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A. K. Mahendra[a]; V. D. Puranik[a]; B. Bhattacharjee[a]
[a] CHEMICAL TECHNOLOGY DIVISION, BHABHA ATOMIC RESEARCH CENTRE, MUMBAI, INDIA

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Separative Power for a Binary Mixture of Isotopes

A. K. MAHENDRA,* V. D. PURANIK, and B. BHATTACHARJEE
CHEMICAL TECHNOLOGY DIVISION
BHABHA ATOMIC RESEARCH CENTRE
MUMBAI-400 085, INDIA

ABSTRACT

A more accurate expression for the separative power of a device separating a binary mixture into two streams with a large separation factor is worked out by taking recourse to the thermodynamic entropy function without any simplification. It is also shown that the expression reduces to the commonly used form under the assumption of close separation.

INTRODUCTION

For a separation device, the separation factor expresses the change in the composition, while the throughput or flow rates indicate the rate at which this change is effected. The separative power of the device is a property which combines both the magnitude of change in composition and the rate at which it is brought about. It is thus a measure which describes the separation performance of the separating device comprehensively. Historically, the expression for the separative power was derived under the assumption of close separation for use in the gaseous-diffusion process, where the separation factor is small. In the present work, a more accurate expression for the separative power for a device having a large separation factor is derived by taking recourse to the thermodynamic entropy function without any simplification.

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* To whom correspondence should be addressed.

SEPARATIVE POWER AND VALUE FUNCTION

The separative power of a device separating a binary isotopic mixture partially into two streams is given by the following expression:

$$\delta U = P_1 V(N_{P_1}) + P_2 V(N_{P_2}) - FV(N_F) \tag{1A}$$

The expression is similar to the one for the conservation of an extrinsic property in a steady-state flow process, the extrinsic property in the present case being the value function. It may be noted that the value function is a function of composition alone, and its functional form is arrived at with the objective of making the separative power of the device independent of composition. The following expression for the value function is derived under the assumption of close separation (1, 2) which allows the terms of order larger than 2 to be neglected (see Appendix 1):

$$V(N) = (2N - 1)\ln[N/(1 - N)] \tag{1B}$$

However, the above expression of the value function is also commonly used to calculate the separative power of a device with a large separation factor. Perhaps one can justify the practice with the notion that a device with a large separation factor can be split into many small subdevices (such that each subdevice is amenable to close separation) and the separative power of each of such subdevices can be subsequently added to get the separative power of the device (because the above expression of the value function has the additivity property). In reality, such a simplification for a large separation case may lead to propagation of significant error in the calculation. In the present study an accurate expression for separative work for large separation factors is derived by relating separative work with the thermodynamic entropy.

SEPARATIVE POWER AND ENTROPY

The separation process is characterized by a decrease in entropy or disorder. But the rate of change of the mixing entropy of the isotopes varies with the composition of the mixture (3), and hence would vary according to the position of separating device in a cascade. The entropy change is greatest when $N_F = 0.5$ and becomes very small when N_F is either close to zero or close to 1. For a mixture containing two isotopes with concentrations N and $(1 - N)$ respectively, the entropy change caused by the separating element is proportional to $N(1 - N)$. This is because of all the fractions of possible pairs of molecules upon which the element does the separation job, it is only the fraction of unlike pairs, i.e., $N(1 - N)$, which results in useful separation. Separation can be visualized as being produced by a Maxwell's demon (4) working in the element. Apart from simply separating the pairs of unlike molecules, Maxwell's demon also works in finding them. In order to find a molecule of a particular isotope, the demon has first to forget the result of its previous observation. The erasure of the previous observation in the brain of the demon working inside the separating element increases the entropy of the combined demon-separating element system (5, 6). (It should be noted that the paradox of the apparent violation of the second law of thermodynamics by Maxwell's demon was resolved as a result of research on the energy requirement of computations.) Thus the information erasure which occurs after every finding of the molecule of the desired isotope leads to the dissipation of energy (7). The information required by the demon for distinguishing between molecules of desired and undesired isotopes depends on the number of unlike pairs. Thus the fruitful work done by Maxwell's demon is based on the entropy change per pair of unlike molecules separated by the demon (8). For a device handling a feed rate of F mol/s with concentration N, the separative work done per unit time by Maxwell's demon of the separative device is proportional to $\Delta S/\{N(1 - N)\}$. The separative power can therefore be defined as

$$\delta U = F\Delta S/\{RN(1 - N)\} \tag{2}$$

The entropy per mole of the mixture of isotopes is greater than the constituents at the same temperature by an amount

$$S(N) = R\{N \ln N + (1 - N)\ln(1 - N)\} \tag{3}$$

For a separative element with a throughout of F mol/s of the mixture with concentration N_F that produces a fraction θF of product P_1 at mole fraction N_{P_1} and $(1 - \theta)F$ of product P_2 at mole fraction N_{P_2} (as in Fig. 1), the total change in entropy per mole is given by

$$\Delta S(N_F) = \theta S(N_{P_1}) + (1 - \theta)S(N_{P_2}) - S(N_F) \tag{4}$$

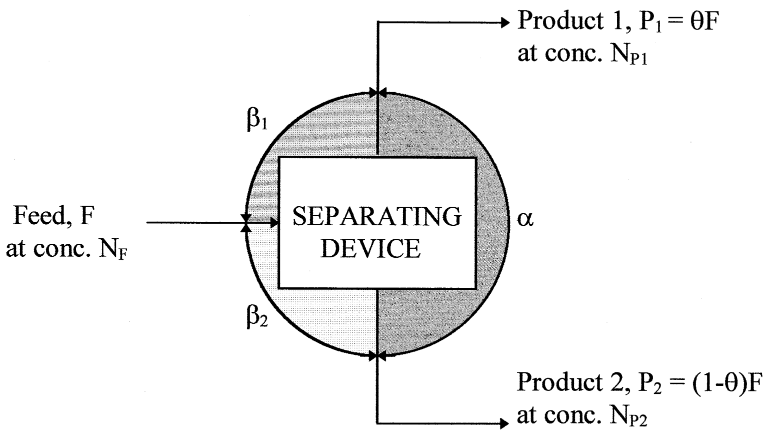

FIG. 1 Separating device.

Expanding $S(N_{P_1})$ and $S(N_{P_2})$ around $S(N_F)$ using the Taylor series, we obtain

$$S(N_{P_1}) = S(N_F) + \sum_{n=1}^{n=\infty} \{(N_{P_1} - N_F)^n/n!\}\{d^n\, S(N_F)/dN_F^n\} \tag{5}$$

$$S(N_{P_2}) = S(N_F) + \sum_{n=1}^{n=\infty} \{(N_{P_2} - N_F)^n/n!\}\{d^n\, S(N_F)/dN_F^n\} \tag{6}$$

From Eqs. (4)–(6) and utilizing mass balance and single component balance, the change in entropy per mole of the feed for the mixture of isotopes works out to be

$$\begin{aligned}\Delta S(N_F) = &\sum_{n=2}^{n=\infty} (1/n!)\{d^n S(N_F)/dN_F^n\}\\ &\times [\theta(N_{P_1} - N_F)^n + (1-\theta)(N_{P_2} - N_F)^n]\end{aligned} \tag{7}$$

Further, from mass balance and single component balance:

$$(N_{P_2} - N_F)^n = (-1)^n[\theta/(1-\theta)]^n(N_{P_1} - N_F)^n \tag{8}$$

$$(N_{P_1} - N_F)^n = N_F^n(1 - N_F)^n(\xi/\theta)^n \tag{9}$$

where

$$\xi = (\beta_1 - 1)(\beta_2 - 1)/(\alpha - 1) \tag{10}$$

With the use of Eqs. (8) and (9), the change in entropy per mole of the feed for the mixture of isotopes can be shown to be

$$\begin{aligned}\Delta S(N_F) = &\sum_{n=2}^{n=\infty} (N_F^n(1 - N_F)^n/n!)\{d^n S\\ &\times (N_F)/dN_F^n\}(\xi/\theta)^n\theta\,[1 + (-1)^n\{\theta/(1-\theta)\}^{n-1}]\end{aligned} \tag{11}$$

By differentiating the entropy function in Eq. (3) and substituting in Eq. (11), we get

$$\Delta S(N_F) = \sum_{m=0}^{m=\infty} RN_F(1 - N_F)\,\chi_m\psi_m/\{(m+2)(m+1)\} \tag{12}$$

where

$$\chi_m = \theta(\xi/\theta)^{m+2} + (-1)^m(1-\theta)\{\xi/(1-\theta)\}^{m+2} \tag{13}$$

and

$$\psi_m = N_F^{m+1} - (-1)^{m+1}(1 - N_F)^{m+1} \tag{14}$$

Thus, the separative power of a separating device per mole of the feed can be written as

$$\delta U(N_F)/F = \Delta S(N_F)/\{RN_F(1 - N_F)\} = \sum_{m=0}^{m=\infty} \chi_m \psi_m/\{(m + 2)(m + 1)\} \tag{15}$$

The solution of Eq. (15) finally leads to

$$\begin{aligned} \delta U(N_F)/F = {} & [(\xi - \theta/N_F) \ln\{\theta/(\theta - \xi N_F)\} + \{\xi \\ & - (1 - \theta)/(1 - N_F)\} \ln[(1 - \theta)/\{(1 - \theta) - \xi \\ & \times (1 - N_F)\}] - \{\xi + (1 - \theta)/N_F\} \ln[(1 - \theta)/\{(1 - \theta) \\ & + \xi N_F)\}] - \{\xi + \theta/(1 - N_F)\} \ln\{\theta/\{\theta + \xi(1 - N_F)\}] \end{aligned} \tag{16}$$

It should be noted from Eq. (10) that ξ is a function of β_1, β_2, and α. Further, β_1 and β_2 can be expressed as functions of α, θ, and N_F as follows:

$$\beta_1 = \{\sqrt{(\lambda^2 + 4N_F(1 - N_F)\alpha)} + \lambda\}/(2N_F) \tag{17}$$

$$\beta_2 = \{\sqrt{(\lambda^2 + 4N_F(1 - N_F)\alpha)} - \lambda\}/\{(2(1 - N_F)\} \tag{18}$$

where

$$\lambda = \alpha(N_F - \theta) + N_F + \theta - 1 \tag{19}$$

It is to be noted that the expression for separative power given by Eq. (16) has been derived from the entropy function and is without the assumption of close separation. The expression for separative power given by Eq. (16) can be used for any isothermal process for a binary ideal solution where separation is taking place. The equation for the case of close separation can be obtained from Eq. (11) as per the details shown in Appendix 2.

A plot of $\delta U/F$ with respect to feed concentration, N_F, and cut, θ, for a case where the value of the overall separation factor is 6 is shown in Fig. 2.

It is clearly observed that the separative power for a device handling a binary mixture with a large separation factor is a function of feed concentration, N_F, overall separation factor, α, and cut, θ. Even for a symmetric separation process (i.e., $\beta_1 = \beta_2 = \beta$), δU is a function of feed concentration, N_F, and overall separation factor, α, and hence δU cannot be made independent of N_F. The expressions for the separative power become much simpler for cases where $N_F \cong 0$, $N_F = 0.5$, and $N_F \cong 1$.

Separative Power for the Case Where $N_F \cong 0$ and $N_F \cong 1$

In the case when $N_F \cong 0$, Eq. (14) reduces to

$$\psi_m = (-1)^m \tag{20}$$

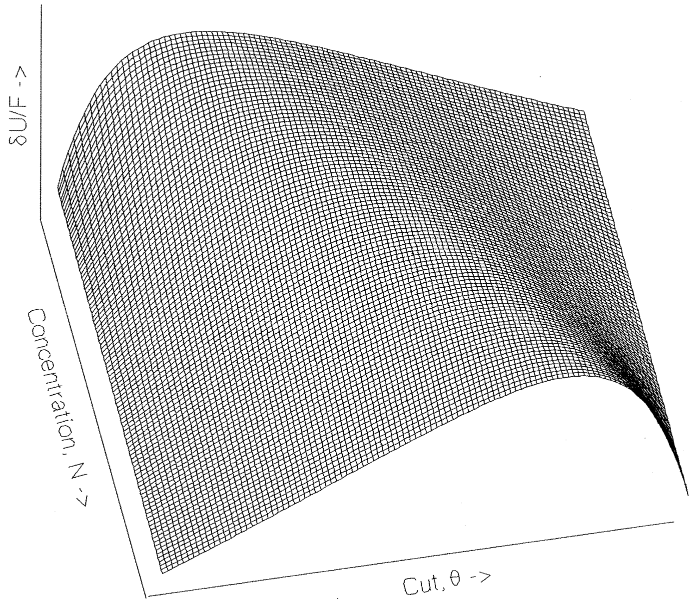

FIG. 2 Plot of $\delta U/F$ with respect to cut θ and concentration N for an overall separation factor $\alpha = 6$.’

which makes the separative power of an element per mole of feed

$$\delta U(0)/F = \Big[(\xi + \theta)\sum_{m=0}^{m=\infty}(-1)^m(\xi/\theta)^{m+1}/(m+1) + (\xi - 1 + \theta)\sum_{m=0}^{m=\infty}\{\xi/(1-\theta)\}^{m+1}/(m+1)\Big] \tag{21}$$

The solution given by Eq. (21) leads to

$$\delta U(0)/F = [-(\xi + \theta)\ln\{\theta/(\xi + \theta)\} + (\xi - 1 + \theta)\ln\{(1-\theta)/(1-\theta-\xi)\}] \tag{22}$$

Further, at $N_F \cong 0$,

$$\beta_1 = \alpha/\{1 + (\alpha - 1)\theta\} \tag{23}$$

$$\beta_2 = 1 + (\alpha - 1)\theta \tag{24}$$

which simplifies the separative power per mole of feed of a separating device to

$$\delta U(0)/F = [\ln(\beta_1) - \{(\beta_1 - 1)/(\alpha - 1)\}\ln(\alpha)] \tag{25}$$

This expression is similar to the one given by Bulang et al. (9) [a printing error in their formula was pointed out by Apelblat and Lehrer-Ilamed (10)]. However, the expression derived by Kanagawa and Yamamoto (13–16) is

$$\delta U(0)/F = [\ln(\beta_2) - \{(\beta_2 - 1)/(\alpha - 1)\}\ln(\alpha)] \tag{26}$$

It may be noted that the expression obtained by us and the one by Bulang et al. (9) for $N_F \cong 0$ is different from the expressions obtained by Kanagawa and Yamamoto (13–16). While on the subject, it may be mentioned that the expressions obtained by Kanagawa and Yamamoto can be obtained from the value function for close separation case (see Appendix 3), and therefore do not represent cases with large separation factors.

For the case when $N_F \cong 0$, the separative power per mole of feed is a function of β_1, the heads separation factor. Similarly for the case when $N_F \cong 1$, the expression for the separative power will be a function of β_2, the tails separation factor. The separative power per mole of feed of a separating device when $N_F \cong 1$ can be written as

$$\delta U(1)/F = [\ln(\beta_2) - \{(\beta_2 - 1)/(\alpha - 1)\}\ln(\alpha)] \tag{27}$$

whereas the expression derived by Kanagawa and Yamamoto (13–16) is

$$\delta U(1)/F = [\ln(\beta_1) - \{(\beta_1 - 1)/(\alpha - 1)\}\ln(\alpha)] \tag{28}$$

It may be noted that the above expression obtained for $N_F \cong 1$ is different from the expression obtained by Kanagawa and Yamamoto (13–16).

Separative Power at $N_F = 0.5$

In the case when $N_F \cong 0.5$, Eq. (14) reduces to

$$\psi_m = (0.5)^{m+1} + (-1)^m(0.5)^{m+1} \tag{29}$$

which makes the separative power of an element per mole of feed

$$\begin{aligned}\delta U(0.5)/F = [&(\xi + 2\theta)\sum_{m=0}^{m=\infty}(\xi/2\theta)^{m+1}/(m+1)\\ &+ (\xi - 2\theta)\sum_{m=0}^{m=\infty}(-1)^m(\xi/2\theta)^{m+1}/(m+1)\\ &+ \{\xi + 2(1-\theta)\}\sum_{m=0}^{m=\infty}\{\xi/2(1-\theta)\}^{m+1}/(m+1)\\ &+ \{\xi - 2(1-\theta)\}\sum_{m=0}^{m=\infty}(-1)^m\{\xi/2(1-\theta)\}^{m+1}/(m+1)]\end{aligned} \tag{30}$$

The solution given by Eq. (30) leads to

$$\begin{aligned}\delta U(0.5)/F = {} & [\xi \ln\{(2\theta + \xi)/(2\theta - \xi)\} + \xi \ln \\ & \times [\{2(1-\theta) + \xi\}/\{(2(1-\theta) - \xi)\}] - 2\theta \ln \\ & \times [(2\theta)^2/\{2\theta + \xi\}\,\{2\theta - \xi\}] - 2(1-\theta) \ln \\ & \times [\{2(1-\theta)\}^2/\{2(1-\theta) + \xi\}\,\{2(1-\theta) - \xi\}]]\end{aligned} \tag{31}$$

By substituting the following expressions for β_1 and β_2 in Eq. (31), one obtains the expression for separative power at $N_F = 0.5$.

$$\beta_1 = \sqrt{(\alpha - 1)^2\,(0.5 - \theta)^2 + \alpha} + (\alpha - 1)(0.5 - \theta) \tag{32}$$

$$\beta_2 = \sqrt{(\alpha - 1)^2\,(0.5 - \theta)^2 + \alpha} - (\alpha - 1)(0.5 - \theta) \tag{33}$$

SEPARATIVE POWER FOR A SYMMETRIC DEVICE

In general, for symmetric cases (i.e., $\beta_1 = \beta_2 = \beta$), the expression for separative power as a function of β and N_F obtained from Eq. (16) is

$$\begin{aligned}[\delta U(N_F, \beta)/F]_{\text{sym}} = {} & \beta \ln \beta/\{(\beta + 1)N_F(1 - N_F)\} \\ & - \{(1 - N_F) + \beta N_F\} \ln\{1 + (\beta - 1)N_F\}/\{(\beta \\ & + 1)N_F(1 - N_F)\} - \{N_F + \beta(1 - N_F)\} \ln\{1 \\ & + \beta(1 - N_F)\}/\{(\beta + 1)N_F(1 - N_F)\}\end{aligned} \tag{34}$$

The above expression simplifies near $N_F \cong 0$ and $N_F \cong 1$ to

$$[\delta U/F]_{\text{sym}} = \{(\beta - 1)/(\beta + 1)\} \ln \beta \tag{35}$$

It simplifies near $N_F \cong 0.5$ to

$$\begin{aligned}[\delta U(0.5, \beta)/F]_{\text{sym}} = {} & \{(\beta - 1)/(\beta + 1)\} \ln \beta \\ & + \{(3\beta + 1)/(\beta + 1)\} \ln \beta + 4 \ln\{2/(1 + \beta)\}\end{aligned} \tag{36}$$

Kanagawa and Yamamoto (13–16) have, however, arrived at an equation identical to Eq. (35) for the entire range of feed concentration. The function given by Eq. (35) is identical to the commonly used expression for symmetric cases.

In order to get an idea of the magnitude of error between the separative power given by Eq. (36) and Eq. (35), the error between them (evaluated at $N_F \cong 0.5$) is plotted in Fig. 3.

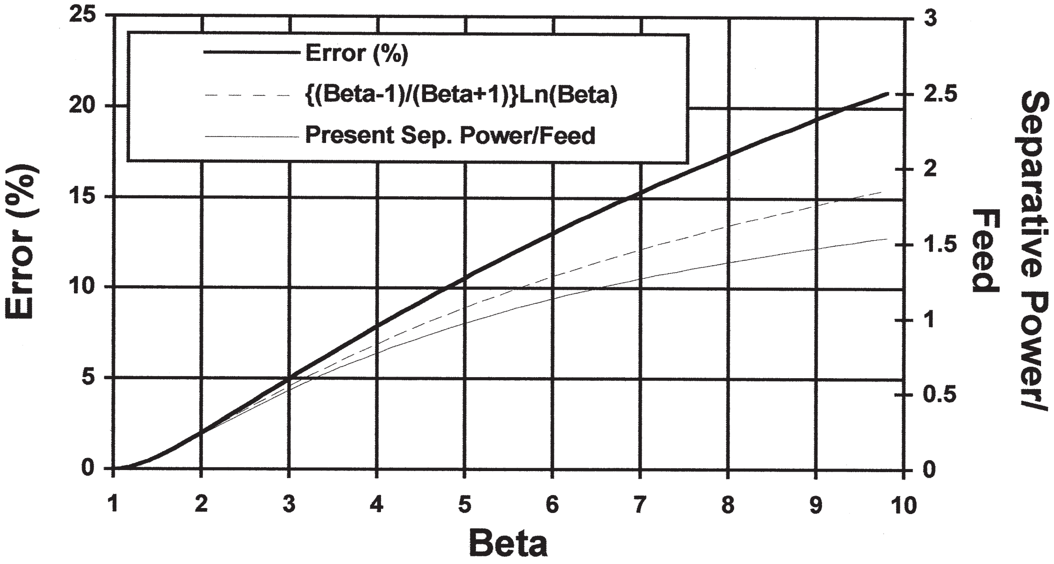

FIG. 3 Graph of separative power and error (%) for symmetric device at feed concentration $N_F = 0.5$.

For instance, consider the case of deutrium exchange between ammonia and hydrogen—a process employed for producing heavy water. This exchange involves seven isotopic species, viz., NH_3, NH_2D, NHD_2, ND_3, H_2, HD, and D_2, and 12 different reactions are possible. The overall separation factor will depend upon any four reactions which involve all the seven species. Thus the following reactions describe the exchange:

$$NH_3 + HD \leftrightarrows NH_2D + H_2 \tag{37}$$

$$NH_3 + NHD_2 \leftrightarrows 2NH_2D \tag{38}$$

$$NH_2D + ND_3 \leftrightarrows 2NHD_2 \tag{39}$$

$$H_2 + D_2 \leftrightarrows 2HD \tag{40}$$

The overall separation factor α in NH_3–H_2 exchange given by the Eqs. (37)–(40) is around 8.571, which corresponds to $\beta = 2.927$ at 193.16 K for a symmetric case (17). This gives an error of nearly 5% in evaluation of separative power per mole of feed using Eq. (35).

DIFFERENCE IN THE PRESENT AND THE CONVENTIONAL VALUE FUNCTION

The present value function of a stream at concentration N is proportional to the entropy per mole $S(N)$ divided by the probability of the entropy change given by the fraction of unlike pairs at the feed concentration of the device,

N_F. Thus, the value function is written

$$V(N) = [N \ln N) + (1 - N) \ln(1 - N) + \ln(2)]/\{N_F(1 - N_F)\} \qquad (41)$$

The extra term, ln(2), which has been added in Eq. (41), does not alter the value of separative power; rather it is done so that the boundary conditions given below are satisfied.

$$V(N)_{N=0.5} = \{dV(N)/dN\}_{N=0.5} = 0 \qquad (42)$$

Figure 4 shows the different value functions plotted against feed concentration. It should be noted that the above graph is symmetric about $N = 0.5$ only because of the imposed boundary condition given by Eq. (42). By imposing a similar boundary condition at any arbitrary concentration other than $N = 0.5$, e.g., given by Eq. (43), the graph shown in Fig. 4 will no longer be symmetric about $N = 0.5$.

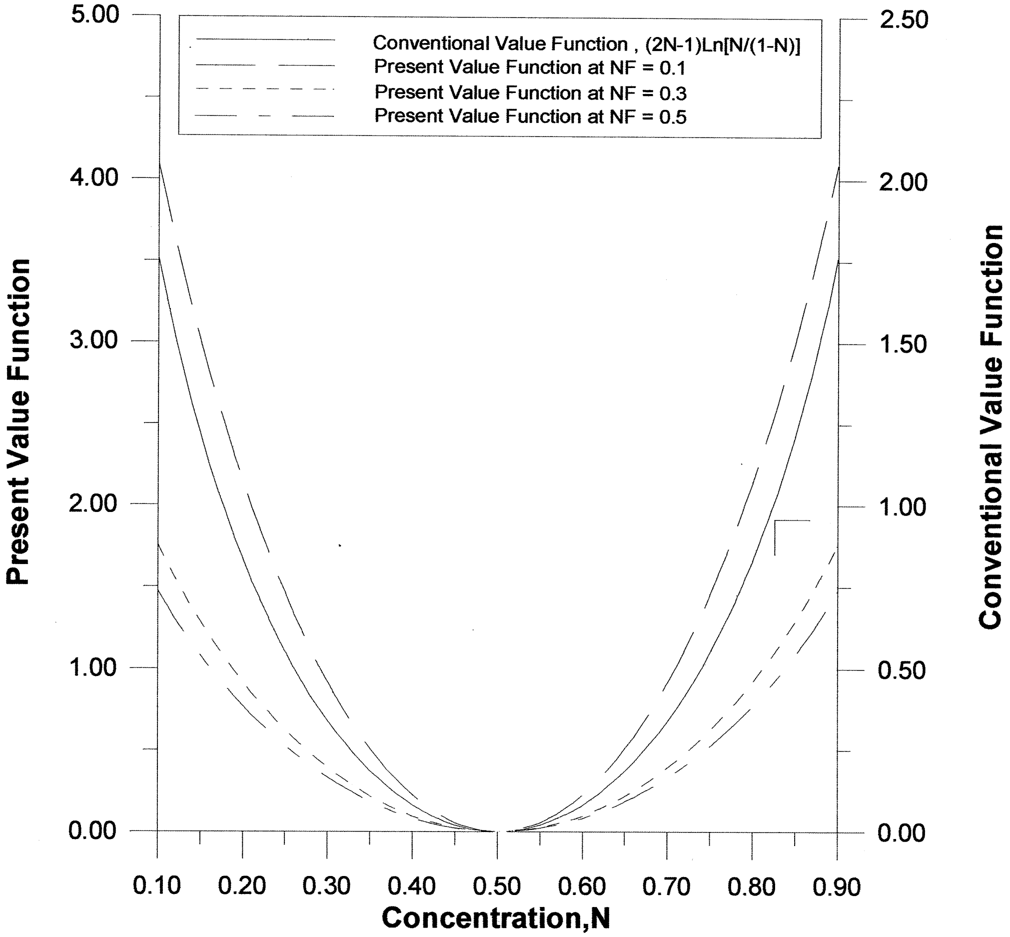

FIG. 4 Graph of the present value function for different feed concentrations as compared to the conventional value function.

$$V(N)_{N\neq 0.5} = \{dV(N)/dN\}_{N\neq 0.5} = 0 \tag{43}$$

The value function for a product stream P_i can thus be written

$$\begin{aligned} V(N)_{Pi} &= S(N)_{Pi}/\{RN_F(1-N_F)\} \\ &= \sum_{n=2}^{n=\infty} [(N_{Pi}-N_F)^n/\{n!RN_F(1-N_F)\}]\{d^nS(N_{\mathrm{F}})/dN_F^n\} \end{aligned} \tag{44}$$

It may be noted that the value function given by Eq. (41) will not assure the additivity of separative powers. This is because the rate of change of the entropy of the isotopes varies with the composition of the mixture and would vary according to the concentration of the feed, N_F.

As mentioned earlier, the conventional value function for the same product stream in a close separation case is given by Eq. (1B), namely.

$$V(N)_{P_i} = (2N-1)\ln[N/(1-N)] \tag{45}$$

It is also to be noted that for close separation cases Eq. (45) is not only additive but it also allows the separative power to be independent of feed concentration.

CONCLUSION

The commonly used expression for the separative power is applicable when the separating device is operating with a small separation factor. The separative power of a separating device is conventionally considered to be a property independent of the concentration level at which the device is operating. Such an expression has a form similar to that of the conservation equation for an extrinsic thermodynamic property for a steady flow process. It is not, however, possible to arrive at an extrinsic form of expression for a general case where the separation factor is large. The expression derived in the present work for the general case has been arrived at from the entropy change for mixtures based on its linkage to the work of separation. However, it does not have the desired additive property. This expression clearly indicates that an error is caused when the usual form of separative power is used for cases where the separation factor is appreciably large. The value function arrived at in the present work takes a form which is dependent on the feed concentration, indicating that a general expression for separative power independent of feed concentration is not possible for the case of a large separation factor. However, in most separation methods based on statistical-molecular processes, the basic separation effect is small and, hence, these are amenable to the usual form of value function (i.e., value function independent of feed concentration). Consequently, for devices with large separation the usual method of calculation of value function and separative power could lead to significant errors.

APPENDIX 1

The value function is determined to satisfy the requirement that the separative power is independent of concentration, and depends only on the separation factor. The separative power δU of a separating device can be defined as the change in the value of material obtained after separation:

$$\delta U = \theta F V(N_{P_1}) + (1 - \theta)\, F V(N_{P_2}) - F V(N_F) \tag{A1}$$

Expanding $V(N_{P_1})$ and $V(N_{P_2})$ around $V(N_F)$ using the Taylor Series

$$V(N_{P_1}) = V(N_F) + \sum_{n=1}^{n=\infty} \{(N_{P_1} - N_F)^n/n!\}\{d^n\, V(N_F)/dN_F^n\} \tag{A2}$$

$$V(N_{P_2}) = V(N_F) + \sum_{n=1}^{n=\infty} \{(N_{P_2} - N_F)^n/n!\}\{d^n\, V(N_F)/dN_F^n\} \tag{A3}$$

Substituting Eqs. (A2) and (A3) in Eq. (A1) and using mass balance and component balance, the change in the value per mole of the feed for the mixture of isotopes is

$$\begin{aligned}\delta U/F = {} & \sum_{n=2}^{n=\infty} (1/n!)\{d^n V(N_F)/dN_F^n\} \\ & \times [\theta(N_{P_1} - N_F)^n + (1 - \theta)(N_{P_2} - N_F)^n]\end{aligned} \tag{A4}$$

Using Eqs. (8) and (9) obtained from mass balance and component balance, Eq. (A4) is simplified as

$$\begin{aligned}\delta U/F = {} & \sum_{n=2}^{n=\infty} (N_F^n(1 - N_F)^n/n!)\{d^n \mathrm{V}(N_F)/dN_F^n\} \\ & \times (\xi/\theta)^n \theta\, [1 + (-1)^n\{\theta/(1 - \theta)\}^{n-1}]\end{aligned} \tag{A5}$$

Since ξ is a function of α, θ, and N_F as shown in Eqs. (17)–(19), for δU to be independent of concentration the mathematical condition imposed is

$$d^n V(N_F)/dN_F^n = \varphi_n/[\xi_n(N_F) N_F^n (1 - N_F)^n]_{\forall n \geq 2 : N_F \varepsilon (0,1)} \tag{A6}$$

where $\xi_n(N_F)$ is a function from ξ containing terms of N_F. In the case of a symmetric device (i.e., $\beta = \beta_1 = \beta_2$), the function $\xi_n(N_F)$ is $(\beta - 1)/(\beta + 1)$ for all N_F. φ_n contains constant terms.

There is no functional form of the value function $V(N)$ which satisfies Eq. (A6) for all values of N_F so long as the value function is monotonic. This implies that it is not possible to define $\delta U/F$ independent of feed concentration N_F.

The value function $(2N - 1)\ln\{N/(1 - N)\}$ is obtained by neglecting terms of order higher than 2 and by introducing boundary condition

$$V(N)_{N=0.5} = \{dV(N)/dN\}_{N=0.5} = 0 \tag{A7}$$

The functional form of $V(N)$, as in Eq. (A1), can also be solved using the difference equation by Pratt (2) or other indirect methods of solution by Lehrer-Ilamed (11), Gantayet and Madhavan (12), and Kanagawa and Yamamoto (13–16). But the solution obtained by these authors assumes that the terms in the functional form of $V(N)$ are only functions of β_1 and β_2. This is not true: for a separating device with given α and θ the heads and tails separation factors β_1 and β_2 are functions of N_F, as shown by Eqs. (17)–(19).

APPENDIX 2

By neglecting the terms of order higher than 2, Eq. (7) can be rewritten

$$\Delta S(N_F) = (1/2!)\{d^2S(N_F)/dN_F^2\}[\theta(N_{P_1} - N_F)^2 + (1 - \theta)(N_{P_2} - N_F)^2] \tag{A8}$$

From Eq. (3) by differentiation:

$$d^2S(N_F)/dN_F^2 = R/\{N_F(1 - N_F)\} \tag{A9}$$

Substituting Eqs. (A9) and (8), Eq. (A8) is simplified to

$$[\Delta S(N_F)]_{\text{close separation}} \cong R/\{2N_F(1 - N_F)\}(\theta/(1 - \theta)(N_{P_1} - N_F)^2 \tag{A10}$$

Using Eq. (2), the separative power δU can be expressed as

$$[\delta U/F]_{\text{close separation}} \cong (\theta/(1 - \theta)(N_{P_1} - N_F)^2/\{2N_F^2(1 - N_F)^2\} \tag{A11}$$

since

$$(N_{P1} - N_F) = (\beta_1 - 1)N_F(1 - N_{P1}) \cong \varepsilon N_F(1 - N_F) \tag{A12}$$

By substituting Eq. (A12), the separative power per unit feed in terms of enrichment factor ε for the close separation case can be shown to be

$$[\delta U/F]_{\text{close separation}} \cong \{(\theta/(1 - \theta)\}\varepsilon^2/2 \tag{A13}$$

APPENDIX 3

By substituting the differentiated form of the value function for the close separation case [i.e., $(2N - 1)\ln\{N/(1 - N)\}$], Eq. (A5) for the separative power is rewritten

$$\delta U(N_F)/F = \sum_{n=2}^{n=\infty} (\phi_n(N_F)/n!)\,(\xi/\theta)^n\,\theta[1 + (-1)^n\{\theta/(1-\theta)\}^{n-1}] \quad \text{(A14)}$$

where

$$\begin{aligned}\phi_n(N_F) = {} & (n-2)!(1-N_F)^n/N_F^2 \\ & \sum_{k=0}^{k=n+2} [(-1)^{n-k}\,(k+1)(n-k-1)\{N_F/(1-N_F)\}^{k+2}]\end{aligned} \quad \text{(A15)}$$

The function $\phi_n(N_F)$ at $N_F \cong 0$ is

$$\phi_n(0) = (-1)^n(n-1)! \quad \text{(A16)}$$

Therefore, at $N_F \cong 0$,

$$\begin{aligned}\delta U(0)/F = \Bigg[& \theta \sum_{m=0}^{m=\infty} (-1)^{m+1}(\xi/\theta)^{\,m+1}/(m+1) \\ & + (1-\theta)\sum_{m=0}^{m=\infty} \{\xi/(1-\theta)\}^{m+1}/(m+1)\Bigg]\end{aligned} \quad \text{(A17)}$$

This is further simplified to

$$\delta U(0)/F = [\theta \ln\{\theta/(\xi+\theta)\} + (1-\theta)\ln\{(1-\theta)/(1-\theta-\xi)\}] \quad \text{(A18)}$$

Using Eqs. (23) and (24), Eq. (A18) is rewritten

$$\delta U(0)/F = [\ln(\beta_2) - \{(\beta_2 - 1)/(\alpha - 1)\}\ln(\alpha)] \quad \text{(A19)}$$

The above expression for $\delta U(0)/F$ is similar to the expression used by Kanagawa and Yamamoto (13–16), and it represents the case of $N_F \cong 0$ for a close separation case.

NOMENCLATURE

δU	separative power (k mol/s)
β_1	heads separation factor of a separating device
β_2	tails separation factor of a separating device
α	overall separation factor of a separating device at a given process condition
β	tails/heads separation factor of a symmetric separating device
ξ	function of separation factors $= (\beta_1 - 1)(\beta_2 - 1)/(\alpha - 1)$
ε	enrichment factor $= (\beta_1 - 1)$
θ	cut for the product $P_1 = P_1/F$
$1 - \theta$	cut for the product $P_2 = P_2/F$

N	general composition (mole fraction)
N_{P_1}	composition of the product P_1 (mole fraction)
N_{P_2}	composition of the product P_2 (mole fraction)
N_F	composition of the feed F (mole fraction)
$V(N)$	value function for any composition N
S	entropy (J/K)
ΔS	change in entropy (J/K)
R	universal gas constant (J/K/kmol)
F	feed rate of the separating device (k mol/s)
P_1	product 1 coming from the separating device (kmol/s)
P_2	product 2 coming from the separating device (kmol/s)

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