T_1	= catalyst bed temperature	[°K]	ρ	= gas density	[kg/m ³]
T_2	= coolant temperature	[°K]	ρ_B	= apparent density of catalyst in the packed bed	[kg/m ³]
T_0	= inlet gas temperature	[°K]	ω	= $\beta(1-x)$	[—]
U	= overall heat transfer coefficient [Kcal/m ² ·hr·°K]				
x	= conversion	[—]			
x_M	= conversion at η_M	[—]			
Z'	= ammonia mol fraction	[—]			
Z'_e	= equilibrium ammonia mol fraction	[—]			
z	= reactor length	[m]			
α	= c	[—]			
β	= ab	[—]			
γ	= $(1+K)/K$	[—]			
η_1	= non-dimensional catalyst temperature (E/RT_0^2)($T_1 - T_0$)	[—]			
η_2	= non-dimensional coolant temperature (E/RT_0^2)($T_2 - T_0$)	[—]			
η_M	= maximum non-dimensional temperature in a reactor	[—]			

Literature Cited

- 1) Baddour R. F., P. L. T. Brain, B. A. Logeais and J. P. Eymery: *Chem. Eng. Sci.*, **20**, 281 (1965).
- 2) Berkelew, C. H.: *Chem. Eng. Progs. Symp. Ser.*, No. 25, 37 (1959).
- 3) Nielsen, A.: "An Investigation on Promoted Iron Catalysts for the Synthesis of Ammonia", 2nd edition, Haldor Topsøe Copenhagen (1956).
- 4) Ohki, Y., T. Kato, H. Inoue, and T. Komiya: *Kagaku Kōgaku*, **32**, 921 (1968).

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A DEFINITION OF SEPARATION EFFICIENCY

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By using the entropy of information theory, a more reasonable separation efficiency can be defined from the point of view of statistics. This newly defined separation efficiency varies from zero for the case of non-separation, in which the mass fractions of valuable component in both product and residuum take the same values as that in feed, to unity for the case of ideal separation, in which the valuable material and useless material in the feed leave the separator as the product and the residuum, respectively, and has sufficient detection sensitivity for even a small change of mass fraction of components in the product or in the residuum. The newly defined separation efficiency, which satisfies the fundamental requirements described above and has clear physical meaning on the basis of its definition, may be useful to evaluate the performance of separation processes.

Introduction

The performance of processes in chemical industries depends in many cases on the efficiency of separators used in the process, and it becomes an important problem how to define the separation efficiency so as to evaluate the performance of separation processes.

The separation efficiency should satisfy the following two requirements. First, the value of separation efficiency is zero for the case of non-separation, in which the mass fractions of valuable component in both product and in residuum take the same values as that in the feed, and unity for the case of ideal

separation, in which the mixture fed to the separator is separated completely into two components, the valuable material and useless material in the feed leaving the separator as the product and the residuum, respectively. Usually, the values of separation efficiency are in the range of zero to unity. Second, it is desirable that the separation efficiency has sufficient detection sensitivity for even a small change of the mass fraction of components in the product or in the residuum. And, additionally, it is advisable that the separation efficiency has clear physical meaning on the basis of its definition.

Various types of separation efficiency have been proposed, and Newton efficiency is most widely used as a suitable and useful one at present²⁻⁴⁾. In the steady-operation separation of a binary mixture as

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shown in Fig. 1, Newton efficiency η_N is defined as

$$\eta_N = \frac{(x_P - x_F)(x_F - x_R)}{x_F(1 - x_F)(x_P - x_R)} \quad (1)$$

where x_F , x_P and x_R are the mass fraction of valuable component in the feed, in the product and in the residuum of the separator, respectively. The basis of definition of this efficiency is generally interpreted as follows.

$\eta_N =$

$$\frac{(\text{yield of product}) \times (\text{qualitative improvement})_{\text{at practical separation}}}{(\text{yield of product}) \times (\text{qualitative improvement})_{\text{at ideal separation}}}$$

$$= \frac{(P/F)\{(x_P - x_F)/x_F\}}{(Fx_F/F)\{(1 - x_F)/x_F\}}$$

or

$$\begin{aligned} \eta_N &= (\text{recovery rate of valuable material}) \\ &\quad - (\text{intermixture rate of useless material in product}) \\ &= Px_P/Fx_F - P(1 - x_P)/F(1 - x_F) \end{aligned}$$

where F , P and R are the mass flow rate of the feed, of the product and of the residuum, respectively.

Newton efficiency satisfies the first requirement mentioned above. However, the second requirement is not sufficiently satisfied, as is described later in detail.

The purpose of this paper is to propose a more suitable and reasonable separation efficiency defined from a statistical point of view.

1. Entropy of Information Theory^{1,5)}

If M_i ($i=V$ or U) are mutually exclusive events and the probabilities that the events will happen are $p(M_i)$, the amount of self-information $I(M_i)$ and the average amount of self-information or self-entropy $H(M)$ are defined as the following equations:

$$I(M_i) = -\log p(M_i) \quad (2)$$

$$\begin{aligned} H(M) &= -\sum_i p(M_i) \log p(M_i) \\ &= -p(M_V) \log p(M_V) - p(M_U) \log p(M_U) \end{aligned} \quad (3)$$

The self-entropy $H(M)$ is the expectation of the amount of self-information $I(M_i)$ obtained from a trial, and represents a kind of uncertainty of the results. In the case of $p(M_V)=1$; $p(M_U)=0$, or $p(M_V)=0$; $p(M_U)=1$, the self-entropy $H(M)$ takes zero value, showing that there is no uncertainty of the results. On the other hand, when the probabilities $p(M_V)$ and $p(M_U)$ are equal to each other, the self-entropy takes the maximum values.

With the combination of the events M_i and other events S_j ($j=P$ or R) which are mutually exclusive and will happen with probabilities $p(S_j)$, the amount of mutual information $I(M_i, S_j)$ and the average amount of mutual information or mutual entropy $I(M; S)$ are defined as follows.

	mass flow rate	mass fraction of valuable component
feed	F	x_F
product	P	x_P
residuum	R	x_R

Fig. 1 Steady-operation separation of a binary mixture

$$\begin{aligned} I(M_i, S_j) &= \log \{p(M_i, S_j)/p(M_i)p(S_j)\} \\ &= \log \{p(M_i/S_j)p(M_i)\} \end{aligned} \quad (4)$$

$$\begin{aligned} I(M; S) &= \sum_i \sum_j p(M_i, S_j) I(M_i, S_j) \\ &= \sum_i \sum_j p(M_i, S_j) \log \{p(M_i/S_j)/p(M_i)\} \\ &= -\sum_i p(M_i) \log p(M_i) \\ &\quad + \sum_i \sum_j p(M_i, S_j) \log p(M_i/S_j) \\ &= H(M) - H(M/S) \end{aligned} \quad (5)$$

In these equations, $p(M_i, S_j)$ is the joint probabilities of events M_i and S_j and represents the probabilities that events M_i and S_j will both happen in the same time, $p(M_i/S_j)$ is the conditional probabilities and represents the probabilities that the events M_i will happen in sub-population S_j and $H(M/S)$ ($= -\sum_i \sum_j p(M_i, S_j) \log p(M_i/S_j)$) is the conditional self-entropy and represents the average amount of conditional self-information $I(M_i/S_j)$. The mutual entropy represents a statistical relationship between $H(M)$ and $H(M/S)$, and is the expectation of the amount of mutual information $I(M_i, S_j)$ obtained from a trial.

2. Definition of Another Separation Efficiency

In the steady-operation separation of a binary mixture as shown in Fig. 1, the events M_i correspond to a mass chosen in the feed mixture being valuable material or useless material, and the probabilities $p(M_i)$ correspond to the mass fraction of valuable or useless component in the feed.

$$p(M_V) = x_F \quad (6)$$

$$p(M_U) = 1 - x_F \quad (7)$$

The events S_j correspond to that the feed mixture leaving the separator as the product or as the residuum, and the probabilities $p(S_j)$ are given as

$$p(S_P) = P/F \quad (8)$$

$$p(S_R) = R/F \quad (9)$$

Table 1 Joint probabilities $p(M_i, S_j)$ and conditional probabilities $p(M_i/S_j)$

$S_j \setminus M_i$	$p(M_i, S_j)$		$p(M_i/S_j)$	
	M_V	M_U	M_V	M_U
S_P	Px_P/F	$P(1-x_P)/F$	x_P	$1-x_P$
S_R	Rx_R/F	$R(1-x_R)/F$	x_R	$1-x_R$

Fig. 2 Example of characteristic curves of newly defined separation efficiency under condition of $x_F=0.4$

with the following two material balance relations.

$$F = P + R \quad (10)$$

$$Fx_F = Px_P + Rx_R \quad (11)$$

In this paper, the quantitative condition of

$$x_P \geq x_F \geq x_R \quad (12)$$

is assumed as a natural requirement. And the joint probabilities $p(M_i, S_j)$ and the conditional probabilities $p(M_i/S_j)$ which will be used are shown in **Table 1**.

From these probabilities, the self-entropy, the conditional self-entropy and the mutual entropy are shown as follows:

$$H(M) = -x_F \log x_F - (1-x_F) \log(1-x_F) \quad (13)$$

$$H(M/S) = (P/F) \{-x_P \log x_P - (1-x_P) \log(1-x_P)\} \\ + (R/F) \{-x_R \log x_R - (1-x_R) \log(1-x_R)\} \quad (14)$$

$$I(M; S) = H(M) - H(M/S) \quad (15)$$

In the case of ideal separation, $x_P=1$ and $x_R=0$, the conditional self-entropy $H(M/S)$ takes the minimum values and the mutual entropy $I(M; S)$ takes the maximum values, that is,

$$H(M/S)_{x_P=1, x_R=0} = H(M/S)_{\min} = 0 \quad (15)$$

$$I(M; S)_{x_P=1, x_R=0} = I(M; S)_{\max} = H(M) \quad (16)$$

In the case of non-separation, $x_P=x_R=x_F$, $H(M/S)$ takes the maximum values and $I(M; S)$ takes the minimum values.

$$H(M/S)_{x_P=x_R=x_F} = H(M/S)_{\max} = H(M) \quad (17)$$

$$I(M; S)_{x_P=x_R=x_F} = I(M; S)_{\min} = 0 \quad (18)$$

The conditional self-entropy $H(M/S)$ represents the reduction of statistical uncertainty of the results after passing through the separator, that is, a decrease of $H(M/S)$ shows an increase of mass fraction of valuable component in the product or its decrease of that in the residuum.

The property of conditional self-entropy and mutual entropy described above suitably represent the performance of separation processes, and a new separation efficiency η can be defined as follows under the first requirement mentioned in the introduction.

$$\eta = \{I(M; S) - I(M; S)_{\min}\} / \{I(M; S)_{\max} - I(M; S)_{\min}\} \\ = \{H(M) - H(M/S)\} / H(M) \\ = 1 - H(M/S) / H(M) \\ = 1 - [P\{-x_P \log x_P - (1-x_P) \log(1-x_P)\} \\ + R\{-x_R \log x_R - (1-x_R) \log(1-x_R)\}] \\ / [F\{-x_F \log x_F - (1-x_F) \log(1-x_F)\}] \quad (19)$$

In the condition of $x_P > x_F > x_R$, Eq. (19) can be rearranged as follows, by substituting Eqs. (10) and (11).

$$\eta = 1 - [(x_F - x_R) \{-x_P \log x_P - (1-x_P) \log(1-x_P)\} \\ + (x_P - x_F) \{-x_R \log x_R - (1-x_R) \log(1-x_R)\}] \\ / [(x_P - x_R) \{-x_F \log x_F - (1-x_F) \log(1-x_F)\}] \quad (20)$$

3. Characteristics of Separation Efficiency

The characteristics of separation efficiency can be shown clearly with characteristic curves as follows. For example, the relationship between the newly defined separation efficiency η and the mass fraction of valuable component in the product x_P under the condition of $x_F=0.4$ is shown in **Fig. 2** with parameter $x_R=0, 0.1, 0.2, 0.3$. These characteristic curves show that the newly defined separation efficiency has sufficient detection sensitivity in a wide range of x_P and satisfies the second requirement described in the introduction.

To compare the newly defined separation efficiency η with Newton efficiency η_N , both characteristic curves in the case of $x_F=0.3$ are shown in **Fig. 3** with parameter $x_R=0, 0.1, 0.2$. As is obvious from this figure, Newton efficiency is too sensitive in the lower range of x_P and has insufficient detection sensitivity in the higher range of x_P , and this tendency is emphasized in the higher range of parameter x_R .

Conclusion

By using the entropy of information theory, a more reasonable separation efficiency can be defined from the point of view of statistics.

This newly defined separation efficiency varies from zero for the case of non-separation to unity for the case of ideal separation. It has sufficient

detection sensitivity for even a small change of the mass fraction of components in the product or in the residuum.

The newly defined separation efficiency, which satisfies the fundamental requirements as described above and has clear physical meaning on the basis of its definition, may be useful to evaluate the performance of separation processes.

Nomenclature

F	= mass flow rate	[g/s]
$H(M)$	= self-entropy	[bit]
$H(M/S)$	= conditional self-entropy	[bit]
$I(M; S)$	= mutual entropy	[bit]
$I(M_i)$	= amount of self-information	[bit]
$I(M_i/S_j)$	= amount of conditional self-information	[bit]
$I(M_i, S_j)$	= amount of mutual information	[bit]
M_i	= event M_P or M_U	[—]
P	= mass flow rate of product	[g/s]
$p(M_i)$	= probabilities that events M_i will happen	[—]
$p(M_i/S_j)$	= probabilities that events M_i will happen in sub-population S_j	[—]
$p(M_i, S_j)$	= probabilities that both events M_i and S_j will happen in the same time	[—]
R	= mass flow rate of residuum	[g/s]
S_j	= event S_P or S_R	[—]
<Subscript>		
F	= feed	
P	= product	
R	= residuum	
U	= useless material

Fig. 3 Comparison of characteristic curves of newly defined separation efficiency with that of Newton efficiency under condition of $x_F=0.3$

V = valuable material

Literature Cited

- 1) Brillouin, L.: "Science and Information Theory", Academic Press (1962).
- 2) Newton, H. W.: *Rock Product*, **35**, 26 (1932).
- 3) Richards, J. C.: *Brit. Coal Utilisat. Res. Assoc.*, **30**, 113 (1967).
- 4) Rietema, K.: *Chem. Eng. Sci.*, **7**, 89 (1957).
- 5) Shannon, C. E.: "The Mathematical Theory of Communication", The Univ. of Illinois Press (1949).