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Effect of Changes in Operating Variables on Stage-wise and Cumulative Separation in Binary Multistage Distillation

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Abstract

The progressive separation that occurs stage-wise within a multistage distillation column is characterized by the cumulative extent of separation, ξ_N; while the contribution of individual stages, δ_N, to the overall separation is given by the difference between ξ_N for successive stages. These indexes permit the "goodness" of separation for individual stages and for the entire column to be compared on an equivalent basis. This paper examines the effects of changing operating variables of reflux ratio, feed rate, feed composition, and feed stage location on the separation obtained in a distillation column containing a fixed number of ideal stages, and how the single-stage contribution changes when these variables are altered from the design value. The calculations show that the reflux ratio (R) is probably the most important variable in determining how well a column makes a separation. Separation declines rapidly as R is reduced below the design value, as the feed rate is increased at constant boil-up rate, and as the feed concentration drops below the design value. Changing the feed stage location of ±5 stages in a 50-stage column has a minimal effect on separation at all feed compositions. δ_N clearly shows how the contribution of individual stages changes when operating variables are varied from the design values.

INTRODUCTION AND BACKGROUND

The "goodness" of separation obtained in binary multistage distillation can be concisely and accurately characterized by applying Rony's extent of separation, ξ, to the two product streams leaving a distillation column.

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ξ varies between 0 (no separation) and 1 (perfect separation) and is a much better measure of separation than the other commonly used separation factors (*1*). The progressive separation accomplished within the column is best characterized by applying ξ to successive multistage sections within the column. This separation index, called the cumulative extent of separation, ξ_N, clearly shows the cumulative effects of the many stages within the column as the separation progressively increases stagewise (*2*). The difference between ξ_N for successive multistage sections gives the contribution of the individual stages, δ_N, to the overall cumulative extent of separation (*3*).

The present paper examines the effects of changing operating variables of reflux ratio, feed rate, feed composition, and feed stage location on the separation obtained in a distillation column containing a fixed number

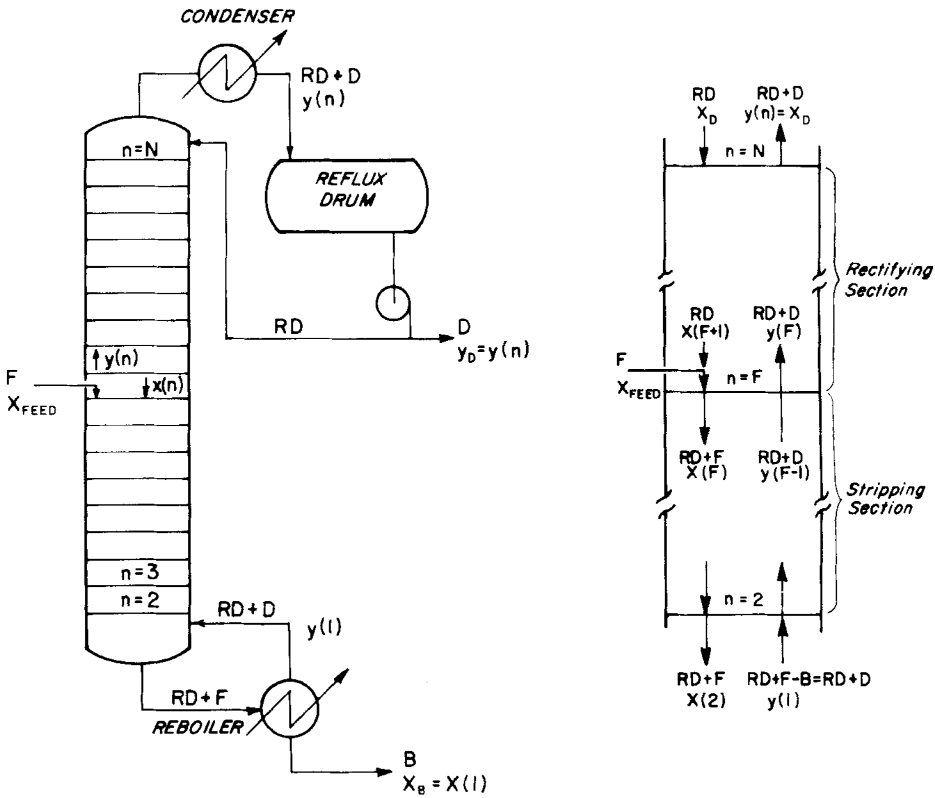

FIG. 1. Equilibrium stage distillation column.

of ideal stages, and how the single stage contributions are distributed among the stages within the column as the variables are changed.

EXTENT OF SEPARATION IN MULTISTAGE DISTILLATION

The different separation indexes are formulated in terms of distribution ratios

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

where n_{im} and n_{ik} are the number of moles of compound i separated to regions m and k, respectively.

For a multistage distillation column the two regions of interest are the bottom and distillate products, but in analyzing the performance of a column we must consider the vapor (Region 3) and liquid (Region 4) streams leaving a multistage section within the column as shown in Fig. 1. This is necessary because the molar rates of the vapor and liquid streams within the columns are different from the product stream rates because of the reflux.

The cumulative extent of separation for the N stages, shown at the right-hand side in Fig. 1, is given by

$$\xi_N(N) = \frac{1}{1 + K_{1N}} - \frac{1}{1 + K_{2N}} \tag{2}$$

where

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

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

The composition of the vapor leaving a stage is given by

$$Y(n) = \frac{\alpha X(n)}{1 + (\alpha - 1)X(n)} \tag{3}$$

Assuming a saturated feed, constant molal overflow, and a total condenser, a material balance yields the composition of the liquid leaving Stages 2 to n for a fixed value of $X_B = X(1)$. For the stripping section, including the stage on which feed is introduced:

$$X(n) = \frac{BX(1) + (RD + D)Y(n - 1)}{RD + F} \quad (4)$$

and for the rectifying section above the feed stage:

$$X(n) = \frac{BX(1) + (RD + D)Y(n - 1) - FX_{\text{Feed}}}{RD} \quad (5)$$

where R is defined as the ratio of moles of reflux to the moles of distillate product.

The single-stage extent of separation is given by using the distribution ratios for the vapor (Region 1) and liquid (Region 2) leaving the stage in equilibrium:

$$\xi_S(n) = \frac{1}{1 + K_1(n)} - \frac{1}{1 + K_2(n)} \quad (6)$$

where

$$K_1(n) = \frac{(RD + F)X(n)}{(RD + D)Y(n)}, \qquad K_2(n) = \alpha K_1(n)$$

The cumulative extent of separation for the n stages is given by

$$\xi_N(n) = \frac{1}{1 + K_{1N}(n)} - \frac{1}{1 + K_{2N}(n)} \quad (7)$$

where

$$K_{1N}(n) = \frac{(RD + F)X(2)}{(RD + D)Y(n)}, \qquad K_{2N}(n) = \frac{(RD + F)[1 - X(2)]}{(RD + D)[1 - Y(n)]}$$

The contribution of stage n to ξ_N is given by

$$\delta_N(n) = \xi_N(n) - \xi_N(n - 1) \quad (8)$$

Calculation Procedure

These equations were programmed on a digital computer and values of ξ_S, ξ_N, and δ_N determined when R, F, X_{Feed} and feed stage were varied from the "design" value for a column containing a fixed number, N, of ideal stages. The solution of the equations requires a trial-and-error procedure:

(1) A value of X_B is assumed and $Y(N)$ is calculated
(2) New values of X_B are assumed until a material balance on the column is satisfied, that is,

$$BX_B + DY(N) = FX_{\text{Feed}} \tag{9}$$

(3) ξ_S, ξ_N, and δ_N are then calculated using the correct value of X_B

The results of these calculations are very sensitive to the value of X_B that is assumed, especially under conditions of low reflux ratio when there are severe pinch zones in the column. In some cases up to 15 significant figures were required in the assumed value of X_B in order for the solution to converge to an acceptable material balance. In all cases the double precision mode was used in the computer calculations.

RESULTS AND DISCUSSION

Many response studies are possible but the following appeared to be the most interesting.

The base case for the calculations were for a column designed to separate a 50% binary mixture, $\alpha = 1.50 =$ constant, into two equal streams, $X_B = .01$ and $Y_D = .99$. With $R = 4.5$ (near the optimum), 50 theoretical stages are required with saturated feed introduced on Stage 25. Thus, $N = 50$ for all of the calculations.

This study shows how changes in these base conditions effect column performance.

A. Effect of Changes in Reflux Ratio

Variable parameter: R between 0 and ∞ (total reflux). Fixed parameters: $N = 50$, $N(F) = 25$, $X_{\text{Feed}} = 0.5$, $F = 2$, $B = D = 1$.

The results of this study are summarized in Figs. 2 through 6. Figure 2 shows how ξ_N increases with stage number as R is increased from 0 to total reflux. At zero reflux there is no separation occurring in the rectifying section of the column, and very little in the stripping section. In the stripping section the liquid stream countercurrent to the vapor is

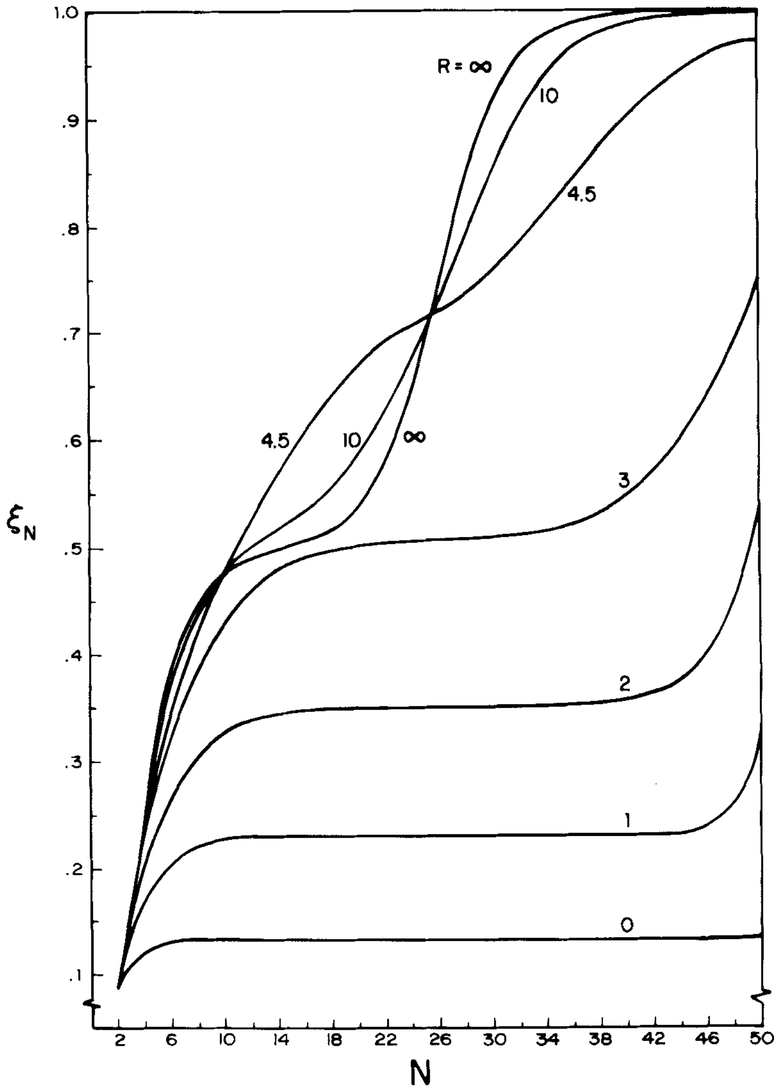

FIG. 2. Cumulative extent of separation as a function of stage number for various reflux ratios. Column contains 50 theoretical stages, α = 1.50.

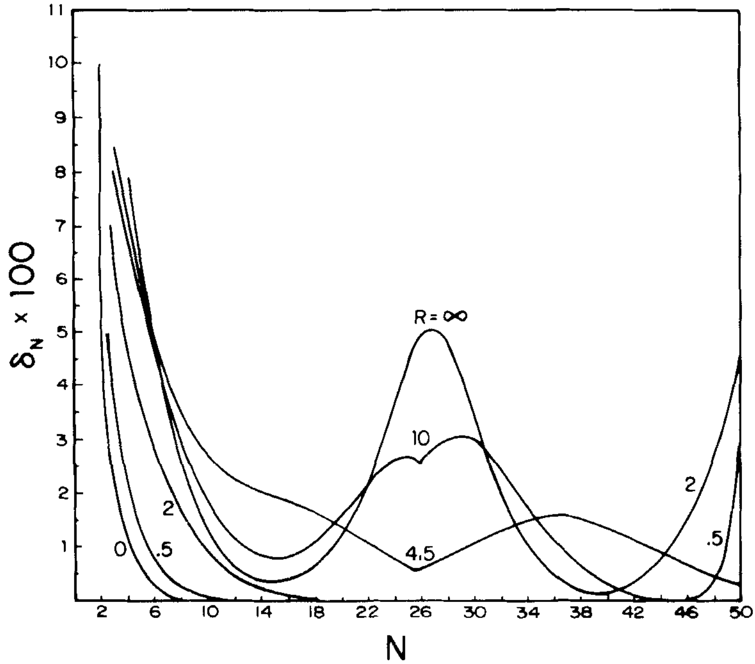

FIG. 3. Individual stage contribution to the cumulative extent of separation for various reflux ratios. Column contains 50 theoretical stages, $\alpha = 1.50$.

provided only by the feed (assumed saturated) and, in the 25 stages of the stripping section, the feed is separated into two streams, $X_B = .400$ and $Y_D = .600$ (equilibrium with the feed, $X_{\text{Feed}} = 0.5$), assuming $B = D = 1$. For this case, almost all of the separation occurs on the bottom few stages because of the severe pinch zone above that point. At finite reflux ratios, there are still severe pinch zones within the column until reflux ratios greater than about 3 are reached. At $R = 4.5$ (the "design" case) the two product streams would have compositions of $X_B = .01$ and $Y_D = Y(50) = .99$. Increasing R above 4.5 does not significantly increase the separation, although the contributions of individual stages are distributed differently as shown in Fig. 3. The overall separation value for the 50-stage column, $\xi_N(50)$, is replotted in Fig. 4 to show the effect of R on the overall separation. As can be seen, the separation decreases rapidly as R is decreased from the design value of 4.5 and increases very little as R is increased above this value.

Figure 3 presents the individual stage contribution, δ_N, to the overall

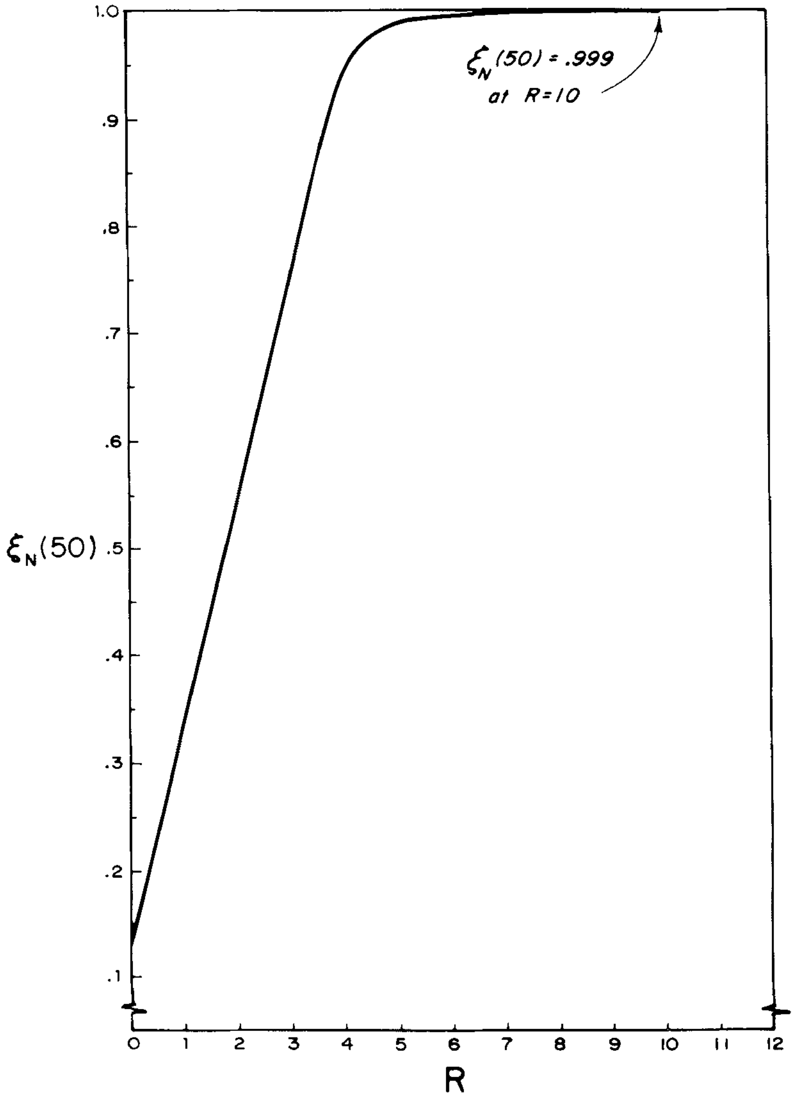

FIG. 4. Overall extent of separation for the 50-stage column as a function of reflux ratio.

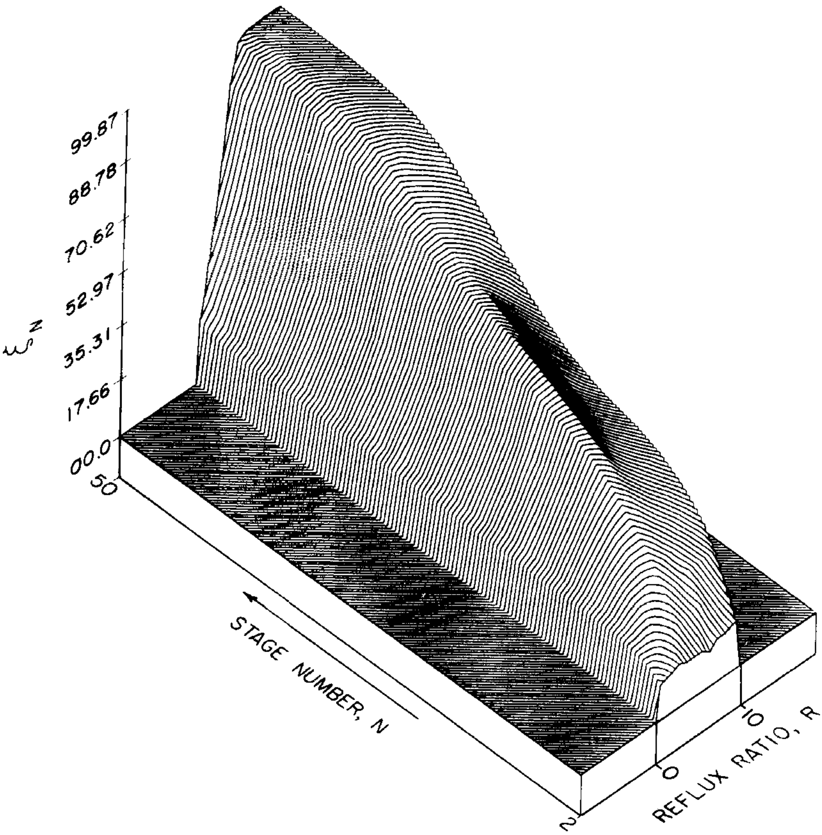

FIG. 5. Cumulative extent of separation as a function of stage number and reflux ratio. This is a three-dimensional plot of part of the data shown in Fig. 2.

separation as a function of N for various values of R. As can be seen, under all conditions the bottom few stages contribute more to the separation than the other stages. At low values of R, stages directly above and below the feed stage contribute little to the separation because of the pinch zone. As R is increased, the center portion of the column contributes more and more to the separation. At higher reflux ratios, relative maxima develop in the δ_N curve in the stages above and below the feed stage. Those maxima converge to the same relative maximum as R is increased to total reflux.

The data that are shown in Figs. 2 and 3 are also presented in Figs. 5 and 6 as three-dimensional plots of ξ_N and δ_N as a function of N and R.

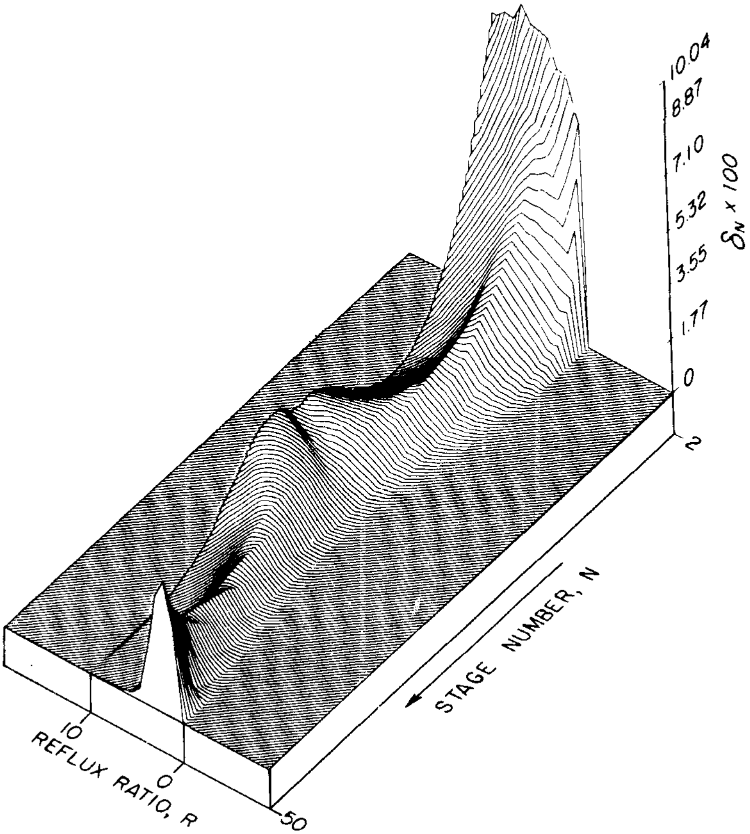

FIG. 6. Individual stage contribution to the cumulative extent of separation as a function of stage number and reflex ratio. This is a three-dimensional plot of part of the data shown in Fig. 3.

These plots were generated from data points representing values of ξ_N and δ_N at 1127 different R and N locations (N from 2 to 50 and R from 0 to 10 at 23 different values of R). Two computer programs were used to make the three-dimensional displays. Both programs were developed at the Harvard Center for Environmental Studies, Harvard University, and are available through the computer at Montana State University. The first program interpolates between point locations to produce a surface in the form of a grid matrix. This matrix is then used by a second program to produce the three-dimensional display on a CALCOMP plotter.

By comparing Figs. 5 and 6 with Figs. 2 and 3, the response of ξ_N and δ_N for different stages within the column to changes in R becomes clearer.

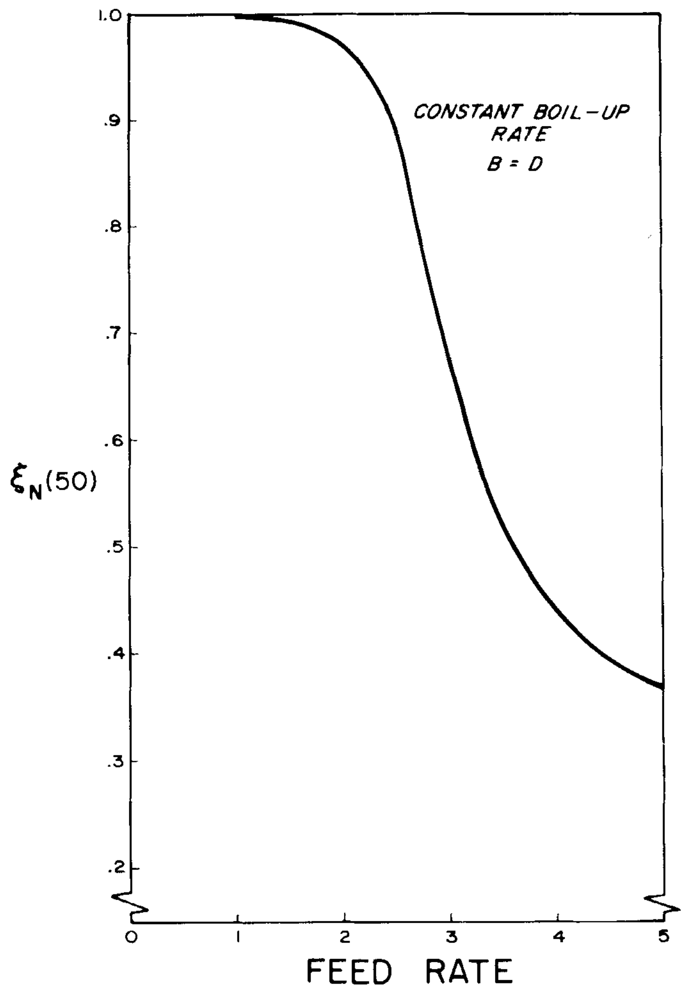

FIG. 7. Overall extent of separation for the 50-stage column as a function of feed rate at constant boil-up rate.

These figures give a good qualitative picture of how reflux ratio affects the separation that occurs in a column containing a fixed number of ideal stages.

B. Effect of Variable Feed Rate

Variable parameter: F between 1 and 5 (base case = 2). Fixed parameters: $N = 50$, $N(F) = 25$, $X_{\text{Feed}} = 0.5$, $B = D = \frac{1}{2}F$.

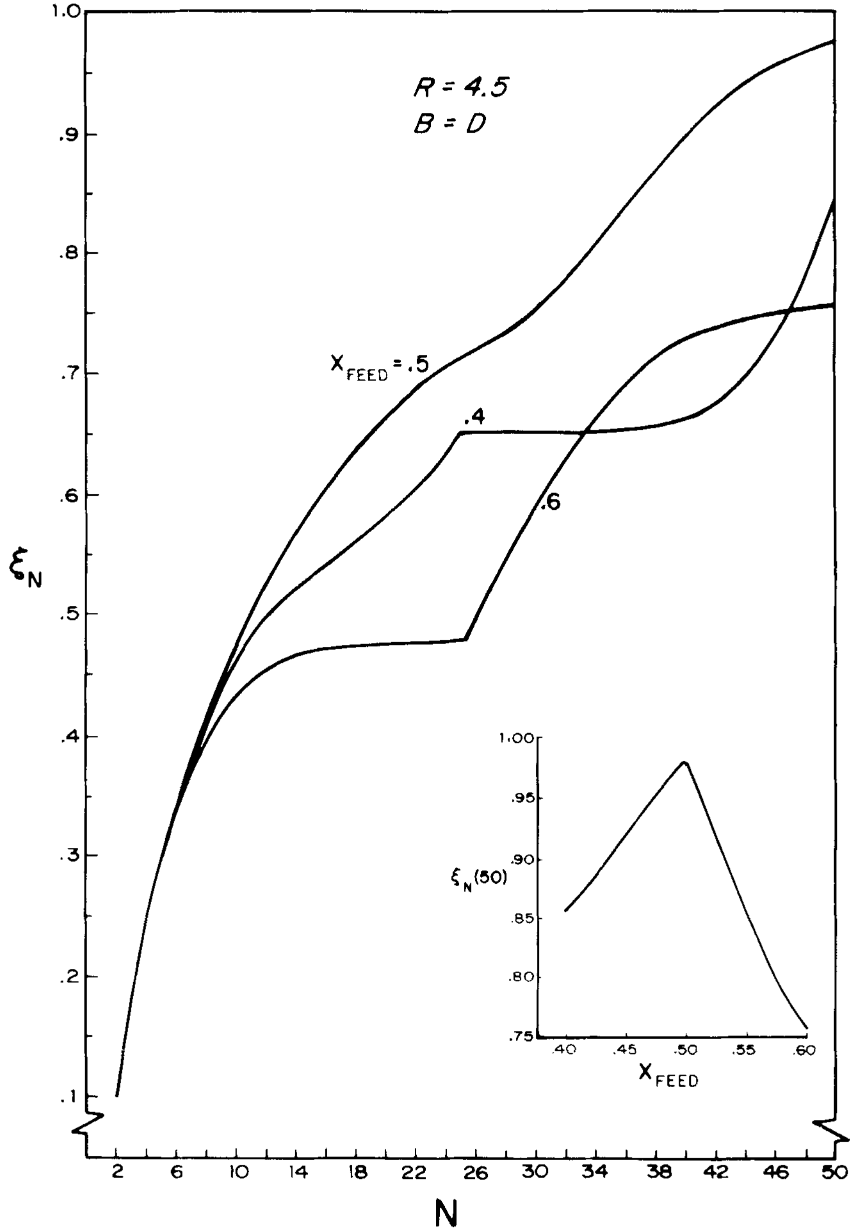

FIG. 8. Cumulative extent of separation as a function of N for various feed compositions. $R = 4.5$, $B = D$.

(a) Constant Boil-up Rate (based on $F = 2$, $R = 4.5$). This case is equivalent to varying the reflux ratio from the base conditions. Thus, for the base case of $F = 2$, $R = 4.5$, the boil-up rate is $(RD + D) = 5.5$, For $F = 1, R = 10$ gives $(RD + D) = 5.5$, and for $F = 5, R = 1.2$ gives $(RD + D) = 5.5$.

The variation in ξ_N for the 50-stage column, $\xi_N(50)$, when the feed rate is varied from 1 to 5 at constant boil-up rate (holding $D = B = \frac{1}{2}F$), is shown in Fig. 7. As can be seen, $\xi_N(50)$ varies from .9989 for $F = 1$ to .3699 for $F = 5$. $\xi_N(50)$ decreases rapidly as F is increased over the design value but increases only slightly at lower values of F.

(b) Constant Reflux Ratio ($R = 4.5$). For this case, as long as $B = D = \frac{1}{2}F$, the separation will be the same as the "design" case of $F = 2$ and $R = 4.5$.

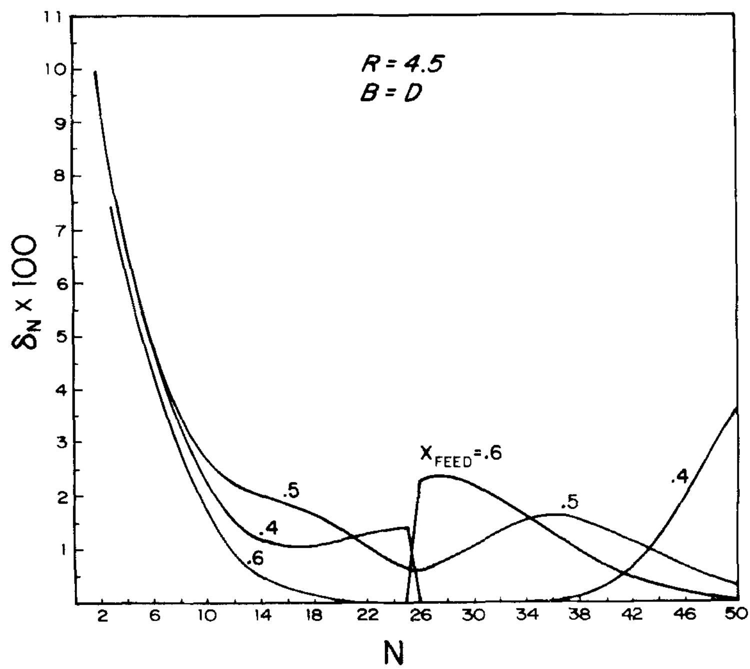

FIG. 9. Individual stage contribution to the cumulative extent of separation for various feed compositions. $R = 4.5$, $B = D$.

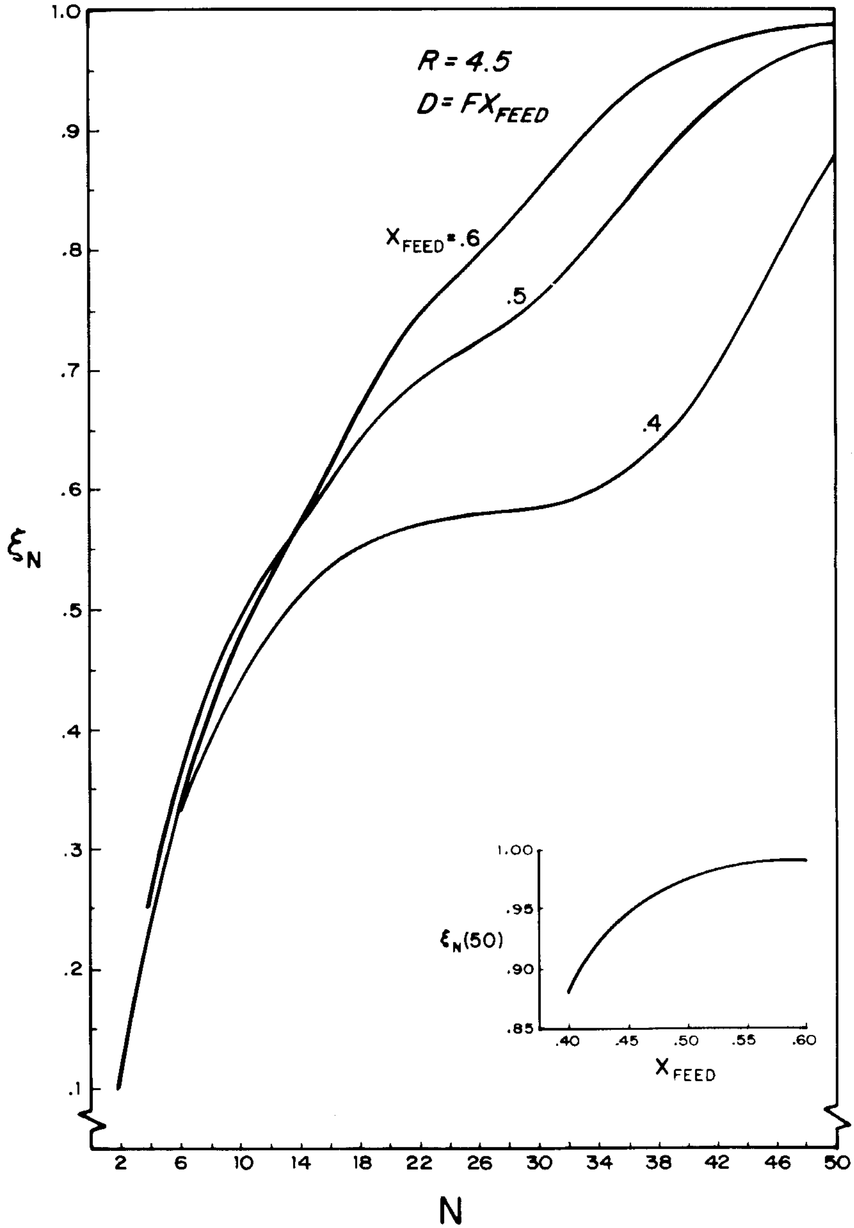

FIG. 10. Cumulative extent of separation as a function of N for various feed compositions. $R = 4.5$, D is proportional to the feed composition.

C. Effect of Variable Feed Composition

Variable parameter: X_{Feed} between 0.4 and 0.6. Fixed parameters: $N = 50, N(F) = 25, R = 4.5, F = 2$.

(a) B = D = ½F. For this case it is assumed that the two product stream rates are maintained at $\frac{1}{2}F$, the same as the design case, when X_{Feed} is varied between 0.4 and 0.6. ξ_N and δ_N curves for this case are shown in Figs. 8 and 9. As can be seen, significant pinch zones are present when X_{Feed} is different from the design value, resulting in a poorer separation. The pinch zone is in the rectifying section of the column directly above the feed stage when $X_{\text{Feed}} < 0.5$ and in the stripping section directly below the feed stage when $X_{\text{Feed}} > 0.5$. Also shown in Fig. 8 is a plot of $\xi_N(50)$ as a function of X_{Feed}. This plot shows that the overall separation for the column drops rapidly as X_{Feed} changes on either side of the design case if B and D are held constant.

(b) B = (1 − X_Feed) F, D = X_Feed F. For this case, D is adjusted so that it is directly proportional to the amount of the lighter component in the feed. The results of these calculations are summarized in Figs. 10 and 11 which show that there is a significant pinch zone in the middle part of the column for $X_{\text{Feed}} = 0.4$, but there is none when $X_{\text{Feed}} \geqslant 0.5$. The cumulative extent of separation for the column, $\xi_N(50)$, increases with increasing feed composition as is also shown by Fig. 10.

D. Effect of Changing Feed Stage Location for Different Values of X_{Feed}

Variable parameter: $N(F)$ from 20 to 30 for different fixed X_{Feed}. Fixed parameters: $N = 50, F = 2, D = X_{\text{Feed}}F$.

The results of this study are summarized in Fig. 12 which shows how ξ_N changes as the feed stage location is moved either up or down the column 5 stages for different fixed values of X_{Feed}. As can be seen, as long as the product stream rates are adjusted to be proportional to the feed composition, the feed stage location (±5 stages from the design case) has little effect on the separation. Figure 12 also shows how $\xi_N(50)$ varies with feed stage location for $X_{\text{Feed}} = 0.4$, 0.5 and 0.6. In all cases the maximum separation occurs when $N(F) = 25$. The variation is smallest for $X_{\text{Feed}} =$ 0.6 (about 0.7%) and greatest for $X_{\text{Feed}} = 0.4$ (1.8%).

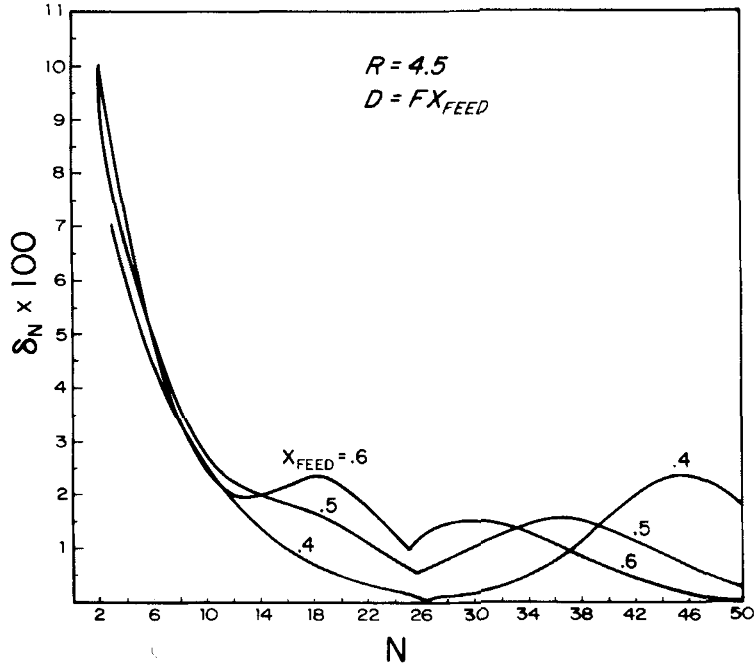

FIG. 11. Individual stage contribution to the cumulative extent of separation for various feed composition. R = 4.5, D is proportional to the feed composition.

E. Effect of Increasing the Reflux Ratio When X_{Feed} Is Below the Design Value

As shown in Section C, separation declines rapidly when the feed composition is lower than the design value of $X_{\text{Feed}} = 0.5$ at constant R. The separation is improved somewhat if the product rates are adjusted to be proportional to the feed composition, but it is still well below the separation that results when X_{Feed} is the design value. This study investigated the effects of increasing R when the feed composition is reduced to $X_{\text{Feed}} = 0.4$. The results are summarized in Fig. 13 which shows that increasing R from 4.5 to 5.5 increases $\xi_N(50)$ from about 0.881 to 0.972, only slightly below the "design" value of 0.9765.

Figure 14 summarizes how the column separation, $\xi_N(50)$, is changed when B, D, and R are varied ($X_{\text{Feed}} = 0.4$). From this figure it is evident that increasing R is the key to maintaining efficient column separation.

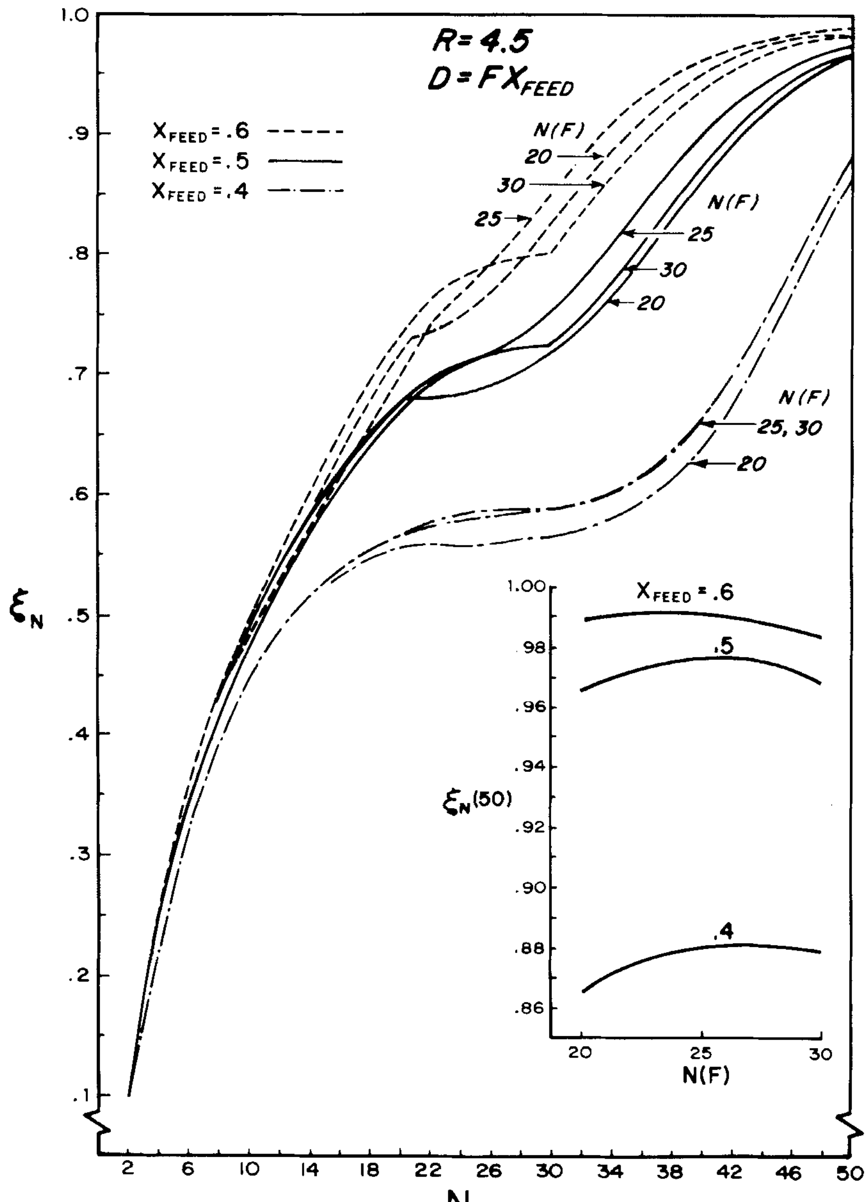

FIG. 12. Effect of feed composition and feed stage location on the cumulative extent of separation. $R = 4.5$. D is proportional to the feed composition.

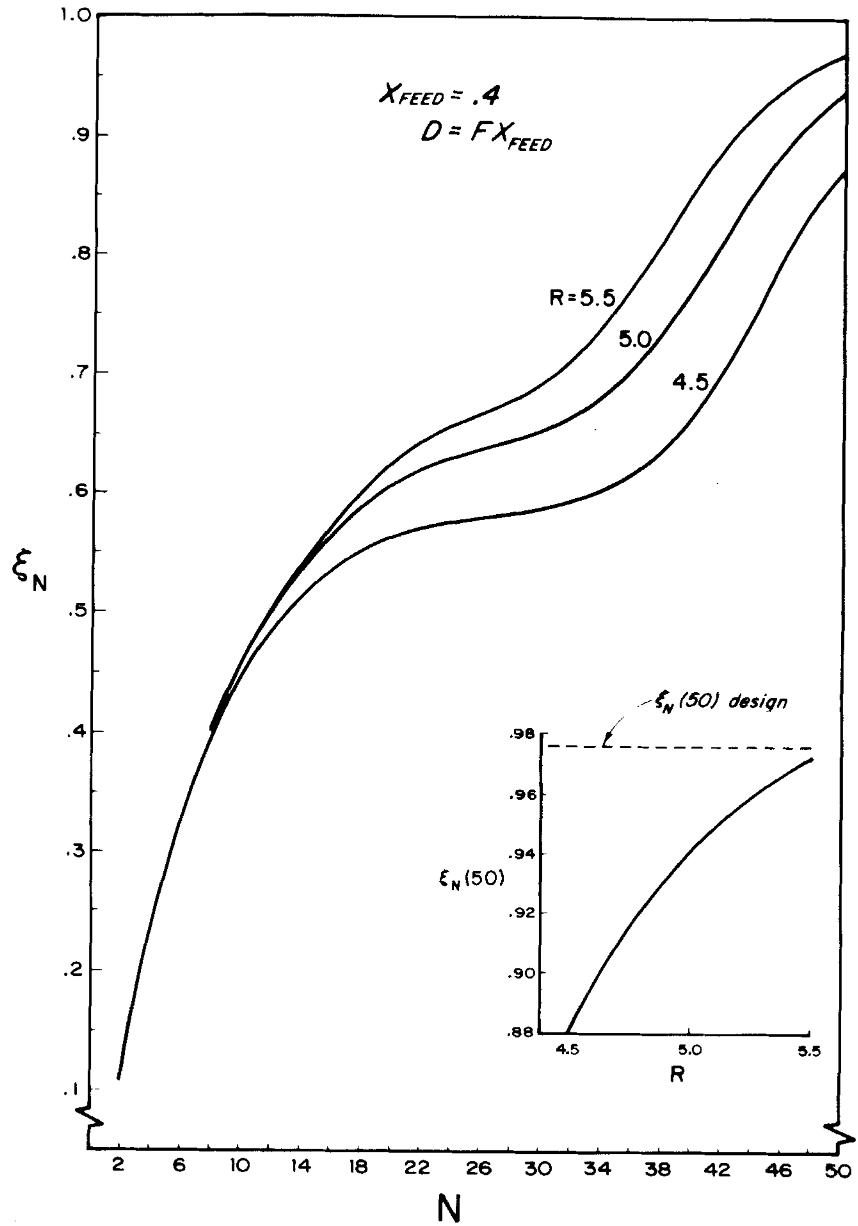

FIG. 13. Effect of increasing reflux ratio on the cumulative extent of separation when the feed composition is below the design value.

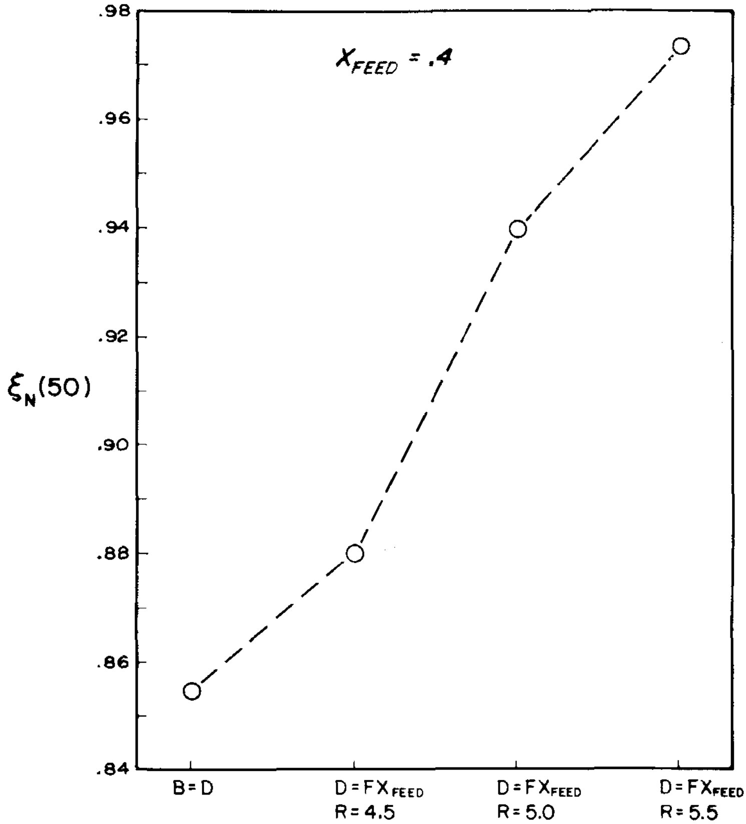

FIG. 14. Effect of reflux ratio on the overall separation when the feed composition is below the design value.

GENERAL DISCUSSION

The previous sections of this paper have shown that the separation obtained under different operating conditions in a multistage distillation column can be meaningfully compared on an equivalent basis using Rony's extent of separation. ξ_N shows how the separation progressively increases stage-wise within the column while δ_N gives the contribution of the individual stages to the overall separation. These indexes clearly show how changes in operating variables affect the "goodness" of separation, indicating where pinch zones occur within the column, and how the areas of the pinch zone change within the column as changes are made in the operating conditions.

These calculations show that reflux ratio is probably the most important variable in determining the goodness of separation in a column containing a fixed number of stages. The separation deteriorates rapidly if R is decreased from the design value while the separation increases only slightly with increases in R over the optimum. For this case, of course, in a real column it may not be possible to increase R indefinitely as was assumed in the present study because at a high enough R, flooding will occur. However, in practice, columns can be designed to accommodate a large variation in vapor and liquid velocities and so the trends shown here are probably meaningful. In any case, the feed rate could be reduced to accommodate higher values of R.

When the feed rate is increased above the design value, while holding the boil-up rate constant, there is a rapid decline in separation, but separation increases only slightly as the feed rate is decreased below the design value. Again, this shows that R is the key to column control for separation.

Changes in feed composition can have a pronounced effect on separation. For example, if product rates and reflux ratio are kept the same, a 20% increase or decrease in X_{Feed} results in 22 and 12% decreases in $\xi_M(50)$, respectively. If product rates are adjusted to be proportional to the feed composition at constant R, then the separation is improved for $X_{\text{Feed}} > 0.5$ but is still about 10% lower than the design case if X_{Feed} is reduced to a value of 0.4. For this case, increasing R from 4.5 to 5.5 improves $\xi_M(50)$ so that it is only about 0.5% lower than the design value.

When the feed stage location is changed 5 stages above or below the "design value, $\xi_M(50)$ declines only slightly (0.6 to 1.8%) at all the feed compositions that were investigated ($X_{\text{Feed}} = 0.4, 0.5, 0.6$). This result was rather surprising since most texts dealing with column design stress the need to match feed composition with the composition of the streams within the column, and it was assumed that the effects of a feed mismatch would be more significant. Again, for this case it appears that increasing R is the key to obtaining the design separation if the feed location is mismatched with the composition within the column.

In summary, $\xi_M(N)$ and δ_N show qualitatively (and possibly quantitatively) how changes in operating variables affect the separation, and where within the column the changes in the separation characteristics are most pronounced. The magnitudes of the effects will, of course, vary with α and the desired product purities, but a study of this nature indicates what corrective measures may be effective in restoring separation efficiency when feed rate, feed composition, or other pertinent feed or operating variables change from the "design" value.

The present study of a hypothetical system illustrates the application of the method. It was by no means exhaustive and a great many additional applications would be possible. For example, the method could easily be applied to systems where α changes with composition and/or where constant molal overflow cannot be assumed. It should also be possible to apply the method to multicomponent systems using the extent of separation between key components. In addition, the method is not restricted to distillation but could easily be applied to other multistage separation systems. Additional hypothetical studies would probably be unproductive, but hopefully this method of viewing separation in a multistage system will eventually find significant application in the real world.

SYMBOLS

B	bottom product rate
D	distillate product rate
F	feed rate, also feed stage
K_i	distribution ratio of component i
$K_{iN}(n)$	distribution ratio of multistage sections for component i
$K_i(n)$	distribution ratio on a single ideal stage N
N	number of stages in a multistage section
n	stage number
R	reflux ratio (moles reflux/moles distillate)
$X(n)$	liquid phase composition (mole fraction) leaving stage n
$Y(n)$	vapor phase composition (mole fraction) leaving stage n

Greek Letters

α	relative volatility $\left(\alpha = \dfrac{Y(1-X)}{X(1-Y)} = \dfrac{K_2(n)}{K_1(n)}\right)$
$\xi_S(n)$	extent of separation for equilibrium stage n
$\xi_N(n)$	cumulative extent of separation stages 2 to n
$\xi_N(50)$	cumulative extent of separation for 50 stage column
$\delta_N(n)$	contribution of stage n to ξ_N

Subscripts

B	bottom product
D	distillate product
Feed	composition of feed stream

i	component i
iN	component i leaving multistage section
N	multistage section

REFERENCES

1. P. R. Rony, in *Recent Advances in Separation Techniques* (AIChE Symposium Series 120), Vol. 68, 1972, pp. 89–104.
2. F. P. McCandless, "The Extent of Separation in Continuous Multistage Binary Distillation," *Sep. Sci. Technol., 17*(12), 1361–1385 (1982–83).
3. F. P. McCandless, "Single-Stage Contribution to the Overall Separation in Binary Multistage Distillation," *Ibid., 18*(9), 803–819 (1983).

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