bypassing effect of the reactant, which is caused by overly effective extraction.

Nomenclature

C	= concentration	[mol/cm ³]
K	= equilibrium constant of first-order reversible reaction	[—]
k	= reaction rate constant	[1/sec]
$k_A a, k_R a$	= capacity coefficient of mass transfer	[1/sec]
m_A, m_R	= distribution coefficient	[1/sec]
$\mathfrak{R}$	= reaction rate	[mol/cm ³ ·sec]
V	= reactor volume	[cm ³]
v	= volumetric flow rate	[cm ³ /sec]
<Subscript>		
A	= component A	
R	= component R	
0	= entrance of reactor	

L = exit of reactor
 l = longitudinal coordinate of reactor
 1 = reactive phase
 2 = extractive phase
 <Dimensionless group>
 $\chi_{A1} = C_{A1}/C_{A1,0}$, $\chi_{A2} = C_{A2}/C_{A1,0}$, $\chi_{R1} = C_{R1}/C_{A1,0}$,
 $\chi_{R2} = C_{R2}/C_{A1,0}$, $\varepsilon = V_2/V_1$, $\zeta = v_2/v_1$,
 $\tau_1 = k_1 V_1/v_1$, $\kappa = k_2/k_1$, $\xi_A = k_A a/k_1$, $\xi_R = k_R a/k_1$,

Literature Cited

- 1) Hofmann, H.: *Chem. Eng. Sci.*, **8**, 113 (1958)
- 2) Piret, E. L., W. H. Penney and P. J. Trambouze: *A.I.Ch.E. Journal*, **6**, 394 (1960)
- 3) Trambouze, P. J. and E. L. Piret: *ibid.*, **6**, 574 (1960)
- 4) Trambouze, P., M. T. Trambouze and E. L. Piret: *ibid.*, **7**, 138 (1961)
- 5) Schoenemann, K.: *Chem. Eng. Sci.*, **14**, 39 (1961)

OPTIMIZATION OF AN EXTRACTIVE STIRRED TANK REACTOR COUPLED WITH SEPARATORS*

SHIGEO GOTO AND MASAKAZU MATSUBARA

Department of Chemical Engineering, Nagoya University, Nagoya, Japan

To assure the profitability of extractive reaction, the optimization of an extractive stirred tank reactor coupled with separators where the manufacturing cost is minimized is investigated.

A diagram which allows immediate choice of the optimal system among three alternatives is provided for first-order reversible reaction.

In the previous paper¹⁾, the efficiency of extractive reaction was proposed and effects of extraction rate and reactor type on the performance of extractive reactor were clarified. A commercial reactor will, however, be operated together with a separator and solvents will be recycled to the reactor. Thus, to assure the profitability of the extractive reaction, the performance of the whole system is to be examined.

In this paper, the minimization of the manufacturing cost of the extractive stirred tank reactor coupled with separators is investigated for first-order reversible reaction. The formulation of the problem with respect to the extractive reactor is identical with that in the previous paper¹⁾ except for the assumption of phase equilibrium or infinite mass transfer rate between two phases.

Three Alternatives of Reactor-Separator System

Three alternatives of reactor-separator system are set up and shown in Fig. 1, that is, Alternative I: a CSTR with extraction, a settler and two distillation units, alternative II: a CSTR with extraction, a

settler and a distillation unit and alternative III: a CSTR without extraction and a distillation unit.

The manufacturing cost is estimated as

$$p_R = \{p_A F_A + p_{S1} \alpha_1 v_1 + p_{S2} \alpha_2 v_2 + p_V V + p_S (v_1 + v_2) + p_{D1} v_1 + p_{D2} v_2\} / F_R \quad (1)$$

for alternative I. The sixth term of the numerator in Eq.(1) should be deleted for alternative II and the third, the fifth and the seventh terms for alternative III.

Using dimensionless groups, Eq.(1) can be reduced to

$$f_I = \{(1+\varepsilon)\tau_1 + \rho_1 + \rho_2 \zeta\} / (\chi_{R1} + \zeta \chi_{R2}) \quad (2)$$

$$f_{II} = \{(1+\varepsilon)\tau_1 + \rho_1' + \rho_2 \zeta\} / \zeta \chi_{R2} \quad (3)$$

$$f_{III} = (\tau_1 + \rho_1'') / \chi_R \quad (4)$$

respectively, for alternative I, II and III.

If the values of ρ_1 , ρ_2 , ρ_1' and ρ_1'' are specified by referring to kinetic and cost data, the value of $f_{I,opt}$, $f_{II,opt}$ and $f_{III,opt}$ can be determined.

Procedure of Numerical Calculation and Results

Solving mass balance equations of the CSTR with extraction for infinite mass transfer rates yields

* Received on September 21, 1971

Fig. 1 Schematic flowsheet of extractive reaction system for three alternatives

Fig. 2 Contours of f_I for $\rho_1=1$, $\rho_2=1$, $m_A=0.1$, $m_R=10$, $\kappa=0.01$ and $K_1=K_2=1/9$

$$\chi_{R1} = \{(\chi_{R1,0} + \zeta \chi_{R2,0})(1 + m_A \zeta) + (1 + \chi_{R1,0} + \zeta \chi_{A2,0} + \zeta \chi_{R2,0})(1 + m_A \kappa \varepsilon) \tau_1\} / [(1 + m_A \zeta)(1 + m_R \zeta)] + \{(1 + m_A \kappa \varepsilon)(1 + m_R \zeta) + (1 + m_A \zeta)(1/K_1 + m_R \kappa \varepsilon/K_2)\} \tau_1] \quad (5)$$

$$\chi_{R2} = m_R \chi_{R1} \quad (6)$$

Boundary conditions for alternative I are

$$\chi_{R1,0}=0, \chi_{A2,0}=0, \chi_{R2,0}=0 \quad (7)$$

while those for alternative II are

$$\chi_{R1,0}=\chi_{R1}, \chi_{A2,0}=0, \chi_{R2,0}=0 \quad (8)$$

On the other hand, solving mass balance equations for the CSTR without extraction yields

$$\chi_R = \{\chi_{R,0} + (1 + \chi_{R,0}) \tau_1\} / \{1 + (1 + 1/K_1) \tau_1\} \quad (9)$$

Boundary conditions for alternative III are

$$\chi_{R,0}=0 \quad (10)$$

By substituting Eqs.(5), (6) and (7) into Eq.(2), f_I for specified values of ρ_1 and ρ_2 becomes a function of τ_1 and ζ if ε is set equal to ζ .

As an example, contours of f_I for $\rho_1=1$ and $\rho_2=1$

Fig. 3 Relation between optimal values of objective function and design variables for alternative I and III, $m_A=0.1$, $m_R=10$, $\kappa=0.01$ and $K_1=K_2=1/9$

Fig. 4 Relation between optimal values of objective function and design variables for alternative II, $m_A=0.1$, $m_R=10$, $\kappa=0.01$ and $K_1=K_2=1/9$

are calculated and shown in Fig. 2. It is seen in this figure that the minimum value of f_I is about 10.4 at $\tau_1=0.6$ and $\zeta=0.4$.

The minimum value of f_I can be obtained by solving the following set of equations.

$$\partial f_I / \partial \tau_1 = 0, \partial f_I / \partial \zeta = 0 \quad (11)$$

Since this set of equations is of second order with respect to τ_1 and of fourth order with respect to ζ , solving them about τ_1 and ζ is very tedious. But if values of τ_1 and ζ are specified, solving the set of

Eq.(11) about ρ_1 and ρ_2 is very easy. Then, $f_{I,opt}$ can be obtained by substituting these values of τ_1 , ζ , ρ_1 and ρ_2 into Eq.(2).

Fig. 3 shows the results obtained in such a manner for $m_A=0.1$, $m_R=10$, $\kappa=0.01$, $K_1=K_2=1/9$.

Alternative III is the special case of alternative I where ζ and ε are set equal to zero. Hence values of $f_{III,opt}$ and τ_1 can be found on the line of $\zeta=0$ in Fig. 3. These can be written as

$$f_{III,opt} = (1 + \sqrt{1 + 1/K_1} \sqrt{\rho_1''})^2 \quad (12)$$

$$\tau_1 = \sqrt{\rho_1'' / (1 + 1/K_1)} \quad (13)$$

χ_{R2} for alternative II can be obtained by solving the set of Eqs.(5), (6) and (8). By substituting this χ_{R2} into Eq.(3), f_I for specified values of ρ_1' and ρ_2 becomes a function of τ_1 and ζ if ε is set equal to ζ . Therefore, the minimum value of f_I can be obtained in a manner similar to that for f_I . The results are shown in **Fig. 4**.

The Choice of the Optimal System

If values of ρ_1 , ρ_2 , ρ_1' and ρ_1'' are estimated, values of $f_{I,opt}$, $f_{II,opt}$ and $f_{III,opt}$ can immediately be obtained from Figs. 3 and 4 and the optimal pattern will be determined. For example, if $\rho_1=1$, $\rho_2=1$, $\rho_1'=0.6$ and $\rho_1''=0.8$, then $f_{I,opt}=10.4$, $f_{II,opt}=9.4$ and $f_{III,opt}=14.7$. Hence alternative II will be chosen and values of design variables will be decided as $\tau_1=0.48$ and $\zeta=0.43$.

It is indicated in Figs. 3 and 4 that a smaller value of ζ must be chosen as the value of ρ_2 becomes larger. This is the natural consequence of ρ_2 being the cost concerning the solvent S_2 and ζ being the relative flow rate of solvent S_2 to S_1 . If the value of ζ must be taken as zero for alternative I, then the system becomes alternative III, which is the limit of alternative I.

Comparison of Figs. 3 and 4 indicates that alternative I is always more profitable than alternative II for a specified value of ρ_2 if ρ_1 is equal to ρ_1' . This

is due to the fact that the product R can be separated from A and S_1 at no cost if $\rho_1 - \rho_1' = 0$. This is because $\rho_1 - \rho_1'$ represents the cost concerning the distillation equipment D_1 which is contained in alternative I but not in alternative II.

Alternative II will become more profitable than alternative I if $\rho_1 - \rho_1'$ becomes larger.

Nomenclature

C	= concentration	[mol/cm ³]
F	= molal flow rate	[mol/sec]
K	= equilibrium constant of first-order reversible reaction	[—]
k	= reaction rate constant	[1/sec]
m_A, m_R	= distribution coefficient	[1/sec]
p_A, p_{S1}, p_{S2}	= price of material	[yen/mol]
p_{D1}, p_{D2}, p_S	= price of equipment proportional to flow rate	[yen/cm ³]
p_V	= price of reactor proportional to volume	[yen/cm ³ ·sec]
V	= reactor volume	[cm ³]
v	= volumetric flow rate	[cm ³ /sec]
α_1, α_2	= ratio of make-up rate to volumetric flow rate	[mol/cm ³]

<Subscript>

A	= component A
R	= component R
$S1$	= solvent S_1
$S2$	= solvent S_2
0	= entrance of reactor
L	= exit of reactor
1	= reactive phase
2	= extractive phase
I	= alternative I
II	= alternative II
III	= alternative III

<Dimensionless group>

$$\begin{aligned} \chi_{A1} &= C_{A1}/C_{A1,0}, \quad \chi_{A2} = C_{A2}/C_{A1,0}, \quad \chi_{R1} = C_{R1}/C_{A1,0}, \\ \chi_{R2} &= C_{R2}/C_{A1,0}, \quad \varepsilon = V_2/V_1, \quad \zeta = v_2/v_1, \quad \tau_1 = k_1 V_1/v_1, \quad \kappa = k_2/k_1, \\ f &= k_1 C_{A1,0} (p_R - p_A)/p_V, \quad \rho_1 = k_1 (p_{S1} \alpha_1 + p_S + p_{D1})/p_V, \\ \rho_2 &= k_1 (p_{S2} \alpha_2 + p_S + p_{D2})/p_V, \quad \rho_1' = k_1 (p_{S1} \alpha_1 + p_S)/p_V, \\ \rho_1'' &= k_1 (p_{S1} \alpha_1 + p_{D1})/p_V \end{aligned}$$

Literature Cited

- 1) Goto, S., M. Matsubara: *J. Chem. Eng. Japan*, **5**, 87 (1972)