SELECTIVITY OF CONSECUTIVE GAS-LIQUID REACTIONS*

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The selectivity of (1, 1) order gas-liquid reactions was studied by taking into account mass transfer in the diffusion film. An approximate method for calculating the yield of an intermediate product and reaction time was presented. Consecutive chlorination of *p*-cresol was carried out in a stirred tank reactor with a constant gas-liquid contacting area, and the effects of various reaction conditions such as stirring speed and dilution of chlorine with air on the yield of the intermediate product were examined.

It was found that experimental results were well explained by the theory, and the approximate solutions could give good estimations for the yield and the reaction time.

Introduction

Most gas-liquid reactions of commercial interest are complicated by side reactions, and we must take into account not only the rate of gas absorption but also the selectivity or the yield of the desired product. Recently several papers¹⁻⁶⁾ have been presented on the selectivity of gas-liquid reactions. In the previous paper¹⁾ of the present authors, a theoretical study was developed on the selectivity of (0, 1) order gas-liquid reactions (zero order with respect to gas component, and first order to liquid components) by taking into account the role of mass transfer, and the effects of various reaction conditions on the yield of an intermediate product were discussed.

In this paper, the theoretical studies are extended to consecutive second order reactions, and the theory is examined by the chlorination of *p*-cresol. The experimental apparatus used was a stirred tank reactor with a constant gas-liquid contacting area. The effects of stirring speed, partial pressure of chlorine, and initial concentration of *p*-cresol were examined, and it was found that the experimental results were in good agreement with the theoretical predictions.

1. Approximate solution for the selectivity of (1, 1) order gas-liquid reactions

1.1 Basic Equations

The reaction scheme considered is

where *A* and *B* are feeds, *R* is the desired intermediate product, and *S* is the undesired final product. If the reactions (1) and (2) are first order with respect to both gas and liquid components, the following differential equations are obtained.

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$$d^2a/d\xi^2 = h_1^2 r_{Bq} b a b + h_2^2 r_{Rq} r a r \quad (3)$$

$$d^2b/d\xi^2 = h_1^2 a b \quad (4)$$

$$d^2r/d\xi^2 = -(r_{Bq} b / r_{Rq} r) h_1^2 a b + h_2^2 a r \quad (5)$$

with boundary conditions:

$$\xi = 0: \quad a = 1 \quad (6)$$

$$db/d\xi = dr/d\xi = 0 \quad (7)$$

$$\xi = 1: \quad a = \alpha \quad (8)$$

$$b = r = 1 \quad (9)$$

$$-da/d\xi = r^2 \alpha \delta \quad (10)$$

van de Vusse⁵⁾ obtained the solution of the above equations on an analog computer for a special case of $\alpha=0$, i. e., he neglected the reactions in the bulk liquid. In the present paper more general solutions will be derived by taking into account both the reactions in the bulk liquid and in the liquid film.

1.2 Approximate solution

As Eqs. (3)~(10) cannot be solved analytically, approximate solutions are derived by applying the method presented by van Krevelen and Hoftijzer⁷⁾, i. e., the concentrations of liquid components *B*, *R* in the terms representing the reaction rates (the right sides of Eqs. (3)~(5)) are assumed to be constant and equal to the concentrations at the gas-liquid interface $b_i (=C_{Bi}/C_{Bi})$, $r_i (=C_{Ri}/C_{Ri})$ respectively. Then Eqs. (3)~(5) are linearized as follows:

$$d^2a/d\xi^2 = \Gamma_A h_1^2 b_i a \quad (3')$$

$$d^2b/d\xi^2 = h_1^2 b_i a \quad (4')$$

$$d^2r/d\xi^2 = \Gamma_R h_1^2 b_i a \quad (5')$$

Elimination of the terms representing reaction rate from Eqs. (3') and (4') gives

$$d^2a/d\xi^2 - \Gamma_A d^2b/d\xi^2 = 0 \quad (11)$$

The above equation is integrated with the boundary conditions (6)~(9) to give

$$(db/d\xi)_{\xi=1} = \beta_f^* / \Gamma_A \quad (12)$$

$$b_i = 1 - (\beta_f^* + \alpha - 1) / \Gamma_A \quad (13)$$

where β_f^* is a modified reaction factor defined by

$$\beta_f^* \equiv N_A / k_{LA} C_{Ai} = - (da/d\xi)_{\xi=0} \quad (14)$$

and β_f^* represents the reaction rate of *A* in the liquid film and is defined as follows

$$\beta_f^* \equiv \beta_f^* - \{ - (da/d\xi)_{\xi=1} \} \quad (15)$$

By the same procedure the following equations are obtained from Eqs. (3') and (5').

$$(dr/d\xi)_{\xi=1} = (\Gamma_R/\Gamma_A)\beta_f^* \quad (16)$$

$$r_i = 1 - (\Gamma_R/\Gamma_A)(\beta_f^* + \alpha - 1) \quad (17)$$

From Eqs. (13) and (17) the relation between b_i and r_i is given by

$$\frac{1 - b_i}{1 - r_i} = \frac{b_i}{\frac{1}{s}r_i - \frac{r_B q_B}{r_R q_R} b_i} \quad (18)$$

The concentration profile of A is derived from Eq. (3') under the conditions of Eqs. (6), (8) and (10):

$$a = [\sinh\{\gamma'(1 - \xi)\} + \alpha \sinh\{\gamma'\xi\}]/\sinh \gamma' \quad (19)$$

where
$$\gamma' = \sqrt{h_1^2 r_B q_B b_i + h_2^2 r_R q_R r_i}$$

$$\alpha = \gamma'/[\gamma' \cosh \gamma' + \gamma^2 \delta \sinh \gamma'] \quad (20)$$

The following equations are obtained by substituting Eq. (19) into Eqs. (14) and (15).

$$\beta^* = \frac{\gamma'}{\tanh \gamma'} \left(1 - \frac{\alpha}{\cosh \gamma'}\right) \quad (21)$$

$$\beta_f^* = \frac{\gamma'}{\tanh \gamma'} (1 + \alpha) \left(1 - \frac{1}{\cosh \gamma'}\right) \quad (22)$$

When the rate of disappearance of B in the liquid film is denoted by N_{Bf} , and the rate of formation of R is denoted by N_{Rf} , these are given by

$$N_{Bf} = D_B(dC_B/dx)_{x=x_i} = k_{lA}C_{Ai}r_B q_B \beta_f^* \Gamma_A \quad (23)$$

$$N_{Rf} = -D_R(dC_R/dx)_{x=x_i} = -k_{lA}C_{Ai}r_R q_R \beta_f^* \Gamma_R/\Gamma_A \quad (24)$$

The reaction rates of B and R in the bulk are

$$N_{Bl} = k_1 C_{Al} C_{Bl} (v - x_i) = k_{lA} C_{Ai} h_1^2 r_B q_B \alpha \delta \quad (25)$$

$$N_{Rl} = (k_1 C_{Al} C_{Bl} - k_2 C_{Al} C_{Rl}) (v - x_i) = k_{lA} C_{Ai} (h_1^2 r_B q_B - h_2^2 r_R q_R) \alpha \delta \quad (26)$$

The instantaneous selectivity of R is represented as follows:

$$\phi \equiv \frac{dC_{Rl}}{-dC_{Bl}} = \frac{dY}{dx_B} = \frac{N_{Rf} + N_{Rl}}{N_{Bf} + N_{Bl}} \quad (27)$$

where x_B is the conversion of B , and Y is the yield of R , and these are defined as follows:

$$x_B = 1 - C_{Bl}/C_{B0}, \quad Y = C_{Rl}/C_{B0}$$

Substitutions of Eqs. (23)~(26) into Eq. (27) gives

$$\frac{dY}{dx_B} = \frac{-(\beta_f^* r_R q_R \Gamma_R/\Gamma_A) + (h_1^2 r_B q_B - h_2^2 r_R q_R) \alpha \delta}{\beta_f^* r_B q_B/\Gamma_A + h_1^2 r_B q_B \alpha \delta} \quad (28)$$

On the other hand, mass balance equation of B for a semibatch reactor is

$$V_l dC_B/dt = -A_r(N_{Bf} + N_{Bl}) \quad (29)$$

where V_l is the liquid volume and A_r is the gas-liquid interfacial area. From Eqs. (23), (25) and (29), the conversion rate of B is obtained in a dimensionless form

$$dx_B/d\theta = r_B(1 - x_B)(\beta_f^*/\Gamma_A + h_1^2 \alpha \delta) \quad (30)$$

where $\theta = k_{lA} a_i t$ and $a_i = A_r/V_l$

The above equations are derived on the assumption of the pseudo-steady state with respect to the concentrations of liquid reactants B and R . Therefore these may give some errors for the cases where the rate of conversion is very fast and the reactions complete within a few minutes. But even for this case rough estimates of the selectivity and the conversion rate might be possible.

For given values of parameters r_B , r_R , q_{B0} ($=C_{B0}/C_{Ai}$),

h_1 , s and δ , the $Y-x_B$ and $\theta-x_B$ relations can be calculated from Eqs. (28) and (30). If the values of x_B and Y at θ are known, q_B and q_R are calculated from the following relations:

$$q_B = q_{B0}(1 - x_B), \quad q_R = q_{B0}Y$$

From Eqs. (13), (18), (20) and (21), the values of b_i and r_i are determined by the trial and error procedure. Then the instantaneous selectivity and the conversion rate can be calculated from Eqs. (28) and (30) respectively. Numerical integrations of these equations give the $Y-x_B$ and $\theta-x_B$ relations.

For continuous operations, Eqs. (20), (28) and (30) are rewritten as follows:

$$\alpha = \gamma'/\{\gamma' \cosh \gamma' + (\gamma^2 \delta + 1/\theta) \sinh \gamma'\} \quad (20')$$

$$\frac{Y}{x_B} = \frac{-(\beta_f^* r_R q_R \Gamma_R/\Gamma_A) + (h_1^2 r_B q_B - h_2^2 r_R q_R) \alpha \delta}{\beta_f^* r_B q_B/\Gamma_A + h_1^2 r_B q_B \alpha \delta} \quad (28')$$

$$\theta = x_B/[r_B(1 - x_B)(\beta_f^*/\Gamma_A + h_1^2 \alpha \delta)] \quad (30')$$

The $Y-x_B$ and $\theta-x_B$ relations can be obtained from these equations by trial and error procedure.

1.3 Computed results

For given values of s , r_B , r_R , q_{B0} , h_1 , and δ , $Y-x_B$ and $\theta-x_B$ curves were computed on a digital computer. The influences of s and h_1 on the yield of the intermediate are analogous to those obtained for (0, 1) order reaction¹¹, that is, an increase in s and a decrease in h_1 result in an improved yield of the intermediate. Here particular attention was paid to the effect of $r_B q_{B0}$.

1.3.1 The effect of $r_B q_{B0}$ ($\equiv \frac{D_B}{D_A} \frac{C_{B0}}{C_{Ai}}$)

This parameter indicates the ratio of the concentration of B in the feed to that of A at the interface. As shown in Fig. 1, the behavior of this parameter is complicated. In Fig. 2 maximum yield of R is plotted against $r_B q_{B0}$. It is seen that in the range of very low and very large values of $r_B q_{B0}$, the yield approaches to that of homogeneous reactions, and in the range of

Fig. 1 Effect of $r_B q_{B0}$ on Y and θ

Table 1 Comparison of approximate solutions with numerical solutions ($s=4$, $\delta+1=100$)

h_1 [—]	r_{BQ_B} [—]	r_{BQ_R} [—]	$\phi_{approx.}$ [—]	$\phi_{num.}$ [—]	Error [%]	$\beta^*_{approx.}$ [—]	$\beta^*_{num.}$ [—]	Error [%]
0.5	0.3243	0.4436	0.6566	0.6567	-0.02	0.9594	0.9594	0.00
1.0	0.8076	0.1773	0.9256	0.9297	-0.44	1.214	1.225	-0.90
2.0	0.8008	0.1637	0.8217	0.8411	-2.31	1.570	1.593	-1.44
5.0	0.8000	0.1031	0.5154	0.5593	-7.85	2.190	2.259	-3.05
10.0	0.5000	0.1557	0.2908	0.3115	-6.65	2.039	2.129	-4.23

 Fig. 2 Effect of $r_B q_{B_0}$ on Y_{max}

intermediate values, it has a minimum value. In Fig. 2 the curve presented by van de Vusse⁵⁾ is also shown. These two curves are in good agreement when $r_B q_{B_0}$ is large, but at small values of $r_B q_{B_0}$ ($r_B q_{B_0} < 1$), the results obtained by van de Vusse give considerably lower values. This is because he neglected the reaction in the bulk liquid, notwithstanding that it is not negligibly small at small values of $r_B q_{B_0}$.

1.3.2 Accuracy of approximation

The method proposed by van Krevelen and Hoftijzer⁶⁾ for obtaining gas absorption rate accompanied by (1, 1) order chemical reaction was shown to give a good approximation. However when this method is extended to consecutive reaction systems, reexamination of accuracy is necessary. The comparison of the calculated values of the approximate solutions with those of numerical solutions of Eqs. (3)~(10) is shown in Table 1. It was noted that the former gives slightly lower values than the latter, but this method is considered to be available for practical use.

2. Experimental Details

2.1 Reaction system

Van de Vusse⁵⁾ carried out the chlorination of *n*-decane for studying the kinetics of gas-liquid consecutive reactions. However in this reaction system, several species of monochlorides and dichlorides are formed. Recently Inoue et al.²⁾ reported the kinetic study on the consecutive chlorination of *p*-cresol in carbon tetrachloride, and found that in this reaction system only one species of monochloride and dichloride was formed because of the strong ortho and para orientation of OH group. Thus the chlorination of *p*-cresol takes exactly the analogous path to that analysed in the previous section. It is represented as follows:

Furthermore both reactions are first order with respect to gas and liquid components²⁾. Therefore this reaction system is considered to be more suitable to verify the theory.

2.2 Apparatus

The schematic diagram of the apparatus is shown in Fig. 3 (a). The reactor was made of glass, the inside diameter was 9cm, and the volume 500ml. It was equipped with a mercury-sealed agitator, a gas inlet, a reflux condenser, a thermometer and a sampling tube. The chlorine gas was not bubbled into the liquid, but introduced over the free surface and absorbed into the liquid. The agitator, as shown in Fig. 3 (b), was a disc stirrer consisting of a disc and four triangular blades, and was driven oscillatorily in 90° interval. Even in the range of considerably high stirring speed, the liquid surface was kept flat without vortex formation and no entrainment of gas bubbles is introduced in the bulk of the solution. Therefore the area of the free surface is considered to be constant.

2.3 Procedure

After 500ml of *p*-cresol solution in carbon tetrachloride was charged in the reactor, chlorine was introduced over the liquid surface, and then stirring was started. The reaction temperature was maintained within $25 \pm 1^\circ\text{C}$. Liquid samples were taken and analysed by gas chromatography. A 2m×4mm stainless column packed with diethylene glycol succinate + H_3PO_4 on Chromosorb W (60~80 mesh) was used for the separation of liquid components. The exit gases from the reactor, which consist of unreacted chlorine, hydrogen chloride formed, and air when feed chlorine was diluted with air, were introduced into the vessel *L* shown in Fig. 3 (a). This vessel was used to obtain the value of C_{Ai} , the chlorine concentration at the gas-liquid interface in the reactor. As the liquid in the vessel was sufficiently stirred, the liquid was assumed to be in equilibrium with the gas from the reactor. Thus the chlorine concentration in the vessel was measured by iodometry and this value

(a) Schematic diagram of apparatus

Fig. 3 Experimental apparatus

(b) Agitator

Fig. 4 $Y-x_B$ relation without the effect of diffusion

Table 2 Experimental conditions

Run No.	n [r. p. m.]	C_{B0} [M]	m [—]	$k_{LA} \times 10^3$ [cm/sec]	$D_A \times 10^5$ [cm ² /sec]	C_{At} [M]	h_1 [—]	$r_{BQ_{B0}}$ [—]	δ [—]
1	300	1.25	0	2.17	2.32	0.794	6.83	0.921	735
2	300	2.50	0	1.51	1.72	0.816	8.83	1.69	690
3	300	3.00	0	1.24	1.44	0.716	9.22	2.31	675
4	300	3.92	0	0.909	1.10	0.799	11.6	2.71	649
5	300	4.66	0	0.715	0.896	0.765	13.0	3.36	627
6	200	2.50	0	1.14	1.72	0.846	11.9	1.63	520
7	140	2.50	0	0.881	1.72	0.855	15.4	1.61	402
8	300	4.66	0.893	0.715	0.896	0.406	9.49	6.34	627
9	300	4.66	1.57	0.715	0.896	0.369	9.05	6.97	627
10	300	4.66	2.55	0.715	0.896	0.269	7.72	9.56	627

was used as a rough estimate of C_{At} .

3. Results and Discussion

3.1 Preliminary Experiment

In order to calculate the parameters h_1 , s , $r_{BQ_{B0}}$ and δ , it is necessary to obtain reaction rate constants, mass transfer coefficients and diffusivities³⁾ in the liquid phase. The rate of reaction of the first step was too rapid to measure by usual methods. Inoue *et al.*²⁾ measured the rate constant by the so called stopped flow method, and this value was used in the present study ($k_1=71/\text{g mole} \cdot \text{sec}$ at 25°C).

The value of s' ($=k_1/k_2$) was determined as follows. In Fig. 4 is shown the yield-conversion relation obtained in the successive chlorination of *p*-cresol carried out in a gas sparged stirred tank reactor. As the rate of mass transfer of chlorine from the gas bubbles to the liquid is considerably higher than the reaction rate, the $Y-x_B$ relation thus obtained was assumed to be almost equal to that obtained under the condition of homogeneous reaction⁴⁾. In Fig. 4 are also presented the theoretical $Y-x_B$ relations for various values of s' , which is given by Eq. (31).

$$Y = \frac{s'}{s' - 1} \{ (1 - x_B)^{1/s'} - (1 - x_B) \} \quad (s' \neq 1) \quad (31)$$

Experimental data deviate to the left side from theoretical curves for homogeneous reactions. A satisfactory explanation could not be found for this phenomenon. Here the value of s' was determined so that the maximum value of Y calculated by Eq. (32) might coincide with the experimental data.

$$Y_{\max} = s'^{1/(1-s')} \quad (32)$$

Thus the value of s' was determined as 110. This value is considerably larger than that obtained by Inoue *et al.*²⁾ ($s'=30 \sim 60$). The liquid phase mass transfer coefficient, k_{LA} , was determined from the measurements of gas absorption rates of carbon dioxide into an aqueous solution of glycerin which had almost the same viscosities as the reacting solution. The experimental results were correlated by the following equation.

$$Sh = 0.0658 Re^{0.725} Sc^{0.3}$$

Mass transfer coefficients of chlorine in the reaction system were calculated by this equation.

3.2 Chlorination of *p*-cresol

Three series of experiments were carried out to examine the effects of the stirring speed, the initial concentration of *p*-cresol, and the degree of dilution of chlorine with air. Fig. 5 indicates the typical kinetic curves of the chlorination of *p*-cresol. The experimental conditions are listed in Table 2, where various parameters corresponding to each reaction condition are also

Fig. 5 Typical kinetic curves of chlorination of *p*-cresol

(a) Experimental results

(b) Computed results

Fig. 6 Effect of stirring speed

presented.

Effect of stirring speed

The effect of stirring speed on the yield of monochloro *p*-cresol is shown in Fig. 6 (a). An increase in stirring speed results in an improved yield of the intermediate product. With an increase in stirring speed, liquid phase mass transfer coefficient increases. As a result the accumulation of the intermediate product in the vicinity of the interface and further chlorination to the final product are prevented. Thus higher stirring speed improves the yield of the intermediate.

Effect of initial concentration of *p*-cresol

The effect of C_{B0} , the initial concentration of *p*-cresol, was examined at a constant stirring speed of 300 r.p.m. Fig. 7 (a) indicates that the yield decreases with an increase in C_{B0} . This is explained as follows. First,

with an increase in the initial concentration of *p*-cresol the viscosity of the liquid increases, and k_l is lowered. Secondly, with an increase in C_{B0} , $r_{BQ_{B0}}$ also increases. It is seen from Fig. 2 that in the range of $r_{BQ_{B0}}$ ($0.9 < r_{BQ_{B0}} < 3.4$), the yield falls with an increase in $r_{BQ_{B0}}$.

Effect of dilution of chlorine with air

To examine the effect of the partial pressure of chlorine on the selectivity, chlorinations were carried out at various dilutions of chlorine with air. The parameter m represents the ratio of molal flow rate of air to that of chlorine. As shown in Fig. 8 (a), an increase in m gives a higher yield of the intermediate. In Fig. 9, maximum yields are plotted against $r_{BQ_{B0}}$ at a constant value of r_0 ($=\sqrt{k_l C_{B0} D_A / k_{lA}}$). It is indicated that as $r_{BQ_{B0}}$ increases, yields are improved under this experimental condition ($3.4 < r_{BQ_{B0}} < 9.6$).

(a) Experimental results

(b) Computed results

Fig. 7 Effect of initial concentration of *p*-cresol

(a) Experimental results

(b) Computed results

Fig. 8 Effect of dilution of chlorine with air

Fig. 9 Effect of $r_B q_{B0}$ on $Y_{\max}$

3.3 Comparison of experimental results with theoretical calculations

The computed results by the approximate method are shown in Fig. 6 (b), 7 (b), and 8 (b). Experimental data are in agreement with the theoretical calculation, though the former give slightly higher values than the latter. As shown in Table 1, the approximate solutions show rather lower values than the rigorous solution. Therefore, if the rigorous solution is compared with the experimental data, the agreement between them would become more satisfactory. The theoretical curves for the concentration of various reactants and the amount of chlorine absorbed during the reaction are shown in Fig. 5. Thus the theoretical calculations give satisfactory predictions for both the yield and the reaction time.

Conclusion

The approximate method for predicting the selectivity of (1, 1) order consecutive gas-liquid reactions was derived by extending van Krevelen's method, and the effect of reaction conditions on the yield of the intermediate product was discussed. The experimental results of the consecutive chlorination of *p*-cresol were well explained by the theory, and they were in good agreement with the computed predictions.

Nomenclature

$a = C_A/C_{Ai}$	[—]
$a_i = \text{gas-liquid interfacial area per unit liquid volum}$	[cm ² /cm ³]
$A_r = \text{total contact area at gas-liquid interface}$	[cm ²]
$b = C_B/C_{Bi}$	[—]
$b_i = C_{Bi}/C_{Bi}$	[—]
$C = \text{concentration}$	[g mole/l]
$D = \text{diffusivity}$	[cm ² /sec]
$d = \text{diameter of agitator}$	[cm]
$h_1 = x_i \sqrt{k_2 C_{Ai}/D_B} = (D_A/k_{LA}) \sqrt{k_2 C_{Ai}/D_B}$	[—]
$h_2 = x_i \sqrt{k_2 C_{Ai}/D_R} = (D_A/k_{LA}) \sqrt{k_2 C_{Ai}/D_R}$	[—]
$k = \text{reaction rate constant}$	[g mole/l·sec]
$k_L = \text{liquid phase mass transfer coefficient}$	[cm/sec]
$m = \text{ratio of mole flow rate of air to that of chlorine}$	[—]
$N = \text{reaction rate per unit interfacial area}$	[g mole/cm ² ·sec]
$n = \text{agitating speed}$	[r. p. s.]
$q_B = C_{Bi}/C_{Ai}$	[—]
$q_{B0} = C_{B0}/C_{Ai}$	[—]
$q_R = C_{Ri}/C_{Ai}$	[—]
$r = C_R/C_{Ri}$	[—]
$r_B = D_B/D_A$	[—]
$Re = d^2 n \rho / \mu$	[—]

$r_i = C_{Ri}/C_{Ri}$	[—]
$r_R = D_R/D_A$	[—]
$s = k_1 D_R / k_2 D_B (= h_1^2 / h_2^2)$	[—]
$s' = k_1 / k_2$	[—]
$S_C = \mu / \rho D$	[—]
$Sh = k_i T / D$	[—]
$T = \text{diameter of reactor}$	[cm]
$t = \text{time}$	[sec]
$v = \text{liquid volume per unit area of gas-liquid interface}$	[cm ³ /cm ²]
$V_L = \text{liquid volume of reactor}$	[cm ³]
$x_B = \text{conversion of component B } (= 1 - C_{Bi}/C_{B0})$	[—]
$x_L = \text{liquid film thickness}$	[cm]
$Y = \text{overall yield of intermediate product R } (= C_{Ri}/C_{B0})$	[—]
$\alpha = C_{Ai}/C_{Ai}$	[—]
$\beta^* = \text{modified reaction factor}$	[—]
$\beta_f^* : \beta^* - \{-(da/d\xi)_{\xi=1}\}$	[—]
$\gamma = \sqrt{h_1^2 r_B q_B + h_2^2 r_R q_R}$	[—]
$\Gamma_A = \gamma^2 / h_1^2 b_i$	[—]
$\Gamma_R = r_i / s b_i - r_B q_B / r_R q_R$	[—]
$\gamma' = \sqrt{h_1^2 r_B q_B b_i + h_2^2 r_R q_R r_i}$	[—]
$\gamma_0 : \sqrt{k_1 C_{B0} D_A / k_{LA}}$	[—]
$\delta = (v - x_i) / x_i$	[—]
$\theta = a_i k_{LA} t$	[—]
$\mu = \text{viscosity of liquid}$	[g/cm·sec]
$\xi = \text{dimensionless distance } (= x/x_L)$	[—]
$\rho = \text{density of liquid}$	[g/cm ³]
$\phi = \text{instantaneous selectivity of intermediate product R}$	[—]

Subscript

$A = \text{component A (chlorine)}$	
$B = \text{component B (p-cresol)}$	
$f = \text{liquid film}$	
$i = \text{gas-liquid interface}$	
$l = \text{bulk liquid}$	
$R = \text{component R (monochloro p-cresol)}$	
$0 = \text{feed}$	
$1 = \text{the first reaction represented by Eq. (1)}$	
$2 = \text{the second reaction represented by Eq. (2)}$	

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