate is as follows. If D'_i and W'_i are the number of moles of each component in the receiver and still, respectively, when the receiver just becomes full, the fractional vaporization of each component, φ_i, at this instant is given as

$$\varphi_i = \frac{D'_i}{W_i^0} = \frac{W_i^0 - W'_i}{W_i^0} = 1 - \left(\frac{W'_i}{W_i^0}\right) \tag{15}$$

Since a relation

$$\frac{W'_1}{W_1^0} = \left(\frac{W'_2}{W_2^0}\right)^{\alpha_{12}} = \cdots = \left(\frac{W'_i}{W_i^0}\right)^{\alpha_{1i}}$$

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or

$$\left(\frac{W'_i}{W^0_i}\right) = \left(\frac{W'_1}{W^0_1}\right)^{1/\alpha_{1i}}, \qquad i = 1, 2, \ldots, n \tag{16}$$

holds for a Rayleigh distillation, φ_i is obtained in terms of φ_1 as

$$\varphi_i = 1 - (1 - \varphi_1)^{1/\alpha_{1i}}, \qquad i = 1, 2, \ldots, n \tag{17}$$

The distillate is then

$$D = \sum_{i=1}^{n} D'_i = \sum_{i=1}^{n} W^0_i \varphi_i = \sum_{i=1}^{n} W^0_i [1 - (1 - \varphi_1)^{1/\alpha_{1i}}] \tag{18}$$

Since W^0_i, α_{1i}, and D are known, φ_l will be obtained from Eq. (18). Using φ_1, the distillate receiver and still compositions at the end of the Rayleigh distillation are calculated as

$$x'_{\mathrm{D}i} = \frac{D'_i}{D} = \frac{W^0_i \varphi_i}{D} = \frac{W^0_i}{D}\left[1 - (1 - \varphi_1)^{1/\alpha_{1i}}\right] \tag{19}$$

$$x'_{\mathrm{W}i} = \frac{W^0_i(1 - \varphi_i)}{W_0 - D} = \frac{W^0_i}{W_0 - D}(1 - \varphi_1)^{1/\alpha_{1i}} \tag{20}$$

During Rayleigh distillation the composition of the distillate receiver varies from $x^0_{\mathrm{D}i}$ to $x'_{\mathrm{D}i}$ while that of the still changes from $x^0_{\mathrm{W}i}$ to $x'_{\mathrm{W}i}$. The variation of the compositions in the receiver and the still can be estimated as follows. Let the amount of each component accumulated in the receiver by Rayleigh distillation up to the time $m\Delta t$ from startup be $D^{(\mathrm{m})}_i$ moles, where m is the time-increment index. When distillation starts, no distillate exists in the receiver. Then $D^{(0)}_i = 0$ and $D^{(\mathrm{m})}_i$ is estimated by the relation

$$D^{(\mathrm{m})}_i = D^{(\mathrm{m}-1)}_i + x^{(\mathrm{m}-1)}_{\mathrm{D}i} \times V \times \Delta t, \qquad m \geq 1 \tag{21}$$

from which the total distillate accumulated in the receiver and the amount of residue remaining in the still become respectively,

$$D^{(\mathrm{m})} = \sum_{i=1}^{n} D^{(\mathrm{m})}_i \tag{22}$$

and

$$W^{(\mathrm{m})} = W_0 - D^{(\mathrm{m})} \tag{23}$$

Then the compositions of the still and the receiver are calculated by

$$x^{(\mathrm{m})}_{\mathrm{W}i} = \frac{W_0 x^0_{\mathrm{W}i} - D^{(\mathrm{m})}_i}{W^{(\mathrm{m})}} \tag{24}$$

and

$$x_{\mathrm{D}i}^{(\mathrm{m})} = D_i^{(\mathrm{m})}/D^{(\mathrm{m})} \tag{25}$$

$x_{\mathrm{D1}}^{(\mathrm{m})}$ is then compared to x'_{D1}, and if $x_{\mathrm{D1}}^{(\mathrm{m})}$ is greater than x'_{D1}, calculation for the next time step is undertaken by substituting the newly obtained $x_{\mathrm{D1}}^{(\mathrm{m})}$ for $x_{\mathrm{D}i}^{(\mathrm{m}-1)}$ in Eq. (21). The calculation is repeated until $x_{\mathrm{D1}}^{(\mathrm{m})}$ becomes x'_{D1}.

2-5-2. Analysis of the Operation under Total Reflux

As distillation proceeds from this point, reflux runs down the column at the same molar rate as the molar vapor boilup rate. As distillation continues, the compositions of the distillate receiver, the still, and the plates vary continuously. The composition of the lightest component in the still, x_{W1}, becomes leaner and that of distillate receiver, x_{D1}, becomes richer, reaching the ultimate values of $x_{\mathrm{D1}}^{\mathrm{F}}$ and $x_{\mathrm{W1}}^{\mathrm{F}}$, respectively, at the end of distillation. This will require a time θ_2. The analysis of this process is as follows. A component material balance for each plate and the distillate receiver are

$$\frac{dx_{ji}}{dt} = \frac{V}{H_{\mathrm{S}}}(x_{j+1i} - x_{ji} + y_{j-1i} - y_{ji}), \qquad j = 1, 2, \ldots, N \tag{26}$$

$$\frac{\mathrm{dx}_{\mathrm{D}i}}{dt} = \frac{\mathrm{V}}{\mathrm{D}}(\mathrm{y}_{\mathrm{N}i} - \mathrm{x}_{\mathrm{D}i}) \tag{27}$$

In finite-difference form, these equations are

$$x_{ji}^{(\mathrm{k}+1)} = x_{ji}^{(\mathrm{k})} + \frac{V}{H_{\mathrm{S}}}\left[x_{j+1i}^{(\mathrm{k})} - x_{ji}^{(\mathrm{k})} + y_{j-1i}^{(\mathrm{k})} - y_{ji}^{(\mathrm{k})}\right]\Delta t, \qquad \mathrm{i} = 1, 2, \ldots, n-1; \qquad j = 1, 2, \ldots, N \tag{28}$$

$$x_{\mathrm{D}i}^{(\mathrm{k}+1)} = x_{\mathrm{D}i}^{(\mathrm{k})} + \frac{V}{D}\left[y_{\mathrm{N}i}^{(\mathrm{k})} - x_{\mathrm{D}i}^{(\mathrm{k})}\right]\Delta t, \qquad i = 1, 2, \ldots, n-1 \tag{29}$$

Then the compositions of the heaviest component are calculated by

$$x_{jn}^{(\mathrm{k}+1)} = 1 - \sum_{i=1}^{n-1} x_{ji}^{(\mathrm{k}+1)}, \qquad j = 1, 2, \ldots, N \tag{30}$$

$$x_{\mathrm{D}n}^{(\mathrm{k}+1)} = 1 - \sum_{i=1}^{n-1} x_{\mathrm{D}i}^{(\mathrm{k}+1)} \tag{31}$$

The expressions for still compositions can be obtained from material balances

$$x_{Wi}^{(k+1)} = \frac{\left[W_0 x_{Wi}^0 - D x_{Di}^{(k+1)} - H_S \sum_{j=1}^{N} x_{ji}^{(k+1)} - H_C y_{Ni}^{(k+1)}\right]}{(W_0 - D - NH_S - H_C)}, \tag{32}$$

$$i = 1, 2, \ldots, n-1$$

and

$$x_{Wn}^{(k+1)} = 1 - \sum_{i=1}^{n-1} x_{Wi}^{(k+1)} \tag{33}$$

In Eqs. (28) to (33), k is the time-increment index. For a given time increment Δt, $x_{ji}^{(k+1)}$, $x_{Di}^{(k+1)}$, and $x_{Wi}^{(k+1)}$ are computed for each component from Eqs. (28) and (30), (29) and (31), and (32) and (33), respectively. The vapor compositions, $y_{ji}^{(k)}$, in Eqs. (28), (29), and (32) are calculated from the relations

$$y_{ji}^{(k)} = \frac{\alpha_{in} x_{ji}^{(k)}}{\sum_{i=1}^{n} \alpha_{in} x_{ji}^{(k)}}, \qquad j = 1, 2, \ldots, N \tag{34}$$

$$y_{j-1i}^{(k)} = y_{Wi}^{(k)} = \frac{\alpha_{in} x_{Wi}^{(k)}}{\sum_{i=1}^{n} \alpha_{in} x_{Wi}^{(k)}}, \qquad j = 1 \tag{35}$$

Calculations are initiated at $k = 0$. At that instant, $x_{Di}^{(k)} = x_{Di}^{(0)} = x'_{Di}$ and $x_{Wi}^{(k)} = x_{Wi}^{(0)} = x'_{Wi}$. However, the calculation procedure requires initial values of liquid compositions for each stage, $x_{ji}^{(0)}$. It is not easy to correctly estimate the initial composition profile of the liquid streams at the precise moment of the onset of reflux flow. In this article, $x_{ji}^{(0)}$ are taken arbitrarily by assuming a linear variation of liquid compositions between x'_{Di} and x'_{Wi}. Initial vapor compositions corresponding to $x_{ji}^{(0)}$ are then calculated from Eqs. (34) and (35), and these are substituted into Eqs. (28) through (33) to estimate new compositions of $x_{Di}^{(k+1)}$, $x_{ji}^{(k+1)}$, and $x_{Wi}^{(k+1)}$. The value $x_{D1}^{(k+1)}$ is then compared to x_{D1}^{F}, and if $x_{D1}^{(k+1)}$ is smaller than x_{D1}^{F}, a new calculation for the next time step is undertaken by substituting the values of $x_{ji}^{(k+1)}$ and $x_{Di}^{(k+1)}$ in place of $x_{ji}^{(k+1)}$ and $x_{Di}^{(k+1)}$ in Eqs. (28) and (29), respectively. The calculation procedure is repeated until $x_{D1}^{(k+1)}$ is greater than or equal to the specified concentration of x_{D1}^{F}. Counting the number of the time-increment index, k, the distillation time required for total reflux operation is calculated by

$$\theta_2 = k\Delta t \tag{36}$$

TABLE 1
Base Conditions for Sample Calculations

Amount of batch charge	$W_0 = 100$ mol			
Initial feed compositions	$X_{W1}^0 = 0.30,$	$X_{W2}^0 = 0.25,$	$X_{W3}^0 = 0.20,$	$X_{W4}^0 = 0.25$
Relative volatilities	$\alpha_{14} = 3.0,$	$\alpha_{24} = 2.0,$	$\alpha_{34} = 1.5$	
Number of equilibrium stages	$N = 5$			
Liquid holdups	$H_S = 1.0$ mol	$H_C = 1.0$ mol		
Vapor boilup rate	$V = 100$ mol/h			
Desired product purity	$X_{D1}^F = 0.85$			
Scaling factor	$f_D = 0.95$			

from which the total distillation time is

$$\theta = \theta_1 + \theta_2 \tag{37}$$

where Δt is the size of the time increment which affects the accuracy of the numerical integration. For the system and conditions shown in Table 1, Δt can be varied up to 0.005 hour. However, an arbitary value of 0.001 hour was used for Δt in this study. The step-by-step calculation procedure is shown in Fig. 2.

2-6. Operation with the Distillate Receiver Initially Filled-up

An alternate procedure is to start the operation with the distillate receiver filled-up with the same liquid as is used for the initial charge. In this procedure the operation is carried out entirely under the condition of total reflux ($\theta = \theta_2$). Analysis of this mode of operation is analogous to that of operation with the receiver initially empty. Equations (26) to (35) are applied again with initial values of $x_{Wi}^{(0)} = x_{Wi}^{(0)}$ and $x_{Di}^{(0)} = x_{Wi}^{(0)}$. The calculation procedure is also summarized in Fig. 2.

3. SIMULATION FOR A QUATERNARY COLUMN

Under the assumptions set out in Section 2-1, the calculation method proposed in this study is applicable to any multicomponent batch distillation operation with a distillate receiver regardless of the number of components in the system. The results of simulation and related discussions for a quaternary column are presented in this article. The base conditions for the sample calculations are summarized in Table 1.

Prior to the start of simulation, the validity of the specified product purity must be checked since x_{D1}^F must be lower than $x_{D1}^{\max}$. By solving Eqs. (5) to (9)

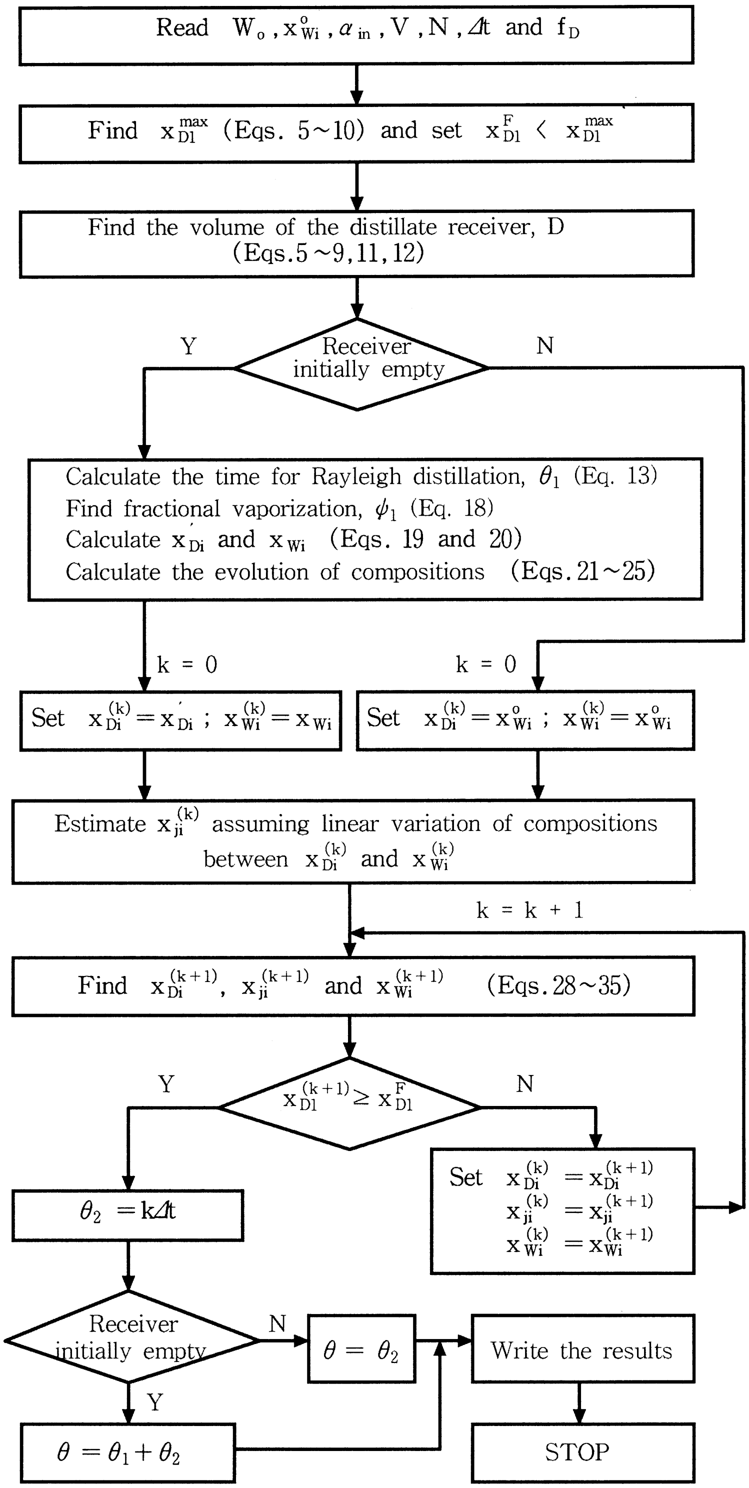

FIG. 2 Flow chart for shortcut calculation.

simultaneously under the condition of $D = 0$, one finds $x_{D1}^{max} = 0.9131$. Thus the specified separation is feasible.

Figure 3 represents the effect of varying the liquid holdup in the column and condenser on x_{D1}^{max}. Since x_{D1}^{max} decreases continuously as the liquid holdup grows, exact estimation of the amount of the total liquid holdup will be important when a high purity distillate is desired. Estimation of x_{W1}^{min} corresponding to x_{D1}^{F} may be worthwhile since x_{W1}^{min} can be specified in place of adjusting the volume of the receiver. Figure 4 shows the variation of x_{W1}^{min} according to x_{D1}^{F} and the tray and condenser liquid holdup. The value x_{W1}^{min} diminishes as x_{D1}^{F} is lowered and/or holdup increases. It seems that the effect of liquid holdup on x_{W1}^{min} is not significant in the case of holdups we tested ($H_S = H_C = 0$–3 mol), but the effect would be considerable if the plate holdup and/or the number of stages in the column were to be increased.

The solution of the simultaneous Eqs. (5) to (9) for the specified purity of x_{D1}^{F} gives the maximum volume of the distillate receiver, D^{max}, as 16.30 moles. Figure 5 represents the variation of D^{max} due to x_{D1}^{F} and the holdup. The amount of D^{max} is dependent primarily upon the specified value of x_{D1}^{F}, but the effect of the liquid holdup is not negligible. The maximum receiver volume decreases gradually as x_{D1}^{F} increases. Figure 5 shows that $D^{max} = 0$ when x_{D1}^{F} is specified to its maximum value, x_{D1}^{max}.

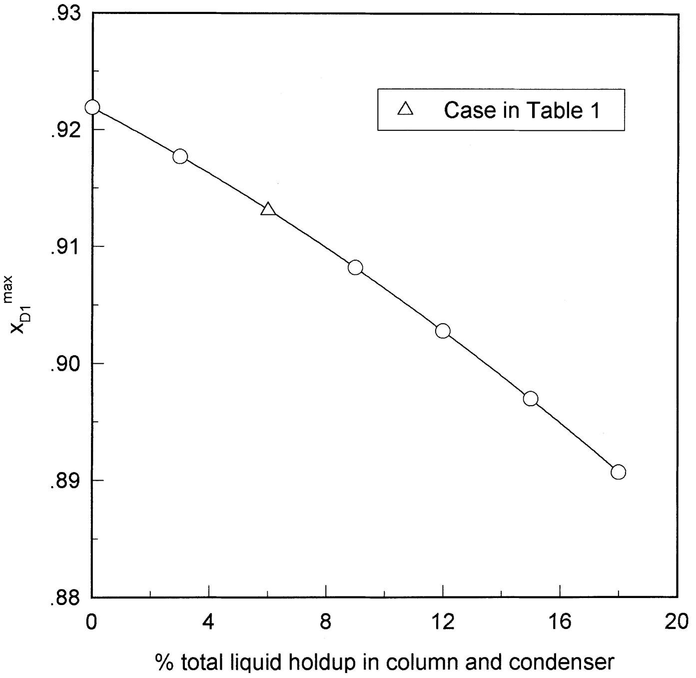

FIG. 3 Effect of % total liquid holdup in the column and condenser on maximum distillate composition, x_{D1}^{max}.

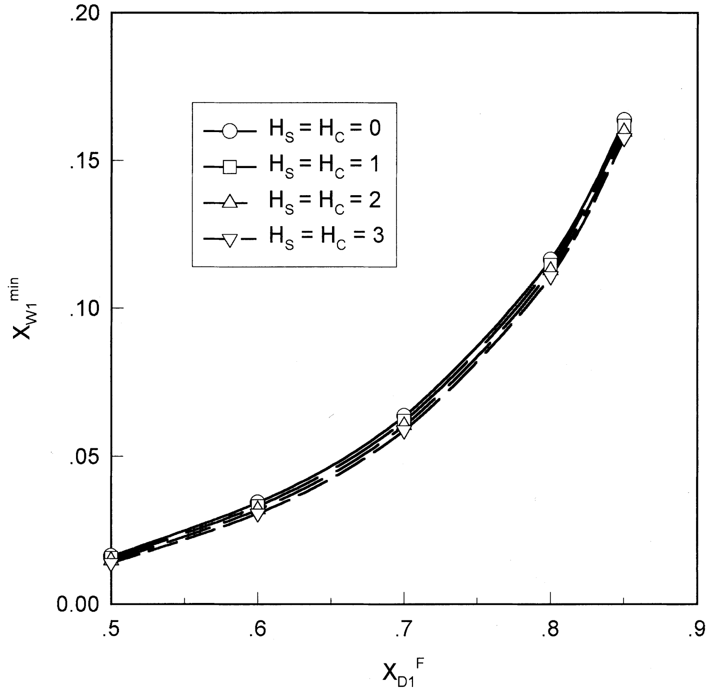

FIG. 4 Variation of the minimum concentration of the lightest component in the still corresponding to the specified distillate composition and holdups for the case in Table 1.

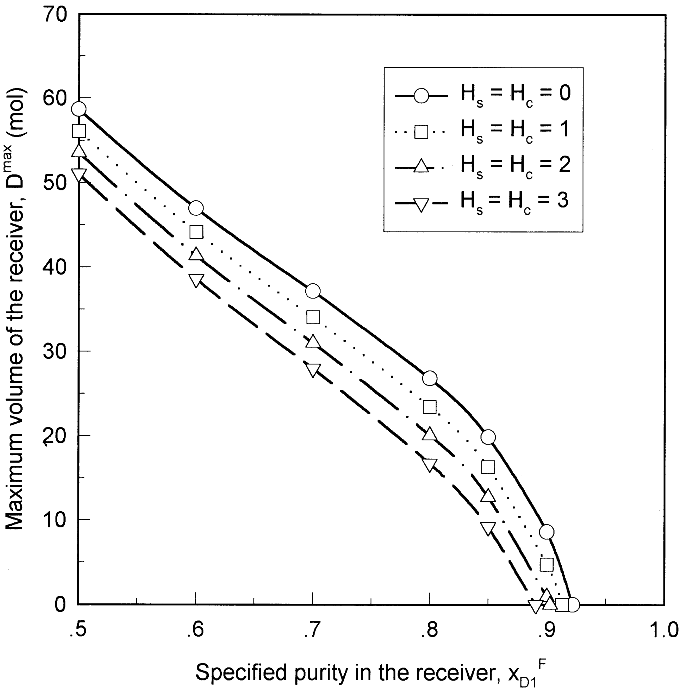

FIG. 5 Maximum volume of the distillate receiver corresponding to the specified purity in the receiver and holdups for the case in Table 1.

As explained in Section 2-4, the distillation time can be shortened considerably by making the volume of the distillate receiver smaller than $D^{\max}$. Figure 6 shows the variation of the batch times due to scaling down the volume of the receiver. The batch time is different according to a specified value of x_{D1}^{F} but in any case the batch time can be shortened considerably if one ignores the gain of a few percent in the maximum volume of the distillate. For example, a batch time of 5.39 hours is required in order to obtain 16.30 moles ($D^{\max}$) of the distillate at a purity of $x_{D1}^{F} = 0.85$. But if one uses a scaling factor of 0.95 ($D = 15.49$ moles), the required time is reduced to 2.61 hours, which is less than half the batch time for $D^{\max}$.

Figure 7 shows the changes in compositions in the receiver and still when the receiver is initially empty. In this case the contents in the still undergo a Rayleigh distillation during $\theta_1 = D/V = 0.95\ D^{\max}/V = 0.155$ hour from startup. The composition of component 1 in the distillate receiver changes from $x_{D1}^{0} = 0.4615$ to $x'_{D1} = 0.4470$ during this period. From this instant the distillation continues under total reflux condition and x_{D1} becomes richer continuously, until ultimately x_{D1} becomes x_{D1}^{F}. The time required for total reflux operation (θ_2) was found to be 2.46 hours. Summation of θ_1 and θ_2 gives the total distillation time as 2.61 hours.

As mentioned in Section 2-6, the operation can be performed with the distillate receiver initially filled-up with the original batch charge. Figure 8

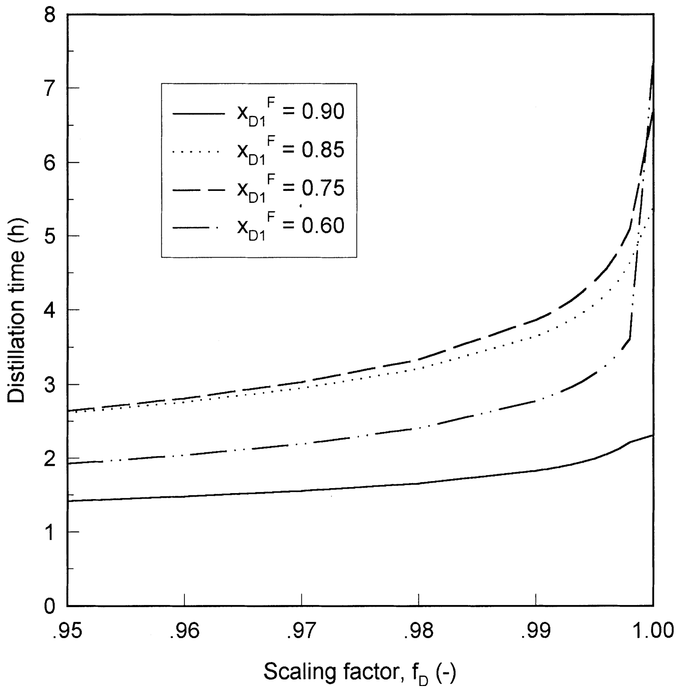

FIG. 6 Effect of scaling down of the volume of the distillate receiver on batch distillation time for the case in Table 1. The receiver is initially empty. $H_S = H_C = 1.0$ mol.

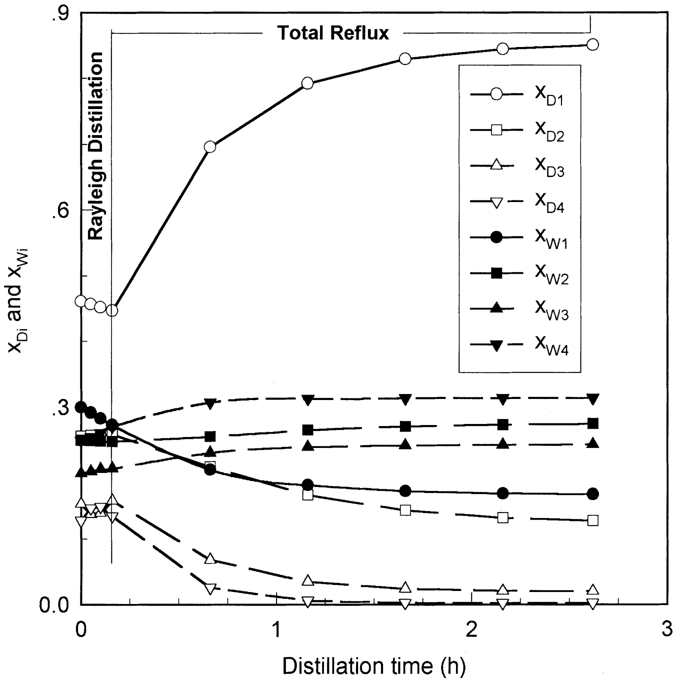

FIG. 7 Changes in compositions in the distillate receiver and the still for $x_{D1}^{F} = 0.85$, $H_S = H_C = 1.0$ mol and $f_D = 0.95$. The receiver is initially empty.

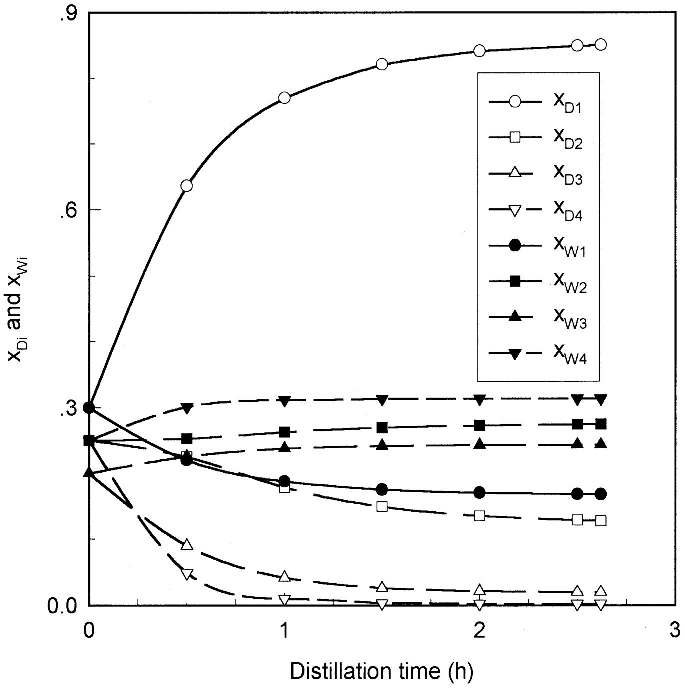

FIG. 8 Changes in compositions in the distillate receiver and the still for $x_{D1}^{F} = 0.85$, $H_S = H_C = 1.0$ mol and $f_D = 0.95$. The receiver is initially filled-up with the batch charge.

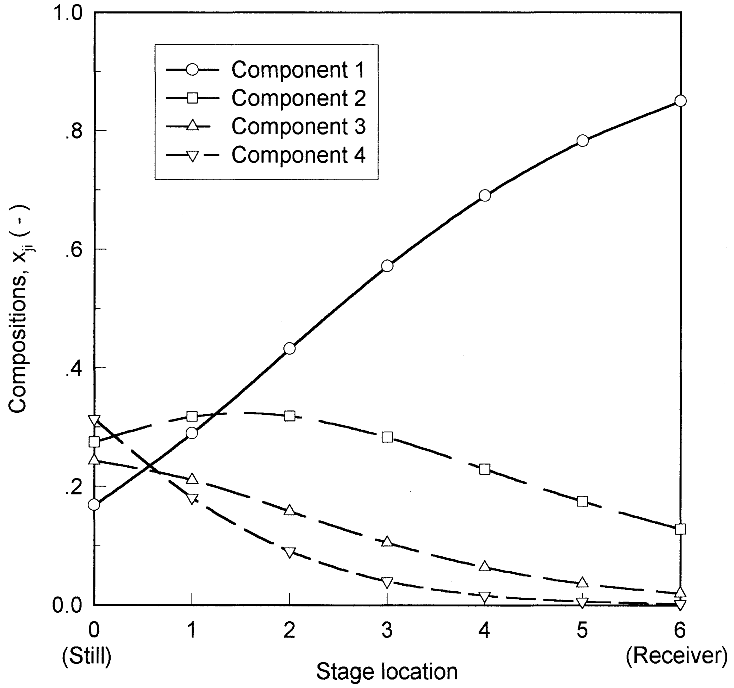

FIG. 9 Composition profiles of the liquid phase at the end of distillation ($x_{D1}^{F} = 0.85, f_D = 0.95$).

shows the trends of the composition change in the distillate receiver and the still. Since the period of Rayleigh distillation does not exist in this case, x_{D1} increases directly from x_{W1}^{0} to x_{D1}^{F}, and the distillation time required in this case is equal to θ_2, which amounts to 2.62 hours.

Figure 9 represents the stagewise composition profiles of the liquid phase at the end of distillation. Naturally, the final profiles are the same regardless of the initial condition of the distillate receiver. Concentration of the lightest component increases continuously from the still toward the receiver while the trend is reversed for the heaviest component. The profile for component 2 shows a maximum concentration in the column, which is typical for a component of intermediate volatility in multicomponent distillations.

4. COMPARISON OF BATCH DISTILLATION TIMES

The batch distillation times required for several specifications of x_{D1}^{F} and f_D are compared in Table 2 for the two initial condition cases of the distillate receiver we investigated. It shows that in all cases of x_{D1}^{F} considered, the total distillation time θ increases as f_D or D increases. It appears that when the volume of the receiver is relatively small, operation using a distillate receiver initially filled-up with the original batch charge takes a little more distillation time θ than does a receiver initially empty. The difference in batch time between the two cases diminishes and then reverses as the volume of the receiver becomes more important. However, Table 2 reveals that the differences are not significant, and it can be concluded, from a practical point of view, that the initial condition of the receiver is not critical for the batch distillation time.

TABLE 2
Comparison of Distillation Times

			Initial state of distillate receiver			
			Empty			Filled-up
X_{D1}^{F}	f_D	D (mol)	θ_1 (h)	θ_2 (h)	θ (h)	θ (h)
0.90	1.0	4.76	0.048	2.26	2.31	2.33
	0.99	4.71	0.047	1.78	1.83	1.85
	0.98	4.67	0.047	1.61	1.66	1.67
	0.97	4.62	0.046	1.51	1.55	1.57
	0.96	4.57	0.046	1.43	1.48	1.50
	0.95	4.52	0.045	1.37	1.42	1.44
0.85	1.0	16.30	0.163	5.23	5.39	5.40
	0.99	16.14	0.161	3.48	3.64	3.65
	0.98	15.98	0.160	3.05	3.21	3.21
	0.97	15.81	0.158	2.79	2.95	2.95
	0.96	15.65	0.157	2.60	2.76	2.77
	0.95	15.49	0.155	2.46	2.61	2.62
0.80	1.0	23.46	0.235	6.30	6.53	6.53
	0.99	23.22	0.230	3.77	4.00	4.00
	0.98	22.99	0.230	3.25	3.48	3.47
	0.97	22.76	0.228	2.94	3.17	3.16
	0.96	22.52	0.225	2.72	2.95	2.94
	0.95	22.29	0.223	2.55	2.78	2.77
0.70	1.0	34.07	0.341	5.99	6.33	6.30
	0.99	33.73	0.337	3.18	3.52	3.48
	0.98	33.39	0.334	2.71	3.04	3.01
	0.97	33.05	0.331	2.43	2.77	2.73
	0.96	32.71	0.327	2.24	2.57	2.54
	0.95	32.37	0.324	2.09	2.42	2.39
0.60	1.0	44.14	0.441	6.95	7.39	7.34
	0.99	43.70	0.437	2.33	2.77	2.70
	0.98	43.26	0.433	1.97	2.41	2.34
	0.97	42.82	0.428	1.76	2.19	2.13
	0.96	42.38	0.424	1.62	2.04	1.98
	0.95	41.94	0.419	1.50	1.92	1.87

Comparison of differences in the batch time due to different modes of operation may be useful to highlight the preference of the operation with a distillate receiver compared to conventional constant reflux or variable reflux operation. Figure 10 shows the variation of batch times for these three modes of operation when the purity of the lightest component in the distillate was specified at 0.85. The batch times for the constant reflux and variable reflux operation, which have an equilibration time of 0.8 hour, were calculated by using a batch distillation simulation package, MultiBatch *DS*. The results show that when the receiver volume is in the neighborhood of its maximum value (16.30 moles), the batch times necessary for the operation with a distillate receiver are longer than the batch times for conventional operations. But if the receiver volume is smaller than 15 moles ($f_D < 0.92$), operation with a distillate receiver takes a shorter time to complete the desired separation. Since the batch times are influenced by the product purity, the amount of distillate, and the relative volatilities of the system, it is not easy to draw a general conclusion on the relative preference between the different modes of operation in regard to the batch distillation time. However, if one desires a distillate with a high degree of purity, one can expect that the mode of operation with a distillate receiver is more suitable for separation since the conventional modes of operation must run at a high reflux ra-

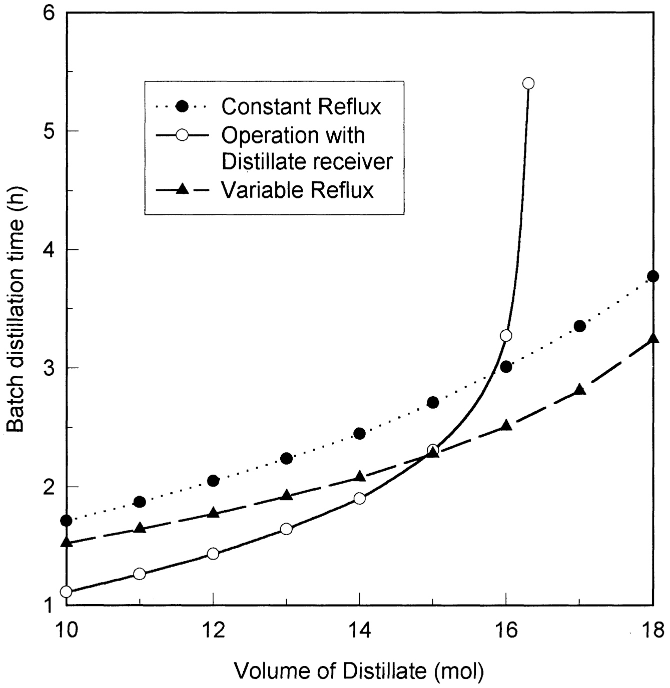

FIG. 10 Comparison of batch distillation times under different modes of operation. The purity of component 1 in the distillate is 0.85.

tio, which results in slow production rate of the distillate needed to meet the required product purity.

5. CONCLUSIONS

Based on the assumptions of constant molal overflows, constant relative volatilities, and constant vapor boilup rates, a calculation method was developed to simulate a multicomponent batch distillation column equipped with a distillate receiver which operates under total reflux condition. Unlike other shortcut methods, the calculation method proposed in this study does not neglect the liquid holdups in the column and the condenser. To start the simulation, the values of some parameters (such as the number of equilibrium stages in the column, amount of the initial batch charge, initial feed compositions, relative volatilities of the system, and a vapor boilup rate) have to be provided. The model first estimates the highest composition of the lightest component in the distillate receiver theoretically attainable under given operating conditions. In consideration of this maximum composition, actual distillate purity and a scaling factor to adjust the volume of the receiver are specified as inputs. Then the proposed model readily estimates the volume of the receiver, the variation of compositions in the receiver and the still, composition profiles of the column, and the total distillation time required to complete the separation for the two cases of the receiver initially empty and initially filled-up with the original batch charge. The calculation procedure was demonstrated for an illustrative example of a quaternary system.

The primary advantage of batch distillation with total reflux through a distillate receiver over conventional constant reflux or variable reflux operation is its expediency. In principle, this mode of operation is applicable to any multicomponent batch distillation used to separate the lightest component from a feed mixture. But it would be more suitable for small-scale distillation operations when the desired product purity is high and the required number of theoretical stages is not important. The calculation procedure developed herein is convenient and useful for those situations.

NOMENCLATURE

D	volume of distillate receiver (mol)
D_i	amount of component i in distillate receiver during Rayleigh distillation (mol)
D_i'	amount of component i in distillate receiver when the receiver is first filled by Rayleigh distillation (mol)
f_D	scaling factor
H_C	liquid holdup in total condenser (mol)

H_S	liquid holdup in each plate (mol)
i	component
k	time-increment index for distillation under the total reflux condition
L	flow rate of liquid phase (mol/h)
N	number of equilibrium stages in column
n	number of components in feed mixture, or heaviest component
t	time (h)
V	vapor boilup rate (mol/h)
W'_i	amount of component i in still when the receiver is first filled by Rayleigh distillation (mol)
W_i^0	amount of component i in feed mixture (mol)
W_0	amount of feed mixture (mol)
x_{D1}^F	specified product purity of the lightest component in distillate receiver
x_{D1}^{max}	maximum possible concentration of the lightest component in distillate receiver
x_{Di}	mole fraction of component i in distillate receiver
x'_{Di}	mole fraction of component i when the distillate receiver just becomes full by Rayleigh distillation
x_{ji}	mole fraction of component i in liquid phase from stage j
x_{W1}^F	final concentration of the lightest component in still
x_{W1}^{min}	minimum possible concentration of the lightest component in still
x_{Wi}	mole fraction of component i in still
x'_{Wi}	mole fraction of component i in still when the distillate receiver just becomes full by Rayleigh distillation
x_{Wi}^0	initial concentration of the batch charge
y_{ji}	mole fraction of component i in vapor phase from stage j

Superscripts

k	time-increment index for the distillation under total reflux condition
m	time-increment index for Rayleigh distillation
max	maximum

Greek Symbols

α_{in}	relative volatility between component i and n
Δt	time increment with a default value of 0.001 (h)
θ	total distillation time (h)
θ_1	time required for Rayleigh distillation (h)
θ_2	time required for total reflux operation (h)
φ_i	fractional vaporization of component i when the receiver is first full

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Received by editor January 26, 1999
Revision received December 1999

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