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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F. P. McCandless[a]
[a] DEPARTMENT OF CHEMICAL ENGINEERING, MONTANA STATE UNIVERSITY, BOZEMAN, MONTANA

To cite this Article McCandless, F. P.(1982) 'The Extent of Separation in Continuous Multistage Binary Distillation', Separation Science and Technology, 17: 12, 1361 — 1385
To link to this Article: DOI: 10.1080/01496398208055626
URL: http://dx.doi.org/10.1080/01496398208055626

SEPARATION SCIENCE AND TECHNOLOGY, 17(12), pp. 1361–1385, 1982-83

The Extent of Separation in Continuous Multistage Binary Distillation

F. P. McCANDLESS

DEPARTMENT OF CHEMICAL ENGINEERING
MONTANA STATE UNIVERSITY
BOZEMAN, MONTANA 59717

Abstract

Rony's extent of seapration has been applied to binary distillation, analyzing both single equilibrium stages and the cumulative separation obtained in a multistage column both at finite and total reflux. Both separation indices depend on relative volatility, reflux ratio, and composition. The cumulative extent of separation clearly shows the influence of reflux ratio on the separation obtained in a continuous distillation column. Small variations in the single-stage extent of separation appear to have a pronounced effect on the cumulation extent of separation and the number of stages required to make a given separation.

INTRODUCTION AND BACKGROUND

Rony (*1*) has suggested that the analysis of all separation processes be through a universal separation index, ξ, the extent of separation. Chaipayungpan (*2*) applied ξ to individual stages in multistage distillation but concluded that it was not a suitable index to characterize the separation because the single-stage separation index does not approach zero on the pinch zone of the column at minimum reflux conditions. However, in this paper it is shown that the cumulative extent of separation describes the multistage separation very well and clearly shows the profound influence of reflux ratio on the separation obtained in a distillation column.

APPLICATION OF ξ TO BINARY MULTISTAGE DISTILLATION

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

$$K_i = n_{im}/n_{ik} \tag{1}$$

For an equilibrium stage within a distillation column the two regions under consideration are the vapor (Region 1) and liquid (Region 2) leaving the stage in equilibrium with each other. For this single equilibrium stage the relative volatility in terms of these distribution ratios is given by

$$\alpha = \frac{n_{22}}{n_{21}} \Big/ \frac{n_{12}}{n_{11}} = K_2/K_1 \tag{2}$$

The extent of separation for a single equilibrium stage is given by

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

For a multistage column the two regions of interest are the distillate and bottoms product streams leaving the column as shown in Fig. 1(a). However, in analyzing the performance of a column in terms of the cumulative extent of separation, it is more convenient to consider the vapor (Region 3) and liquid (Region 4) streams leaving a multistage section within the column as shown in Fig. 1(b). This is necessary 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.

For this case the cumulative extent of separation for the N stages within the column shown in Fig. 1(b) is given by

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

where

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

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

For convenience, x and y in the following discussion will refer to the more volatile component ($i = 1$). Again, for this analysis, only the column (not including the reboiler) as shown in Fig. 1(b), will be considered.

For an equilibrium stage in the stripping section of the column, assuming a fixed bottoms composition of $x_B = x_1$, then

$$y_1 = \frac{\alpha x_B}{1 + (\alpha - 1)x_B} \tag{7}$$

A material balance around the bottom part of the column gives for stage number $n = 2, \ldots, F$ (including the feed tray):

$$x_n = x_B + \left(\frac{R+1}{R+2}\right)y_{n-1}, \qquad y_n = \frac{\alpha x_n}{1 + (\alpha - 1)x_n} \tag{8}$$

$$K_1 = \left(\frac{R+2}{R+1}\right)\left(\frac{x_n}{y_n}\right), \qquad K_2 = \left(\frac{R+2}{R+1}\right)\left(\frac{1-x_n}{1-y_n}\right) = \alpha K_1 \tag{9}$$

$$\xi_s = \left|\frac{1}{1+K_1} - \frac{1}{1+K_2}\right| \tag{10}$$

$$K_{1N} = \left(\frac{R+2}{R+1}\right)\left(\frac{x_2}{y_n}\right), \qquad K_{2N} = \left(\frac{R+2}{R+1}\right)\left(\frac{1-x_2}{1-Y_n}\right) \tag{11}$$

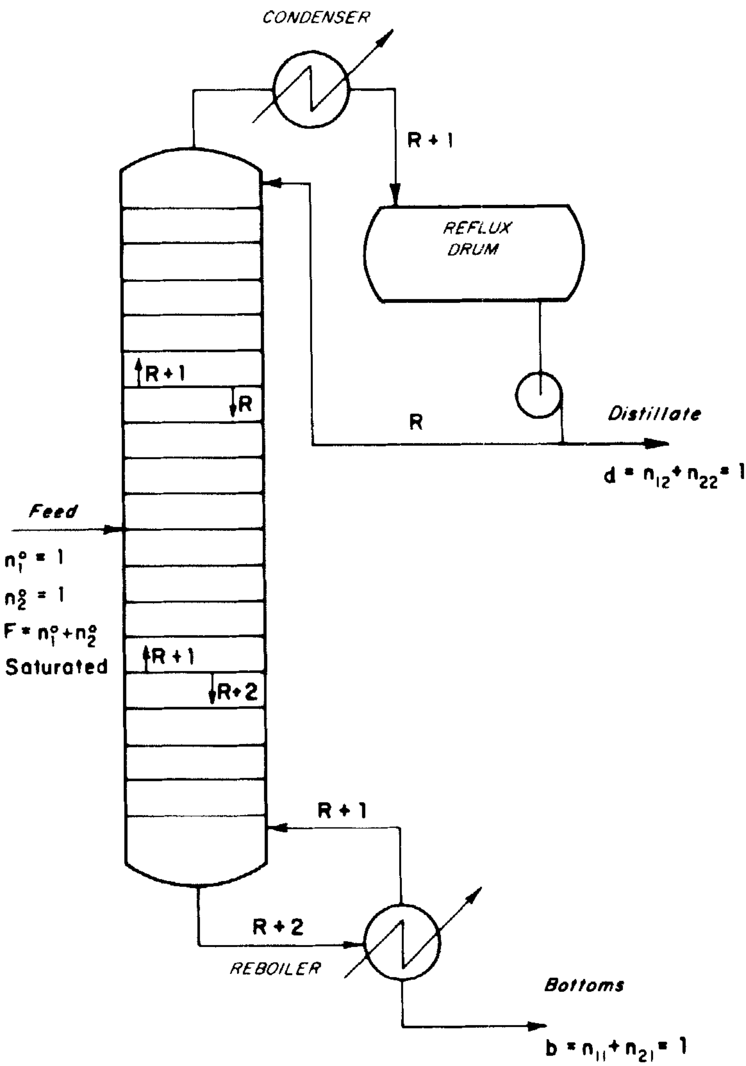
$$\xi_N = \left|\frac{1}{1+K_{1N}} - \frac{1}{1+K_{2N}}\right| \tag{12}$$

Here ξ_s represents the extent of separation by the single equilibrium distillation stage n and ξ_N represents the cumulative extent of separation by the n stages of the stripping section of the column, not including the reboiler (Stage 1).

A material balance on the feed tray yields the composition of the liquid coming to the feed tray from the tray above:

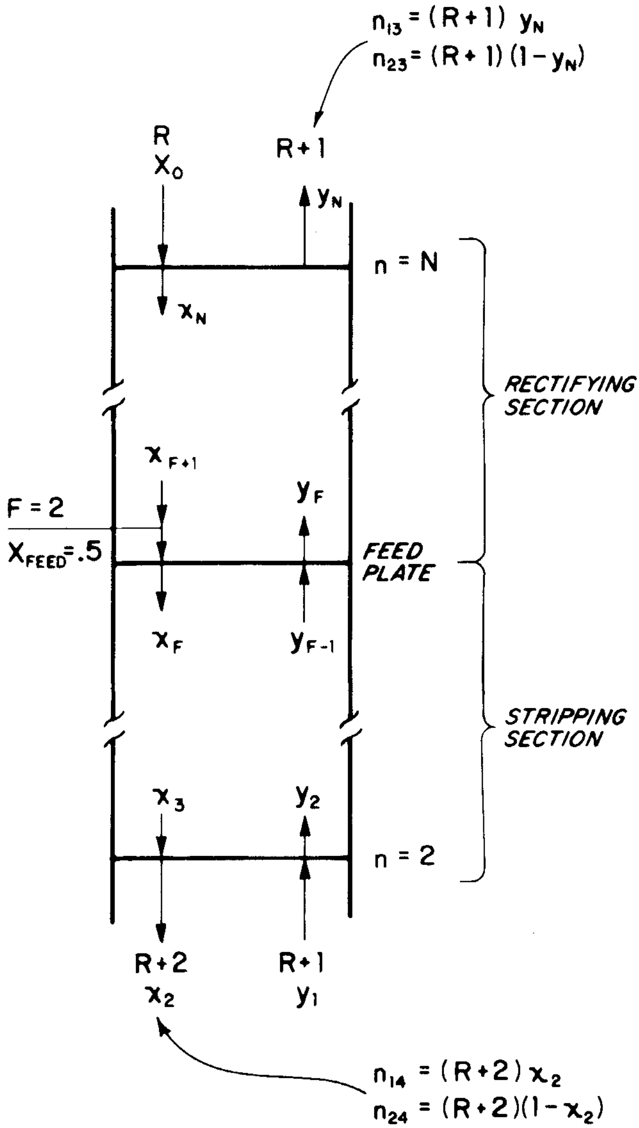
$$x_{F+1} = \frac{(R+2)x_F + (R+1)(y_F \div y_{F-1}) - Fx_{\text{feed}}}{R} \tag{13}$$

and equilibrium gives



(A)

FIG. 1. Equilibrium stage distillation column with saturated feed and finite reflux.



(B)

FIG. 1 (continued)

$$y_{F+1} = \frac{\alpha x_{F+1}}{1 + (\alpha - 1)x_{F+1}} \tag{14}$$

In general, for a stage in the rectifying section of the column, the compositions of the streams leaving the stage are given by

$$x_n = \frac{(R + 2)x_F + (R + 1)(y_{n-1} - y_{F-1}) - Fx_{\text{feed}}}{R} \tag{15}$$

$$y_n = \frac{\alpha x_n}{1 + (\alpha - 1)x_n} \tag{16}$$

$$K_1 = \left(\frac{R}{R + 1}\right)\left(\frac{x_n}{y_n}\right), \qquad K_2 = \left(\frac{R}{R + 1}\right)\left(\frac{1 - x_n}{1 - y_n}\right) = \alpha K_1 \tag{17}$$

$$\xi_s = \left|\frac{1}{1 + K_1} + \frac{1}{1 + K_2}\right| \tag{18}$$

Again, the cumulative extent of separation by the n-stage column excluding the reboiler will be given by Eqs. (11) and (12).

Thus both ξ_s and ξ_N depend on relative volatility and on reflux ratio.

The above equations were programmed on a digital computer, and ξ_s and ξ_N were determined for various values of α at different reflux ratios. The following assumptions were made:

(*a*) Constant relative volatility
(*b*) Constant molal overflow
(*c*) Bottom product composition, $x_B = 0.01$
(*d*) Overhead composition, $y_N \geq 0.99$
(*e*) Feed rate $F = 2$, $x_{\text{feed}} = 0.5$, saturated liquid
(*f*) Total condenser

Calculations were carried out for the stripping section of the column (Eqs. 7 through 12 to a point where $x_n = x_F$ was closest to the feed composition ($x = 0.5$). The appropriate values of x_F and y_{F-1} were then used in Eqs. (14) through (18) to calculate ξ_s and ξ_N in the rectifying section up to a point where $y_N \geq 0.99$.

Calculations were made for relative volatilities between 1.1 and 2.0 at reflux ratios from less than the minimum to total reflux. The minimum reflux ratio is given by

$$R_{\min} = \frac{\dfrac{x_D}{x_{\text{feed}}} - \dfrac{\alpha x_B}{x_{\text{feed}}}}{\alpha - 1} \tag{19}$$

At $R_{\min}$ the stripping and rectifying section operating lines intersect at a pinch point on the equilibrium curve equal to the feed composition.

The results of these calculations are summarized in Figs. 2 through 4 which show ξ_N and ξ_s as a function of N, the stage number.

CUMULATIVE EXTENT OF SEPARATION, ξ_N

As can be seen, the ξ_N curves very clearly indicate the influence of reflux ratio on the separation. At reflux ratios less than or equal to the minimum,

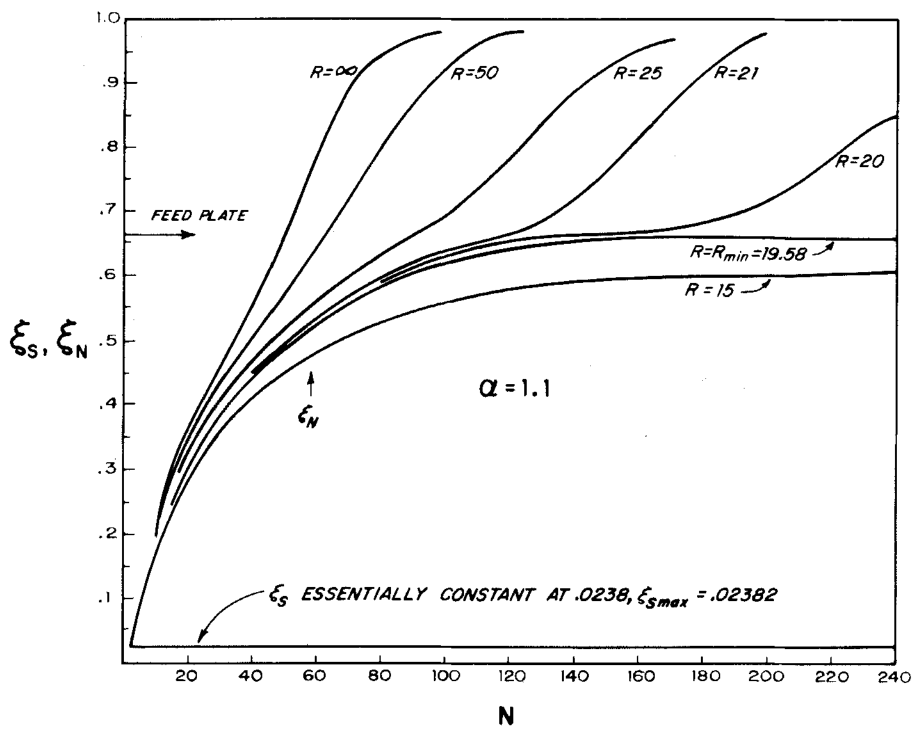


FIG. 2. Cumulative extent of separation and the single-stage extent of separation as a function of stage number for various reflux ratios, $\alpha = 1.1$.

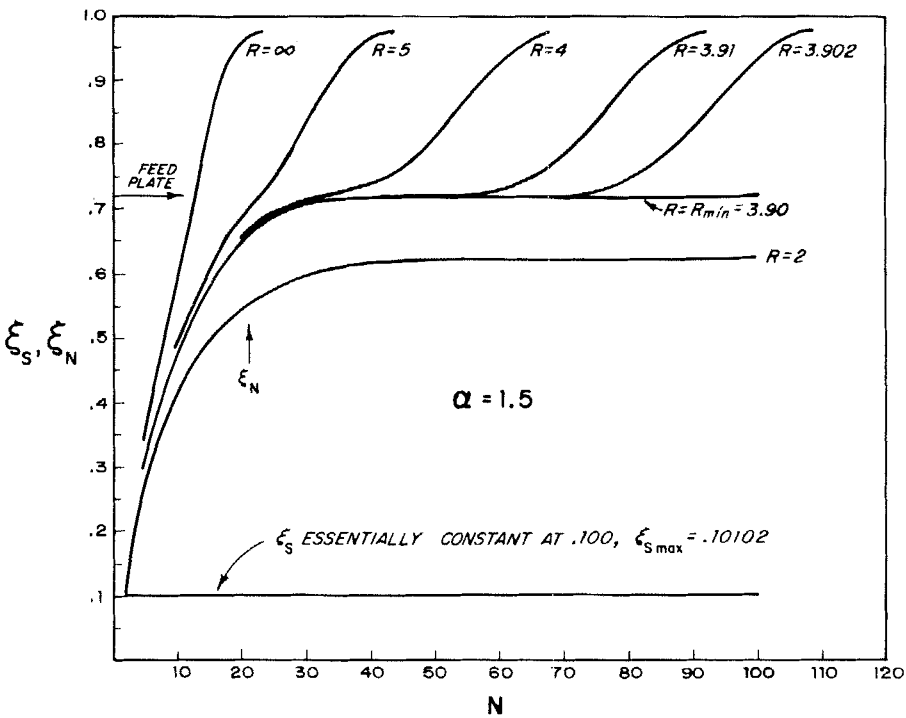


FIG. 3. Cumulative extent of separation and the single-stage extent separation as a function of stage number for various reflux ratios, $\alpha = 1.5$.

there is a pinch zone in the stripping section of the column. An infinite number of stages would be required to reach the feed composition in the stripping section of the column at the minimum reflux conditions, while at reflux ratios below the minimum, the pinch zone will be below the feed tray at a composition less than that of feed. Under the conditions of minimum reflux, ξ_N approaches a value representing separation into two streams, the bottom liquid stream having a composition of x_2 and the top vapor stream having a composition that is in equilibrium with $x_F = 0.5$. At less than the minimum reflux ratio the vapor stream would have a composition less than this value and hence the maximum ξ_N would be less.

At reflux ratios only slightly greater than the minimum it takes a great number of stages (especially at low values of α) to increase the vapor composition over that in the pinch zone at minimum reflux. At higher ratios there is no pinch zone to hinder separation and ξ_N increases rapidly with the number of stages to the material balance limit.

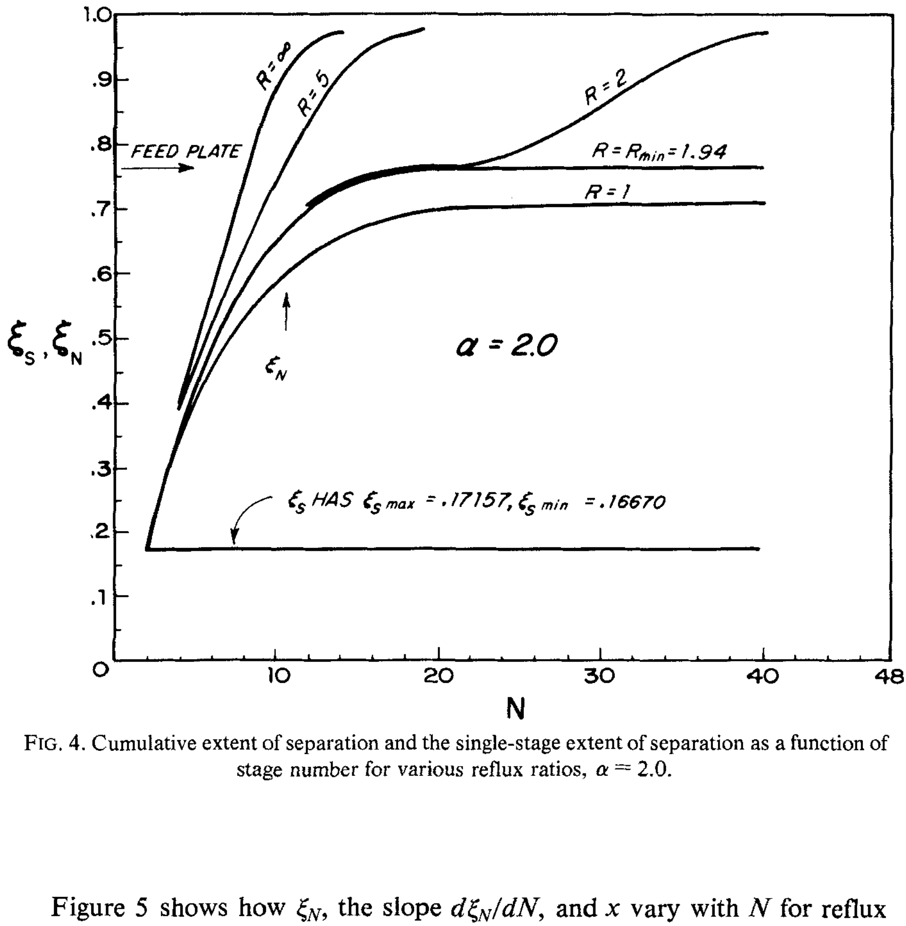


FIG. 4. Cumulative extent of separation and the single-stage extent of separation as a function of stage number for various reflux ratios, $\alpha = 2.0$.

Figure 5 shows how ξ_N, the slope $d\xi_N/dN$, and x vary with N for reflux ratios increasing from $R_{\min}$ to total reflux for the case where $\alpha = 1.1$. The variation in the shape of the $d\xi_N/dN$ curve is interesting and must reflect changes in the relative magnitudes of the two distribution ratios, K_{1N} and K_{2N}, which determine how ξ_N varies with stage number. At minimum reflux conditions ($R = 19.58$) the slope $d\xi_N/dN$ decreases steadily, approaching zero asymptotically in the pinch zone. In the stripping section, at reflux ratios somewhat higher than the minimum (R = 20, 21, 25), the effects of the pinch zone are not as pronounced although the slope decreases monotonically in the stripping section and is a minimum at the feed plate. In all of these curves (Fig. 5a, b, c, d) there are sections where the slope tends to level off. In this area the second derivative, $d^2\xi_N/dN^2$ (which is negative in all cases for these reflux ratios) goes through a relative minimum, and in that section of the column, ξ_N increases more rapidly. For $R = 50$ (Fig. 5e) there is a relative

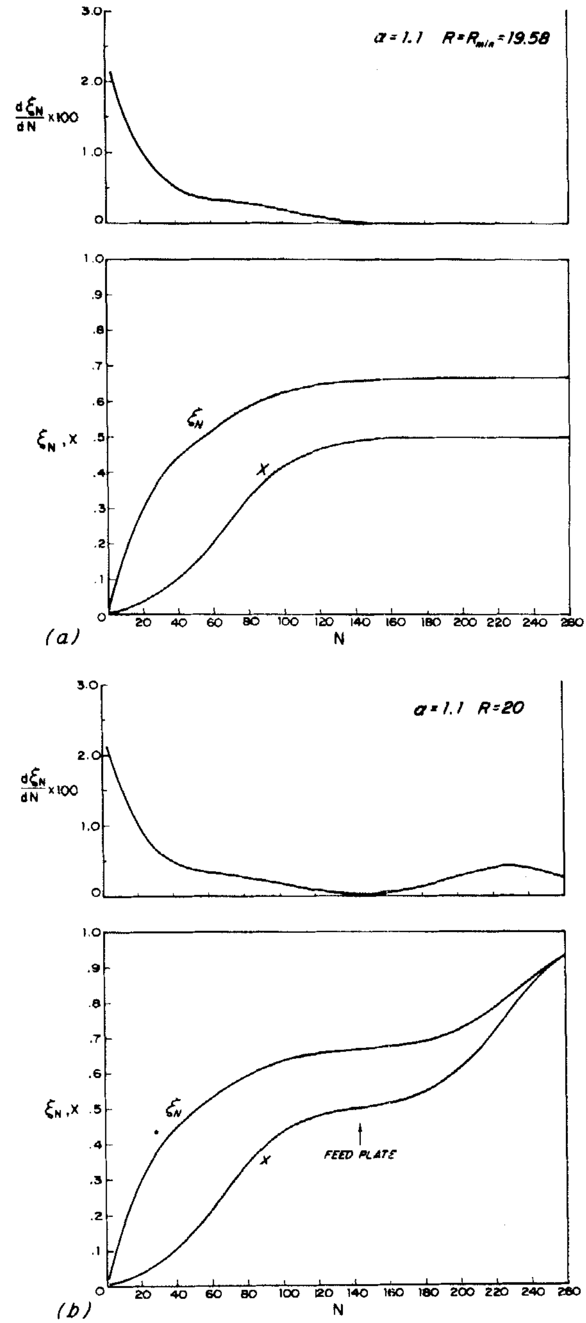


FIG. 5. Cumulative extent of separation, the liquid composition, and the slope of the ξ_N curve as a function of stage number for various reflux ratios, $\alpha = 1.1$.

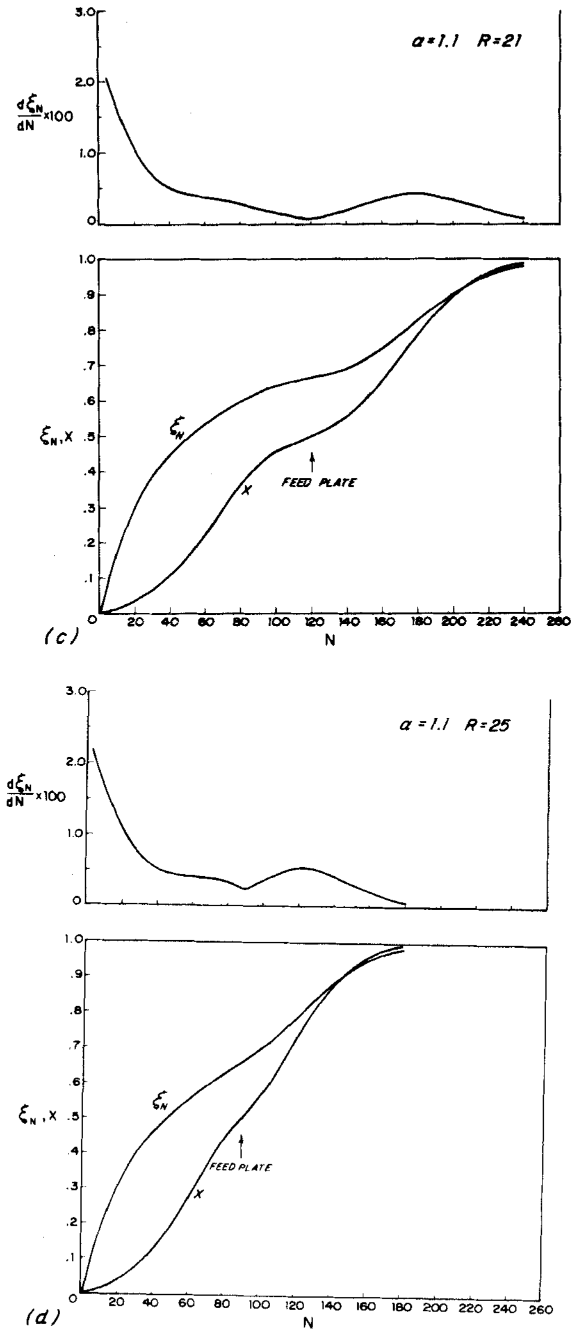


FIG. 5 (continued)

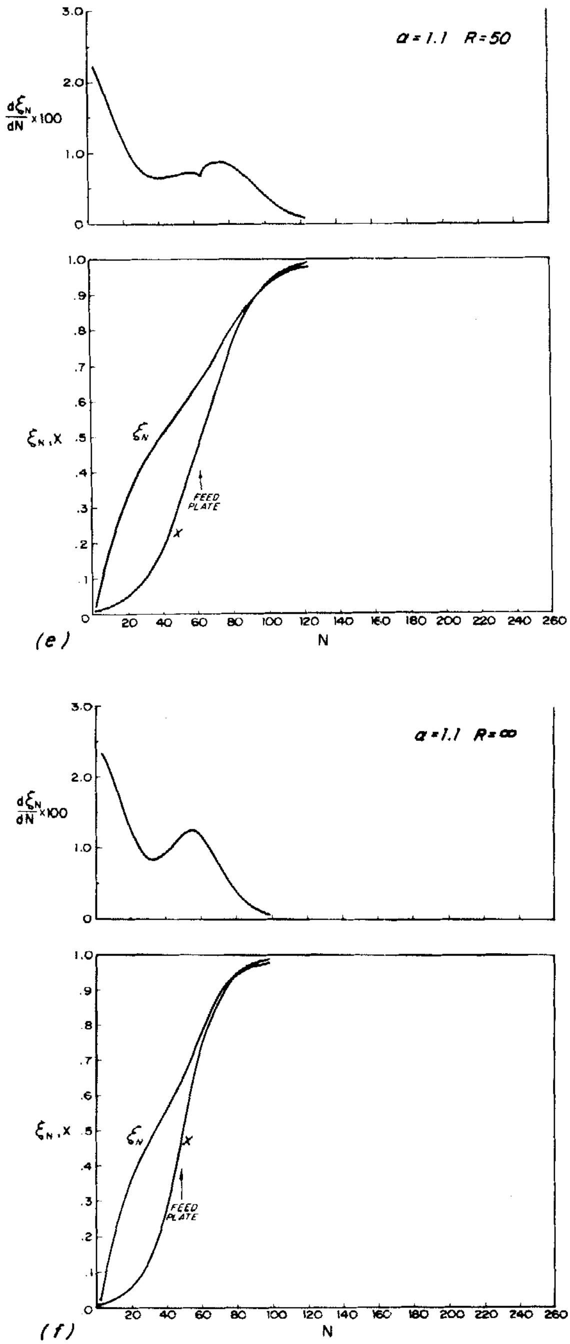


FIG. 5 (continued)

minimum in the $d\xi_N/dN$ curve at about $N = 41$ and goes through a maximum at $N = 58$. In this region the second derivative is positive.

At reflux ratios greater than $R_{\min}$ there is always a maximum in the $d\xi_N/dN$ curve in the rectifying section.

The variation in ξ_N and $d\xi_N/dN$ with N can be explained by considering how the relative magnitudes of the two distribution ratios change with composition. For example, for the case of total reflux the volumes of the two product streams are equal and the distribution ratios become

$$K_{1N} = \frac{0.01}{y_N}, \qquad K_{2N} = \frac{0.99}{(1 - y_N)} \tag{20}$$

For small values of N, as N increases, there is a rapid decrease in K_{1N} while K_{2N} increases only slightly. In this area the increase in ξ_N with N is due mostly to decreases in K_{1N} because of y_N increasing rapidly. Here the slope starts out at a high value and decreases as y_N increases. As N (and y_N) increases further, a point is reached where the changes in ξ_N due to changes in K_{1N} and K_{2N} are the same magnitude, and in this area the slope changes little with composition and goes through a relative minimum. With further increases in N, K_{2N} increases rapidly while K_{1N} changes very little. In this area there is an increase in the slope. Finally, the slope must decrease toward zero as ξ_N approaches the maximum value possible with the fixed bottoms composition.

ξ_N AT TOTAL REFLUX

Although the same results can be obtained by letting $R \to \infty$ in the previous calculations, for the special case of total reflux the number of equilibrium stages required to effect a given separation can be easily calculated using the Fenske-Underwood equation (*3*). This gives the minimum number of stages required to accomplish that separation.

Consider the distillation column operating at total reflux, again assuming constant molal overflow and relative volatility, shown in Fig. 6. Assume that the column is operated such that a composition x_B is maintained in the reboiler. For this case the Fenske-Underwood equation can be used to calculate the composition of the distillate ($y_d = y_n$). Hence ξ_N, the extent of separation for a column containing N equilibrium stages, can be determined:

$$N = \frac{\ln\left[\left(\frac{y_n}{1 - y_n}\right)\left(\frac{1 - x_B}{x_B}\right)\right]}{\ln \alpha} \qquad \text{(Fenske-Underwood equation)} \tag{21}$$

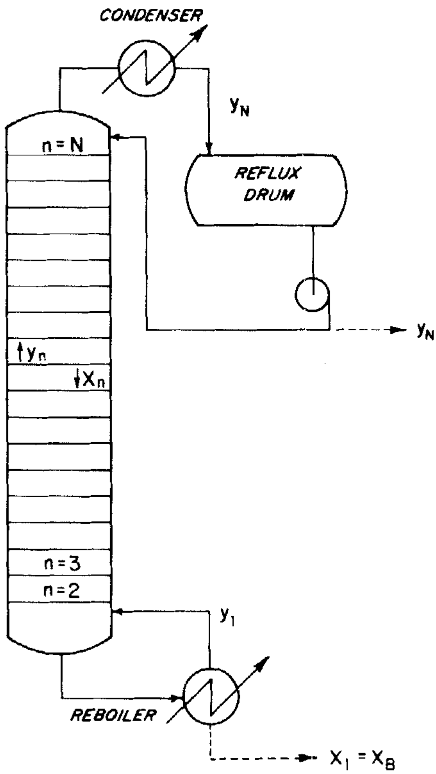


FIG. 6. Equilibrium stage distillation column at total reflux.

or

$$y_n = \frac{\alpha^n \left(\dfrac{x_B}{1 - x_B}\right)}{1 + \alpha^n \left(\dfrac{x_B}{1 - x_B}\right)} = \frac{\alpha^n}{\alpha^n + \left(\dfrac{1 - x_B}{x_B}\right)}, \qquad n = 1, 2, 3, \ldots N \tag{22}$$

This equation relates y_N, the composition of the distillate for N stages at total reflux, to α, with N assuming a fixed x_B.

Since the vapor and liquid streams leaving a stage are equal, the cumulative extent of separation ξ_N for the N stage column can be calculated from the distribution ratio's:

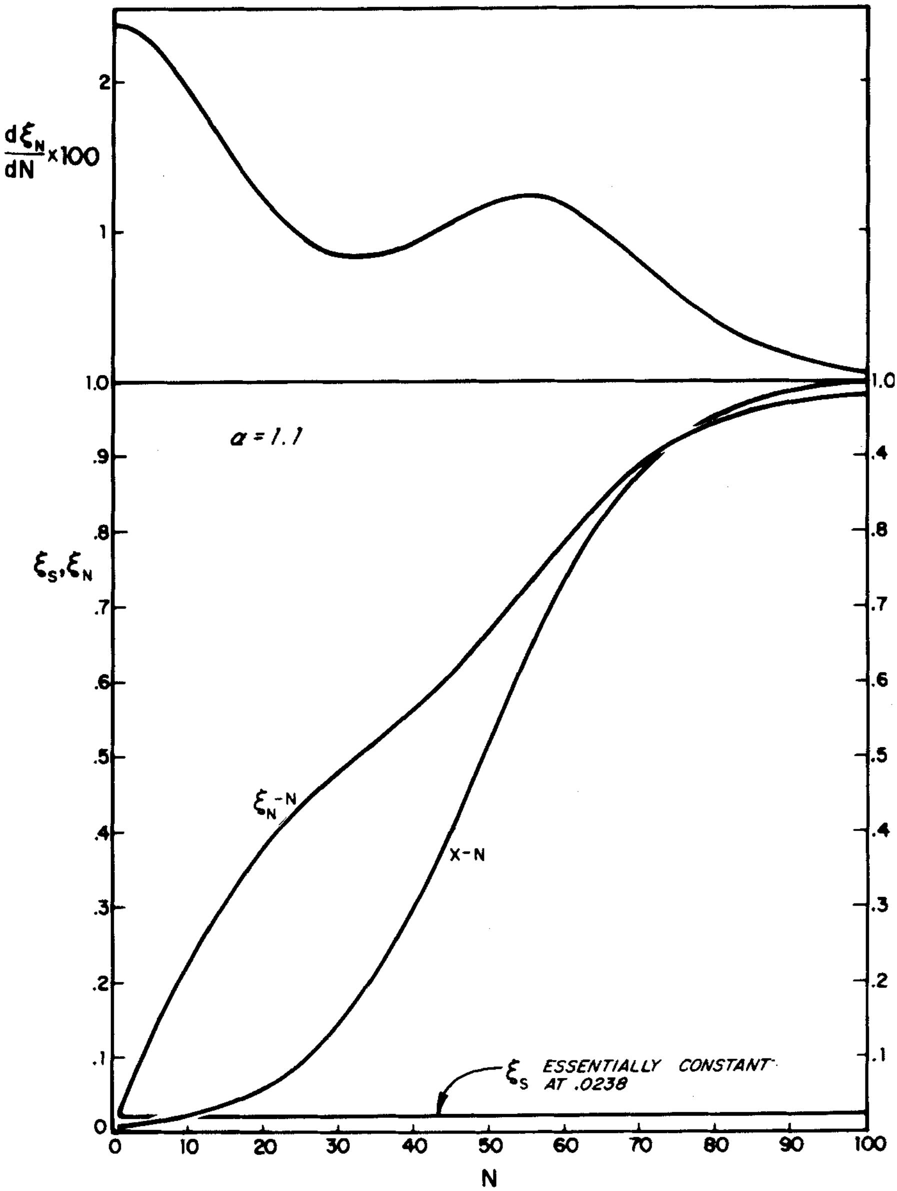


FIG. 7. Cumulative extent of separation and its slope, single-stage extent of separation, the liquid composition leaving the Nth stage as a function of stage number at total reflux, $\alpha = 1.1$.

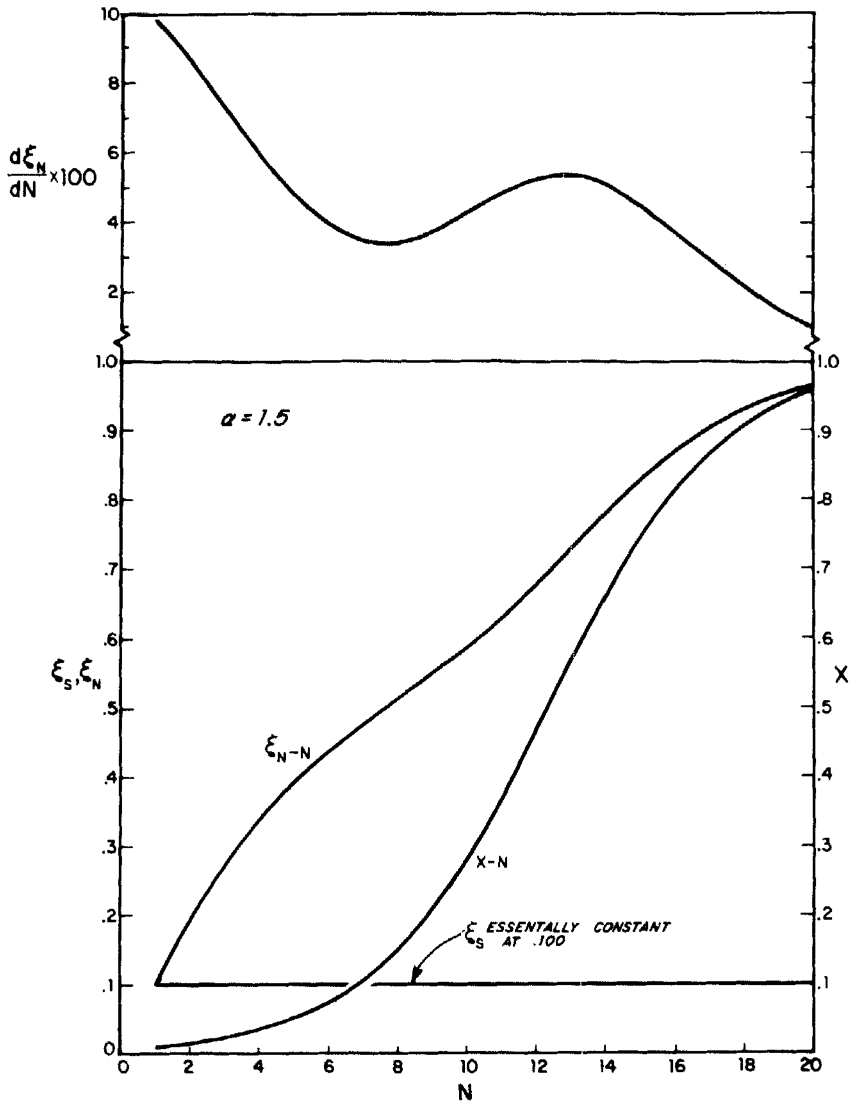


FIG. 8. Cumulative extent of separation and its slope, single-stage extent of separations, and liquid composition leaving the Nth stage as a function of stage number at total reflux, $\alpha = 1.5$.

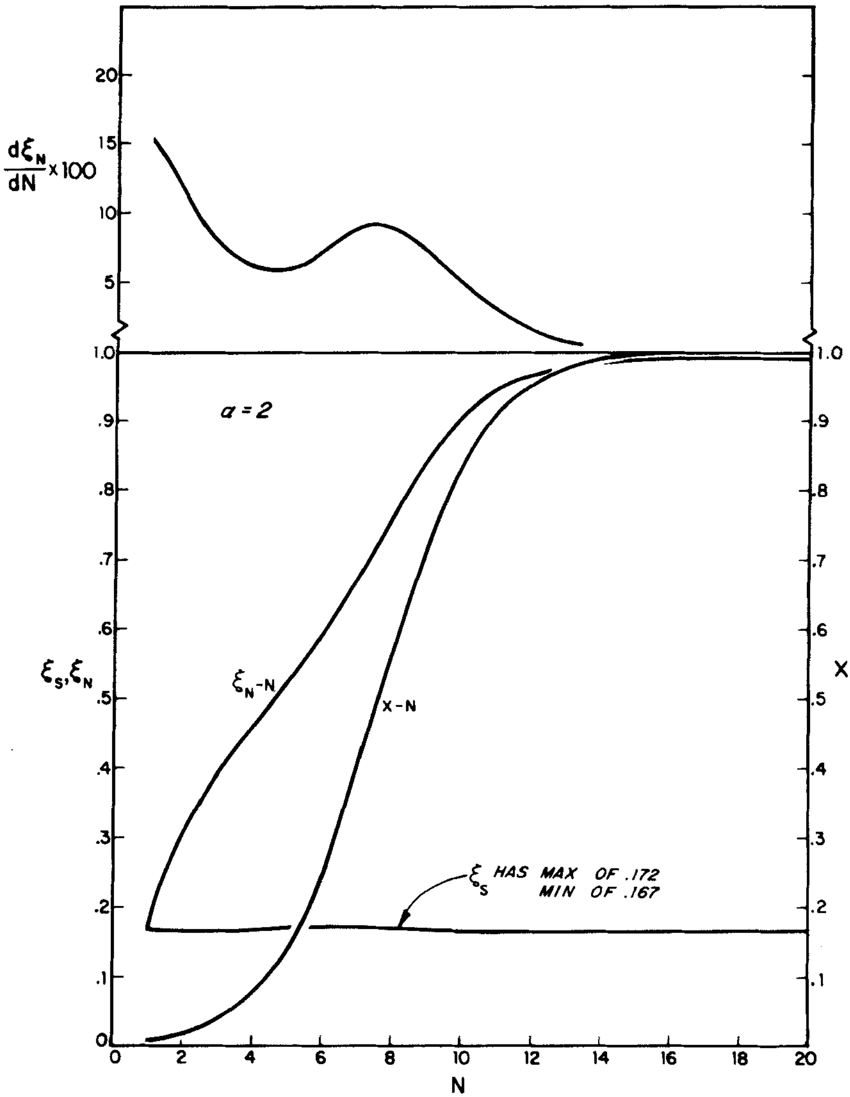


FIG. 9. Cumulative extent of separation and its slope, single-stage extent of separation, and liquid composition leaving the Nth stage as a function of stage number at total reflux, $\alpha = 2$.

$$K_{1N} = \frac{x_B}{y_N}, \qquad K_{2N} = \frac{1 - x_B}{1 - y_N} \tag{23}$$

Also, the single-stage extent of separation, ξ_s, for each equilibrium stage or plate is calculated from the distribution ratios for the streams leaving each stage:

$$K_1 = \frac{x_n}{y_n}, \qquad K_2 = \frac{1 - x_n}{1 - y_n} \tag{24}$$

where

$$x_n = \frac{y_n}{\alpha - (\alpha - 1)y_n} \tag{25}$$

Figures 7 through 9 show ξ_N, ξ_s, and x as a function of N for several values of α. All of these plots assume a composition in the reboiler of $x_B = 0.01$. Also shown is the slope of this cumulative extent of separation curve, $d\xi_N/d_N$, which in this case can easily be calculated by differentiating the expression for ξ_N. Figure 7 is identical to Fig. 5(f). As can be seen, the curves for different values of α all have essentially the same shape.

VARIATION OF ξ_s WITH N AND REFLUX RATIO

Figure 10 shows the variation of the single-stage extent of separation with stage number for various reflux ratios for $\alpha = 2.0$. Curves of this type were first obtained by Chaipayungpan (*2*). As shown in Fig. 10, ξ_s changes very little with stage number although it is different in the two sections of the column because the relative volumes of the vapor and liquid streams are different. The maximum value of $(\xi_s)_{max}$ is given by

$$\xi_{s\ max} = \frac{\sqrt{\alpha} - 1}{\sqrt{\alpha} + 1} \tag{26}$$

and thus depends only on relative volatility and is independent of reflux ratio. However, the location on the x–y diagram where the maximum occurs does depend on reflux ratio. The maximum will occur at

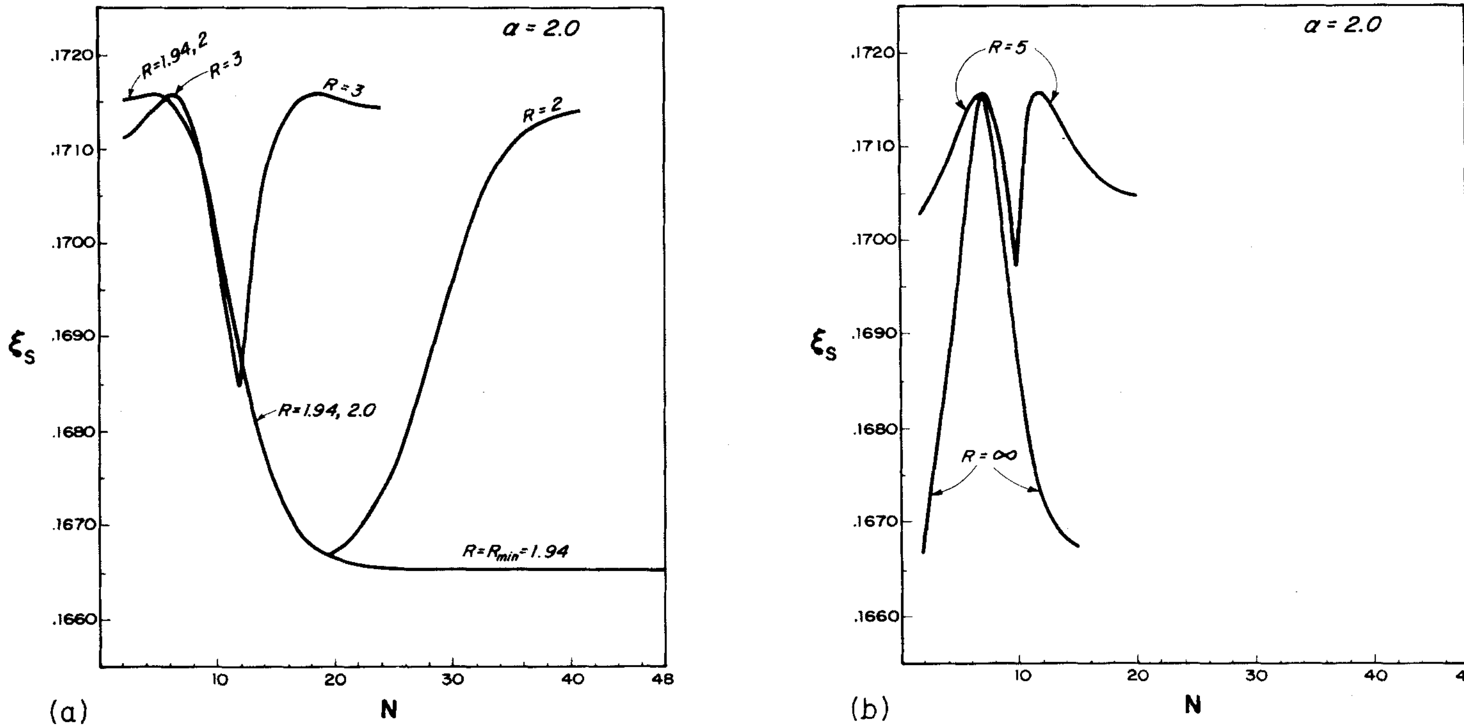


FIG. 10. Variation of the single-stage extent of separation as a function of stage number for various reflux ratios, $\alpha = 2.0$. (The two figures are shown for clarity.)

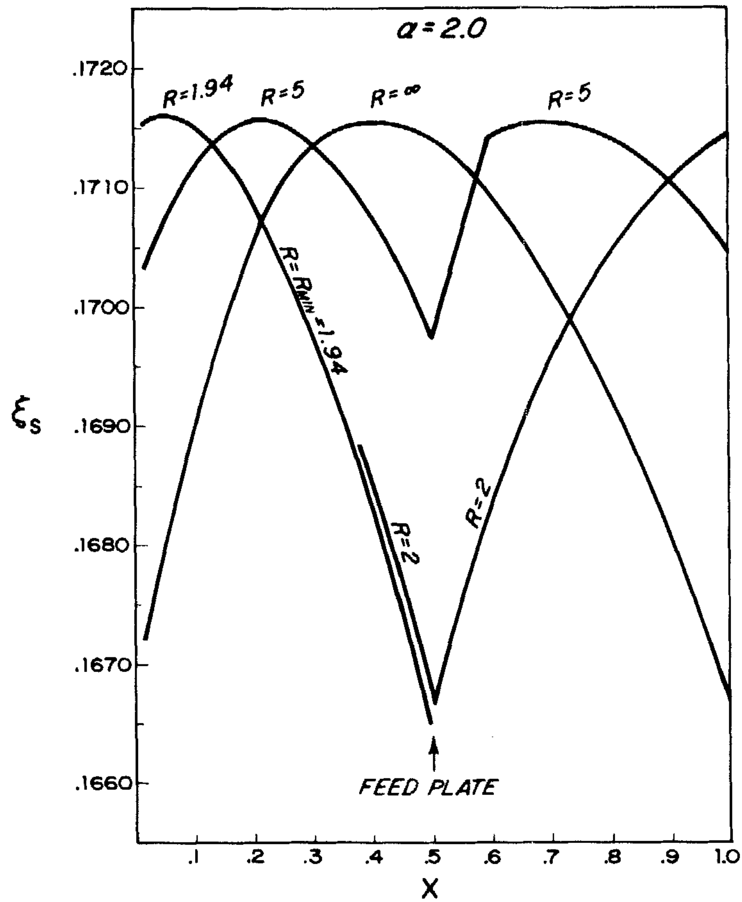


FIG. 11. Variation of the single-stage extent of separation as a function of liquid composition for various reflux ratios, $\alpha = 2.0$.

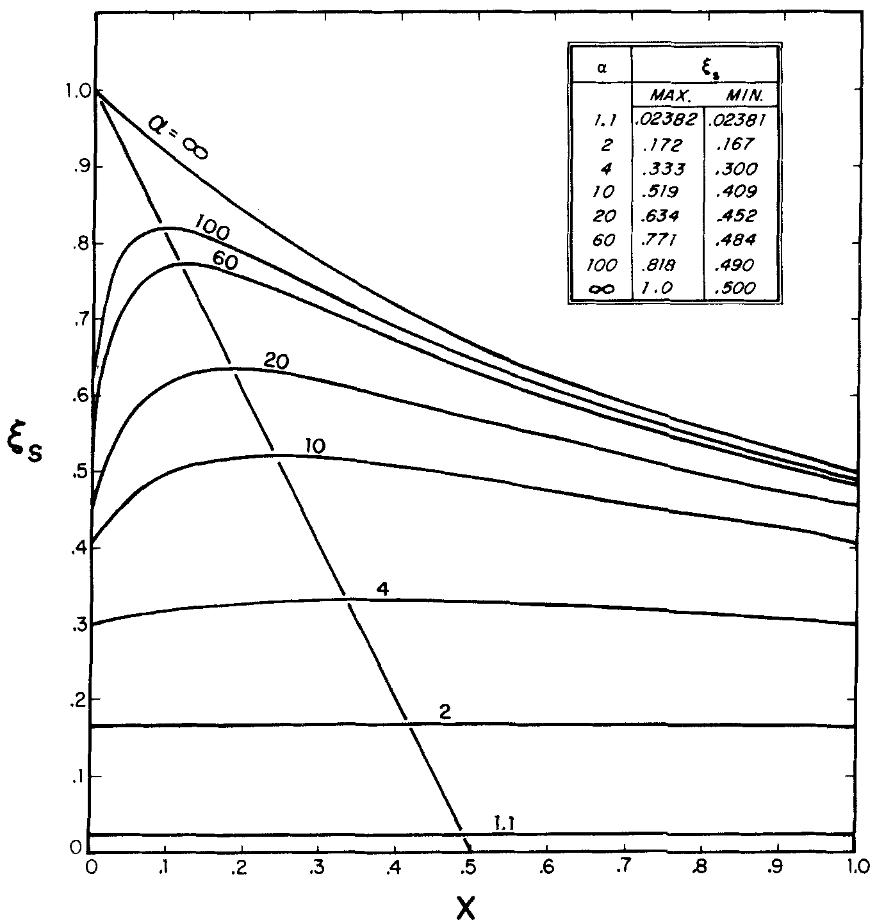
$$x_{\max\xi_s} = \frac{\left(\dfrac{R+1}{R+2}\right)\sqrt{\alpha} - 1}{\alpha - 1} \quad \text{in the stripping section}$$

and

$$x_{\max\xi_s} = \frac{\left(\dfrac{R+1}{R}\right)\sqrt{\alpha} - 1}{\alpha - 1} \quad \text{in the rectifying section}$$

subject to the constraint that $0 \leq x \leq 1$. Thus, depending on the values of α and R, the curves may not go through a maximum.

The same data shown in Fig. 10 are also shown in Fig. 11 where ξ_s is plotted vs x rather than N. For $R > 1.414$ there is a maximum in the curve in the stripping section and for $R > 2.414$ there is a maximum in the rectifying section also. At $R_{min} = 1.94$, ξ_s goes through a maximum at $x = 0.055$ ($\xi_{s\,max} = 0.17157$) and then decreases to the low constant value in the pitch zone. At reflux ratios greater than 2.414, there is a maximum in both the stripping and rectifying sections with the maxima approaching the same point



α	ξ_s MAX.	ξ_s MIN.
1.1	.02382	.02381
2	.172	.167
4	.333	.300
10	.519	.409
20	.634	.452
60	.771	.484
100	.818	.490
∞	1.0	.500

FIG. 12. Variation of the single-stage extent of separation as a function of liquid phase composition at total reflux for various values of α.

at total reflux. For $\alpha = 2$ the maximum at total reflux occurs at $x = 0.414$ as shown in Fig. 11.

The variation in ξ_s with x for values of α varying from 1 to ∞ for the case of total reflux is shown in Fig. 12. Here ξ_s was calculated from the Eq. (10) which for this case reduces to

$$(\xi_s)_{Tr} = \frac{\alpha}{\alpha + 1 + (\alpha - 1)x} - \frac{1}{1 + 1 + (\alpha - 1)x} \tag{27}$$

Again $(\xi_s)_{\max} = (\sqrt{\alpha} - 1)/(\sqrt{\alpha} + 1)$, and this will now occur at $x = (\sqrt{\alpha} - 1)/(\alpha - 1)$. As can be seen in Fig. 12, at low values of the relative volatility, ξ_s does not vary much with composition but the variation is significant for higher values of α. The locus of maxima is given by the equation $\xi_s = 1 - 2x$. In addition, it can be seen that for large values of α, $\xi_s \rightarrow 0.5$ as $x \rightarrow 0$, but for very small, finite values of x, $\xi_s \rightarrow 1$ as α gets larger and larger. This can be explained by considering the vapor and liquid streams leaving the stage, the liquid stream containing only a trace of the more volatile component. Since α is large, the composition of the vapor is essentially 100% of the more volatile component and, since the volume of the two streams are equal, $\xi_s \rightarrow 1$. However, for a fixed large value of α, $\xi_s \rightarrow 0.5$ in the limit as x approaches 0 or 1.

Although ξ_s changes very little with N and R (Fig. 10 shows a variation of only about 3%), the trends in the variation are interesting and the small derivations appear to have a pronounced effect on ξ_N and the number of stages required to make a separation. Figure 13 presents a plot of the average single-stage extent of separation in the column as a function of reflux ratio. Here the average is defined

$$(\xi_s)_{\text{ave}} = \sum_N \xi_s/N \tag{28}$$

Where N is the number of stages required to reach a composition $y_N \geq 0.99$. The number of stages, N, required to reach this composition is also shown in Fig. 13.

As can be seen, $(\xi_s)_{\text{ave}}$ goes through a maximum at $R \sim 4$ and then decreases to the average value at total reflux. It is interesting to note that $R = 4$ appears to be near the optimum reflux ratio since the number of stages required to make the separation decreases very little with increasing reflux ratio above this point.

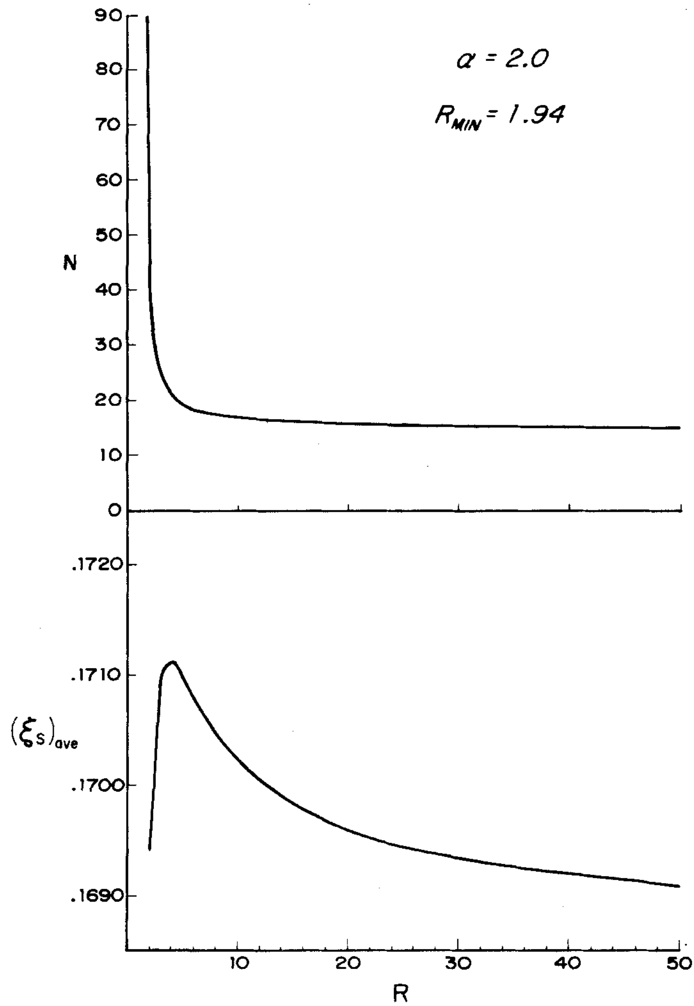


FIG. 13. Average single stage-extent of separation and the number of stages required to reach a composition of $y_N \geq 0.99$ as a function of reflux ratio, $\alpha = 2.0$.

DISCUSSION

The previous sections have demonstrated that the concept of the extent of separation can readily be applied to continuous binary distillation and that different distillation schemes can easily be compared on the same basis.

The cumulative extent of separation, ξ_N, clearly shows the profound influence of reflux ratio on the separation obtained in a multistage distillation column. The variation in the single-stage extent of separation, ξ_s, with reflux ratio is interesting, and a maximum in $(\xi_s)_{ave}$ may indicate some sort of optimum reflux ratio.

Although this paper has dealt only with the simple cases of how the single equilibrium stage extent of separation varies with composition and reflux ratio, it should be possible to apply the concept to more complicated situations. The case where α and molal overflow are not constant could easily be incorporated into the analysis by assuming new values of α and L/V on each stage.

SYMBOLS

b	bottom product
d	distillate product
K_i	distribution ratio of component i on a ideal single for calculation of ξ_s
K_{iN}	distribution ratios for component i in a multistage column for calculation of ξ_N
L	moles liquid product leaving a stage
n_{ij}	number of moles of species i in region j
n_i^0	total number of moles of species i in feed stream
n	stage number in a multistage column
N	total number of stages in a multistage column
R	reflux ratio (moles reflux/moles distillate)
V	moles vapor product leaving a stage
x	liquid phase composition (mole fraction)
y	vapor phase composition (mole fraction)

Greek Letters

α	relative volatility $\left(\alpha = \dfrac{y(1-x)}{x(1-y)} = K_2/K_1\right)$
ξ	extent of separation
ξ_s	extent of separation for a single equilibrium stage
ξ_N	extent of separation for N stages in a distillation column
$(\xi_s)_{ave}$	average value of ξ_s in a column of N stages (Eq. 28)

Subscripts

B	bottoms product
D	distillate product
F	composition leaving feed plate
i	component i
j, k, m	regions j, k, m
n	stage number
N	distillate product composition, also K_i and ξ for N total stages
r	rectifying section of column
s	stripping section of column
Tr	total reflux
max	maximum value for ξ
ave	average value for ξ_s

Acknowledgment

The author is indebted to Prof Peter Rony for his many helpful suggestions during the revision of this paper.

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Received by editor November 6, 1980
Revised May 3, 1982