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## Single-Stage Contribution to the Overall Separation in Binary Multistage Distillation

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### Abstract

The contributions of individual stages to the overall separation obtained in a multistage distillation column are calculated by taking the difference between the cumulative extent of separation for successive stages. The calculations clearly show how the reflux ratio effects the number of stages required for the separation, the contribution of individual stages to the overall separation, and how the stage contributions are distributed as the number of stages required to make the separation decreases with increasing reflux ratio. The individual stage contribution is closely related to the stage-wise derivative of the cumulative extent of separation.

### INTRODUCTION AND BACKGROUND

Rony's extent of separation,  $\xi_s$  (1), varies little with stage number and reflux ratio when it is applied to individual equilibrium stages in a multistage distillation column when separating a binary mixture with constant relative volatility. For example, for  $\alpha = 2.0$ ,  $\xi_s$  varies between 0.16670 and 0.17157 between the minimum and total reflux conditions, a difference of only about 3% (2, 3). The variation in  $\xi_s$  is even smaller for more difficult separations. However, the number of stages required to make a separation decreases rapidly when the reflux ratio is increased from the minimum up to the optimum; that is, the same separation is obtained using fewer stages. Thus the contribution of individual stages to the overall separation must change with the reflux ratio. This paper examines this contribution to the overall separation obtained in a multistage distillation column, and the dependence of the stage separation on reflux ratio and relative volatility.

## CUMULATIVE EXTENT OF SEPARATION AND SINGLE-STAGE CONTRIBUTION IN MULTISTAGE

Questions involving the contribution of individual stages to multistage separations can be answered by analyzing the separation in terms of the cumulative extent of separation,  $\xi_N$ . This separation factor is a modification of Rony's single equilibrium stage index, applied to successive multistage sections of the column (2).

For two components  $i = 1, 2$  distributed between two regions  $j = k, m$  as a result of a separation process,  $n_{ij}$  is the number of moles of component  $i$  in region  $j$ . The distribution ratio for component  $i$  is defined as

$$K_i = \frac{n_{im}}{n_{ik}} \quad (1)$$

For an equilibrium stage the relative volatility in terms of these distribution ratios is given by

$$\alpha = K_2 / K_1 \quad (2)$$

For an equilibrium stage within a distillation column, the two regions of interest are the vapor (Region 1) and the liquid (Region 2), leaving the stage in equilibrium with each other. For this stage  $\xi_s$  is given by

$$\xi_s = \left| \frac{1}{1 + K_1} - \frac{1}{1 + K_2} \right| \quad (3)$$

For a multistage column the two regions of interest are the distillate and bottoms product streams leaving the column. However, in analyzing the performance of the column, it is necessary to consider the vapor (Region 3), and liquid (Region 4) streams leaving a multistage section within the column as shown in Fig. 1. This must be done because, within the column where the separation is taking place, the flow rates of the vapor and liquid streams are not the same as the flow rates of the product streams because of the reflux.

For this case the cumulative extent of separation for the  $N$  stages within the column is given by

$$\xi_N = \left| \frac{1}{1 + K_{1N}} - \frac{1}{1 + K_{2N}} \right| \quad (4)$$

where

$$K_{1N} = \frac{n_{14}}{n_{13}} = \frac{\text{moles of Component 1 in the liquid leaving Stage 2}}{\text{moles of Component 1 in the vapor leaving Stage } N} \quad (5)$$

$$K_{2N} = \frac{n_{24}}{n_{23}} = \frac{\text{moles of Component 2 in the liquid leaving Stage 2}}{\text{moles of Component 2 in the vapor leaving Stage } N} \quad (6)$$

For simplification, the following assumptions are made:

- (a) Constant relative volatility
- (b) Constant molal overflow
- (c) Feed rate,  $F = 2$ ,  $X_{\text{Feed}} = 0.5$ , saturated liquid
- (d) Total condenser

Assume that the column is operating so that  $X_B = X(1) = 0.01$  and  $y_D = y(N) \geq 0.99$ . Equilibrium gives the composition of the vapor leaving Stage 1, the reboiler:

$$y(1) = \frac{\alpha X(1)}{1 + (\alpha - 1)X(1)} \quad (7)$$

A material balance gives the composition of the liquid leaving Stage 2, the first stage within the column:

$$X(2) = \frac{X(1) + (R + 1)y(1)}{(R + 2)} \quad (8)$$

The extent of separation for the entire multistage column shown in Fig. 1 with  $y(N) = 0.99$  is given by

$$\xi_{\text{COL}} = \left| \frac{1}{1 + K_{1NT}} - \frac{1}{1 + K_{2NT}} \right| \quad (9)$$

where

$$K_{1NT} = \frac{\left(\frac{R + 2}{R + 1}\right)X(2)}{0.99}, \quad K_{2NT} = \frac{\left(\frac{R + 2}{R + 1}\right)[1 - X(2)]}{0.01} \quad (10)$$

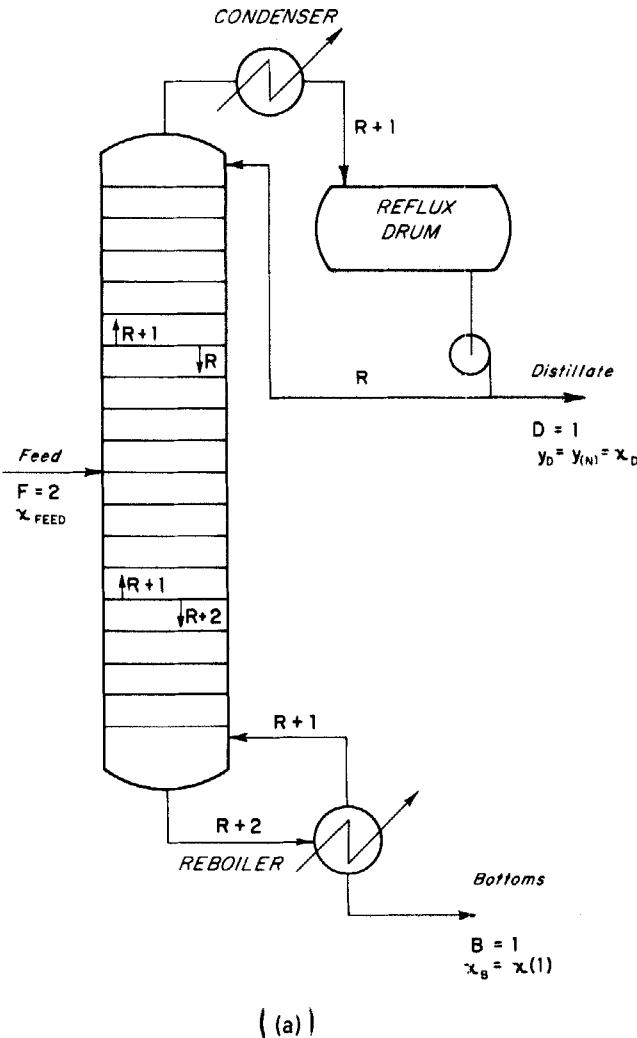
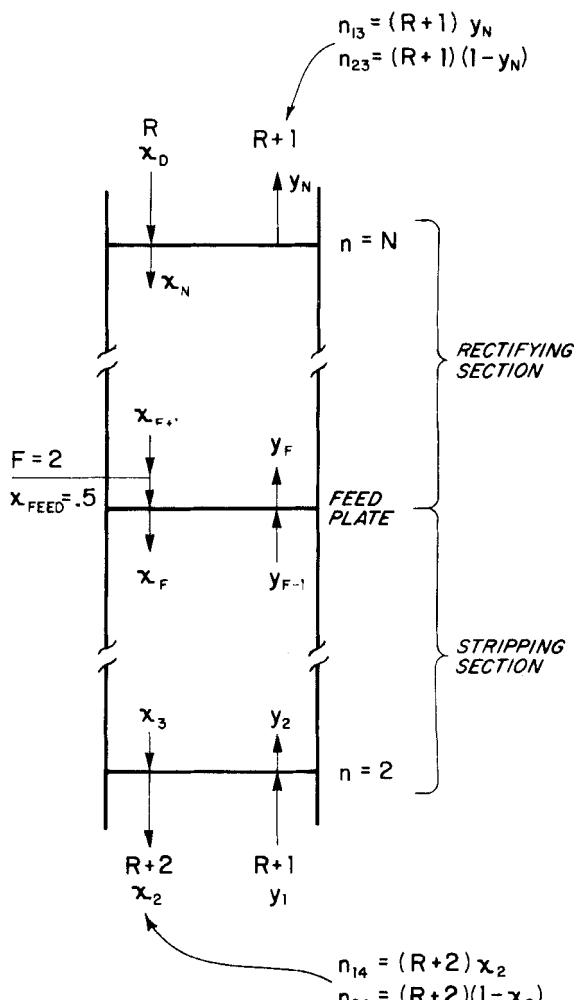


FIG. 1. Equilibrium stage distillation column showing a multistage section within the column.



(b)

FIG. 1 (continued)

$X(2)$  and hence  $\xi_{\text{Col}}$  are slightly different for each reflux ratio.

Proceeding stage-wise up the column for  $N = 2, \dots$ , including the feed stage:

$$X(N) = \frac{X_B + (R + 1)y(N)}{(R + 2)}, \quad y(N) = \frac{\alpha X(N)}{1 + (\alpha - 1)X(N)} \quad (11)$$

$$K_{1N} = \left( \frac{R + 2}{R + 1} \right) \frac{X(2)}{y(N)}, \quad K_{2N} = \left( \frac{R + 2}{R + 1} \right) \left[ \frac{1 - X(2)}{1 - y(N)} \right] \quad (12)$$

The cumulative extent of separation is given by

$$\xi_N = \left| \frac{1}{1 + K_{1N}} - \frac{1}{1 + K_{2N}} \right| \quad (13)$$

Here  $\xi_N$  represents the cumulative extent of separation by the  $N$  stages of the stripping section of the column, not including the reboiler.

The contribution of stage  $N$  to the extent of separation is given by

$$\delta(N) = \xi_N(N) - \xi_N(N - 1) \quad (14)$$

and the fractional contribution by

$$F(N) = \delta(N)/\xi_{\text{COL}} \quad (15)$$

This procedure is continued up the column to the feed tray where the stage liquid composition is closest to the feed composition,  $X_F = 0.5$  for this case. The calculations are then continued stage-wise up the rectifying section in a similar manner with the liquid stream composition given by a material balance:

$$X(N) = \frac{X_B + (R + 1)y(N - 1) - FX_{\text{Feed}}}{R} \quad (16)$$

Again,  $F(N)$  is calculated using Eqs. (12) through (15). Calculations are stopped when  $y(N) \geq 0.99$ . When  $y(N) = 0.99$ , the sum  $\sum_N F(N) = 1$  exactly.

These equations were programmed on a digital computer and calculations made for values of  $\alpha$  between 1.1 and 3.0 from the minimum reflux ratio up to total reflux. The results are summarized in Figs. 2 through 9. In these figures, each curve represents a distillation column operating at a different

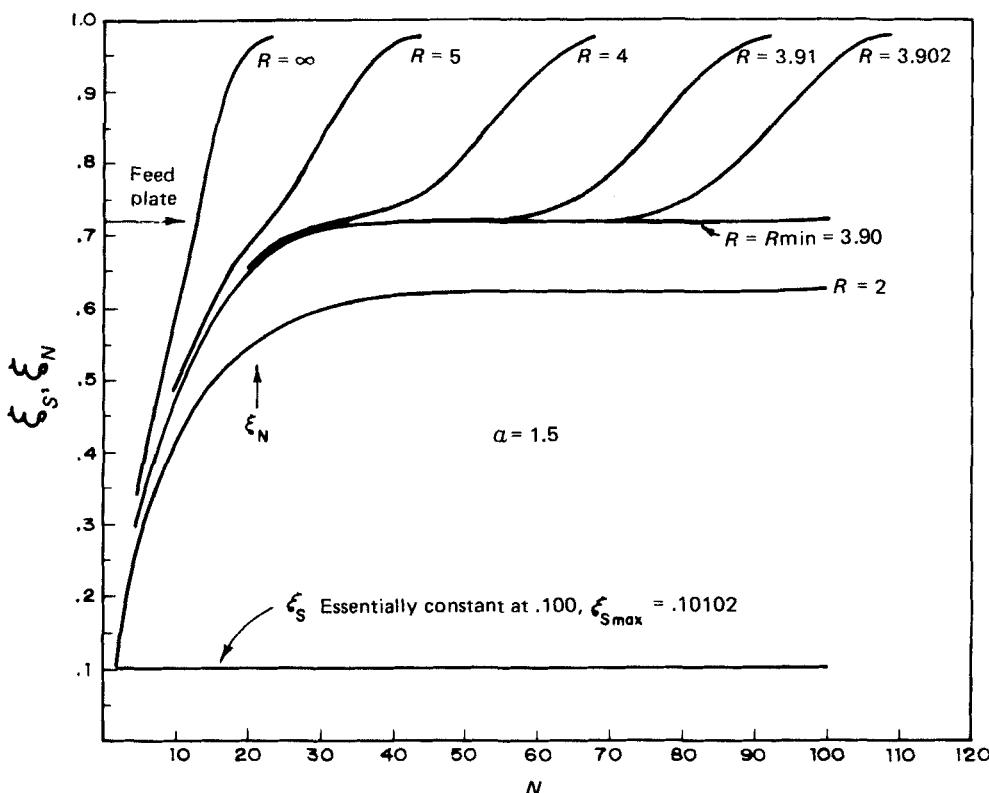


FIG. 2. Cumulative extent of separation and single-stage extent of separation as a function of stage number for various reflux ratios,  $\alpha = 1.5$ .

reflux ratio, and the number of stages required to make the separation is different for each case.

Figure 2 shows the typical ( $\alpha = 1.5$ ) cumulative extent of separation curves for different reflux ratios. Plots of this nature were first presented by McCandless (2). As can be seen from this plot, at reflux ratios less than or equal to the minimum, there is a pinch zone in the stripping section of the column. Under minimum reflux conditions an infinite number of stages would be required to reach the feed composition, while at reflux ratios below the minimum the pinch zone will be below the feed stage at a composition less than that of the feed. At reflux ratios only slightly greater than the minimum, it takes a large number of stages to increase the composition over that in the pinch zone at minimum reflux. At higher values of  $R$  there is no

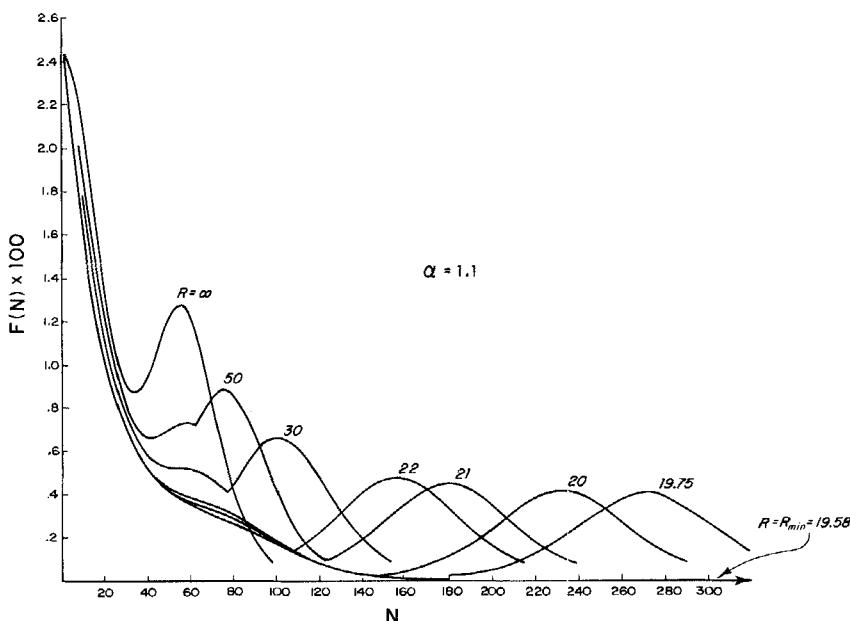


FIG. 3. Fractional separation as a function of stage number for various reflux ratios,  $\alpha = 1.1$ .

pronounced pinch zone to hinder the separation and  $\xi_N$  increases rapidly throughout the column.

Figures 3 through 5 show how  $F(N)$  varies with stage number and  $R$ . As can be seen,  $F(N)$  starts at a relatively high value at  $N = 2$  and, at constant reflux ratio, decreases rapidly in the stripping section of the column. At  $R = R_{\min}$ ,  $F(N)$  rapidly approaches zero in the stripping section of the column and the separation cannot be made even with an infinite number of stages because of the pinch zone approaching the feed stage. For  $R > R_{\min}$ ,  $F(N)$  also rapidly decreases in the stripping section, but after reaching a minimum value at the feed stage it increases and goes through a relative maximum in the rectifying section. At higher values of  $R$ , there is also a relative maximum in the stripping section. The two maxima approach the same point as  $R \rightarrow \infty$ , where the number of stages required to make the separation is a minimum. The curves for all values of  $\alpha$  are similar, with the magnitude of  $F(N)$  increasing with  $\alpha$  since fewer stages are required to make the separation at higher reflux ratios.

The shapes of these curves are interesting because they are very similar to the  $d\xi_N/dN$  vs  $N$  curves presented in a previous paper (2). This point is further discussed in the total reflux section that follows.

Most of the separation occurs in the stripping section of the column as shown in Fig. 6. This plot shows the fraction of the total column separation occurring in the stripping section of the column, including the feed stage as a function of  $\alpha$ . This fraction varies somewhat for different values of  $R$ , and there is some variation because the liquid composition on the feed stage usually differs from the feed composition. As can be seen, the fractional separation for the  $N$  stages in the stripping section increases linearly from about 0.68 for  $\alpha = 1.1$  to 0.85 for  $\alpha = 3.0$ , although in all cases the stripping section, including the reboiler, contains only 50% of the total stages.

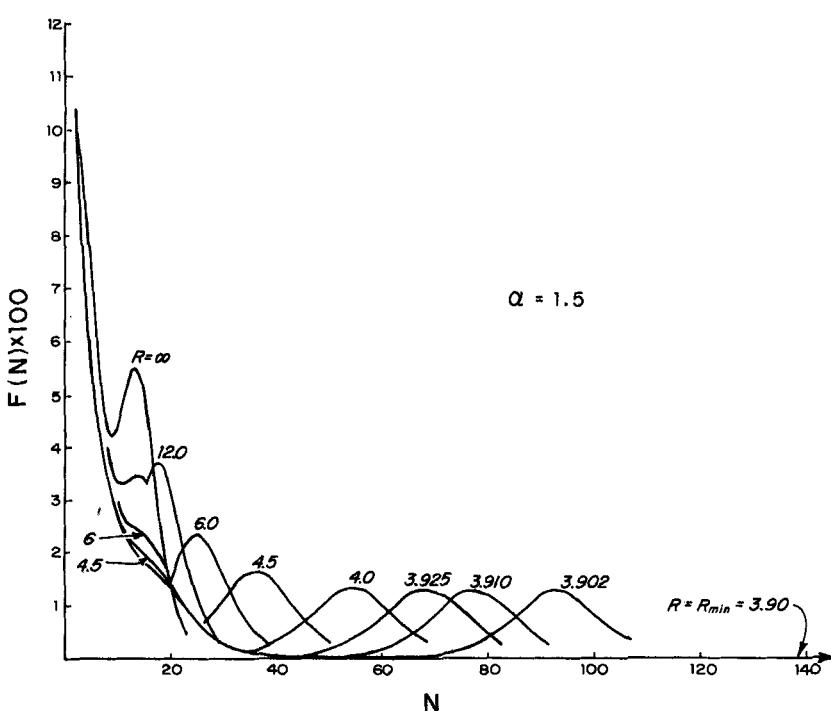


FIG. 4. Fractional separation as a function of stage number for various reflux ratios,  $\alpha = 1.5$ .

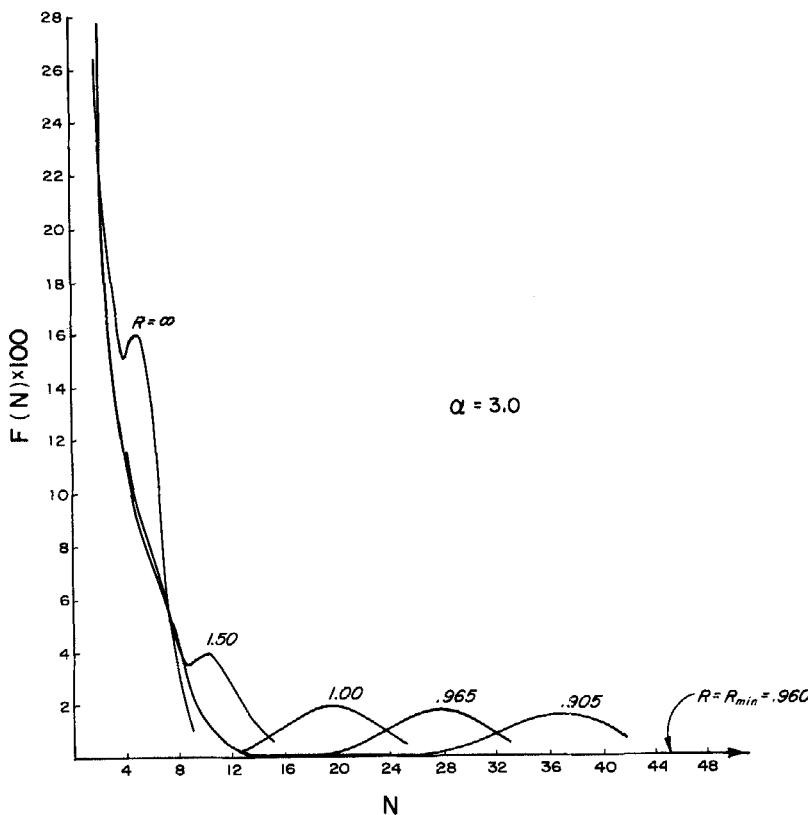


FIG. 5. Fractional separation as a function of stage number for various reflux ratios,  $\alpha = 3.0$ .

### TOTAL REFLUX CASE

As mentioned earlier, when  $F(N)$  is plotted vs  $N$  for a constant value of  $R$ , the shape of the curve is very similar to the shape of the  $d\xi_N/dN$  vs  $N$  curve. For the case of total reflux the equations for the  $\delta(N)$  and  $d\xi_N/dN$  curves can be easily compared by using the Fenske-Underwood equation in the calculations.

The Fenske-Underwood equation in re-arranged form yields a value for  $y(N)$  as a function of  $N$ :

$$y(N) = \frac{\left(\frac{X_B}{1-X_B}\right) \alpha^N}{1 + \left(\frac{X_B}{1-X_B}\right) \alpha^N} \quad (17)$$

A material balance at total reflux yields

$$X(N) = y(N-1) \quad (18)$$

The use of these values in Eqs. (13) and (14) yields the following:

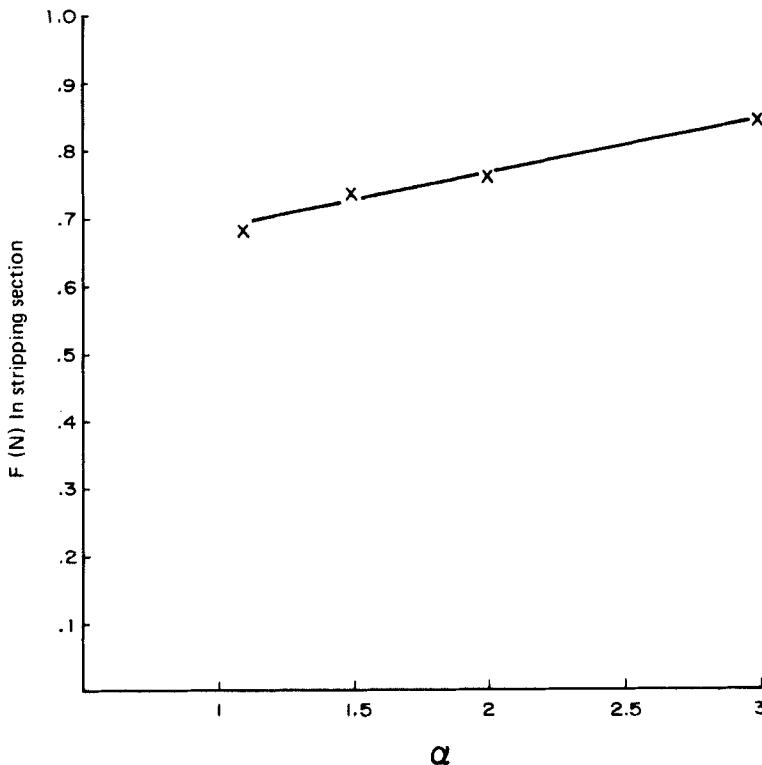


FIG. 6. Fraction of separation occurring in the stripping section as a function of relative volatility.

$$\xi_N(N) = \frac{\alpha^N}{(1 - X_B) + (1 + X_B)\alpha^N} - \frac{1}{(2 - X_B) + X_B\alpha^N} \quad (19)$$

$$\frac{d\xi_N}{dN} = \alpha^N \ln \alpha \frac{1 - X_B}{[(1 - X_B) + (1 + X_B)\alpha^N]^2} + \frac{X_B}{[(2 - X_B) + X_B\alpha^N]^2} \quad (20)$$

$$\delta(N) = \alpha^N \left( 1 - \frac{1}{\alpha} \right)$$

$$\begin{aligned} & \times \frac{1 - X_B}{[(1 - X_B) + (1 + X_B)\alpha^N] [(1 - X_B) + (1 + X_B)\alpha^{N-1}]} \\ & + \frac{X_B}{[(2 - X_B) + X_B\alpha^N] [(2 - X_B) + X_B\alpha^{N-1}]} \end{aligned} \quad (21)$$

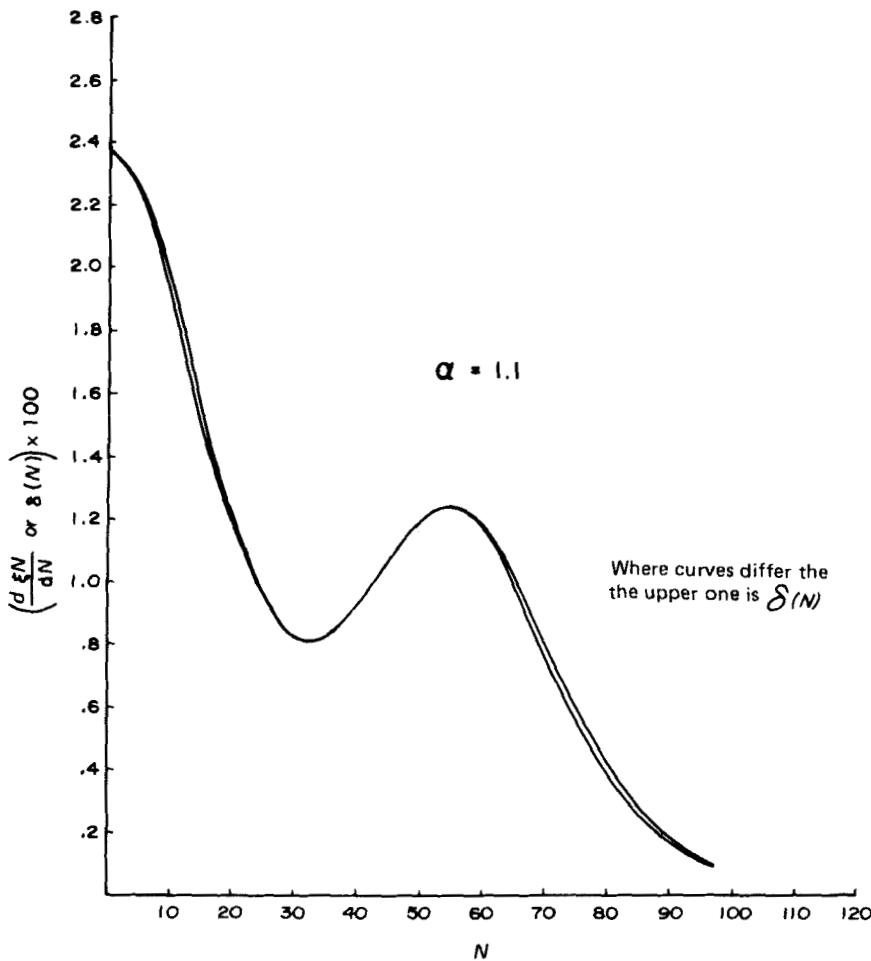
For the case of total reflux there are no feed and product streams, and vapor and liquid streams are equal throughout the column, including stage number 1.

Plots showing both  $d\xi_N/dN$  and  $\delta(N)$  vs  $N$  are shown in Figs. 7 through 9. As can be seen, for  $\alpha = 1.1$  the curves are nearly identical, but the difference is significant for larger values of  $\alpha$ . In the limit, for the case of total reflux the  $d\xi_N/dN$  and the  $\delta(N)$  curves become identical as  $\alpha \rightarrow 1$ . For very large values of  $\alpha$ ,  $(d\xi_N/dN) \rightarrow 0$  and  $\delta(N) \rightarrow 0.98$  where it would take only one equilibrium stage to obtain the assumed separation ( $X_B = 0.01$ ,  $y_D = 0.99$ ). For this case,  $\xi_s$ ,  $\xi_N$ , and  $\delta(N)$  are all identical.

## GENERAL DISCUSSION

The previous sections have demonstrated that the fractional contribution of individual stages to the overall separation in multistage distillation can be easily determined as the difference between the cumulative extent of separation for successive stages. This method could easily be extended to cases where  $\alpha$  and vapor and liquid flow rates are not constant within the column by using new values of these variables at each stage. A similar method should be useful in determining stage contributions to overall separation in all multistage separations.

This study investigated only the special case of column requirements for a fixed separation, and so the number of stages required to make the separation varied with each reflux ratio. The results are useful in understanding how

FIG. 7. Comparison of  $d\xi_N/dN$  and  $\delta(N)$  curves,  $\alpha = 1.1$ .

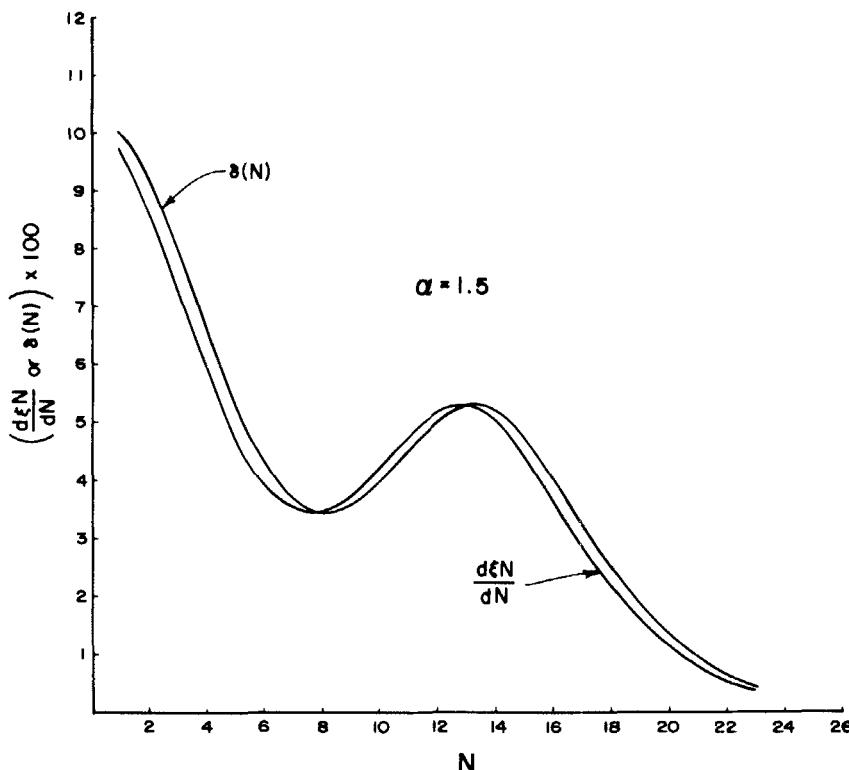
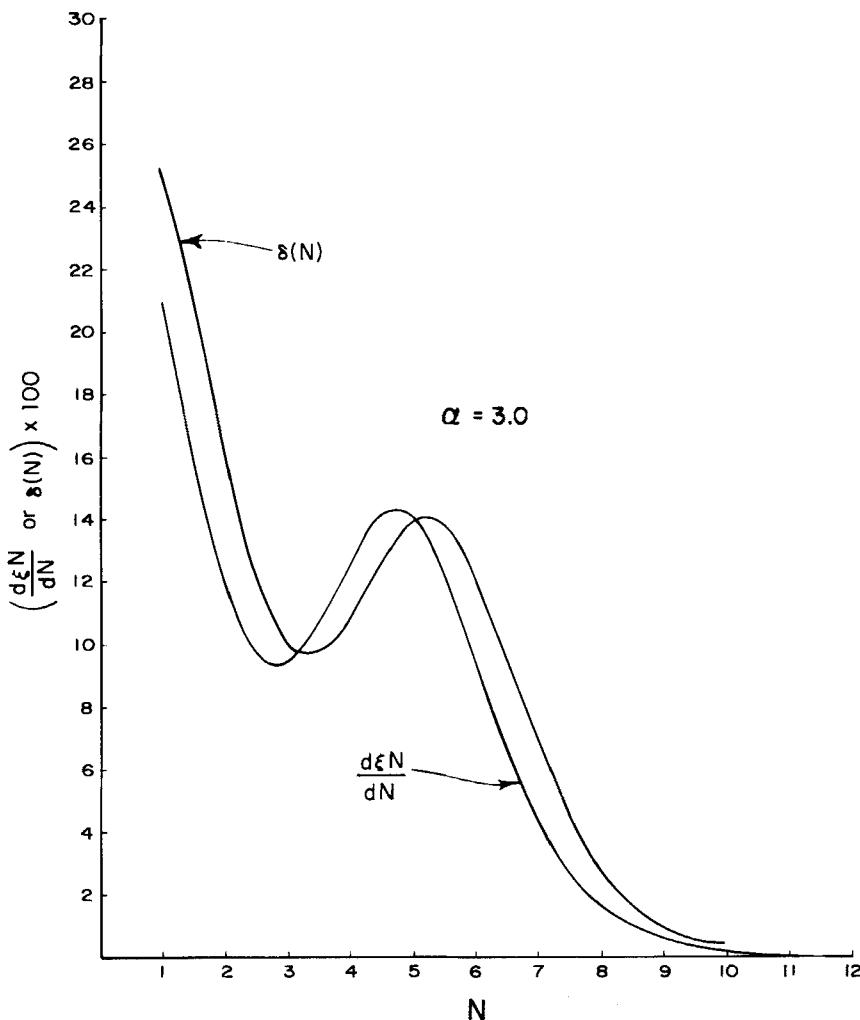


FIG. 8. Comparison of  $d\xi_N/dN$  and  $\delta(N)$  curves,  $\alpha = 1.5$ .

individual stage contributions and the number of stages required to make the separation are interrelated for various relative volatilities and reflux ratios. It should be possible to extend this method to investigate how  $\delta(N)$  and  $\xi_N$  vary when changes are made in the operating conditions of feed rate, feed composition, feed stage location, and reflux ratio for a column containing a fixed number of ideal stages. This will be the topic of a future publication.

## SYMBOLS

<i>B</i>	bottoms product rate
<i>D</i>	distillate product rate
<i>F</i>	feed rate

FIG. 9. Comparison of  $d\xi_N/dN$  and  $\delta(N)$  curves,  $\alpha = 3.0$ .

$F(N)$	fractional contribution of stage $N$
$K_i$	distribution ratio of component $i$
$K_{in}$	distribution ratio of multistage section for component $i$
$n_{ij}$	moles of species $i$ in region $j$
$N$	number of stages in a multistage section, also stage number
$R$	reflux ratio (moles reflux/moles distillate)
$X$	liquid phase composition (mole fraction)
$Y$	vapor phase composition (mole fraction)

## Greek Letters

$\alpha$	relative volatility $\left( \alpha = \frac{Y(1-X)}{X(1-Y)} = \frac{K_2}{K_1} \right)$
$\xi_s$	extent of separation for an equilibrium stage
$\xi_N(N)$	extent of separation for a multistage section
$\delta(N)$	contribution of stage $N$ to $\xi_N(N)$

## Subscripts

$B$	bottoms product
$D$	distillate product
Col	$\xi_N$ for entire column
$F$	composition of liquid leaving feed stage
Feed	composition of feed stream
$i$	component $i$
$iN$	component $i$ leaving multistage section
$iNT$	component $i$ leaving column
$N$	multistage section
max	maximum value for $\xi_s$
min	minimum reflux ratio

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