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89. Yoshiharu Miura : Mass Transfer with Chemical Reaction and Longitudinal Dispersion in Two-Phase Continuous-Flow Operations. I.

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The evaluations of the concentration distributions necessary for predicting the extents of chemical reaction and mass transfer and the length of the apparatus required for obtaining the desired completions of the chemical reaction and mass transfer are permitted by a general theoretical treatment, taken into consideration the effect of longitudinal dispersion of both fluids for two-phase continuous-flow systems accompanying general second order chemical reaction, mass transfer and longitudinal dispersion. The general solutions for the concentration distributions were numerically obtained by a digital computer. The effects of stage number in the finite difference equation, chemical reaction rate and residence time on the concentration distribution were shown by numerical calculations through Equations (11) to (13).

The influence of chemical reaction rate on the concentration distribution is less as the resistance to mass transfer in phase with chemical reaction is less than that in the other phase without chemical reaction and for example, the reaction rate or the mass transfer rate in the phase with chemical reaction is higher. The concentration distribution can be estimated analytically in the case where the resistance to mass transfer in the phase without chemical reaction is controlling or the degree of longitudinal dispersion is very high.

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It is widely known that simultaneous mass transfer and chemical reaction in continuous-flow operations is a very important process in pharmaceutical and other chemical industries. In continuous-flow operations such as absorption, extraction and chemical reaction, it is generally recognized that the efficiencies of mass transfer and chemical reaction are lowered by the phenomenon of longitudinal dispersion, especially if a high degree of completion is needed, and the phenomenon has great influence on performance and scale-up of the apparatus.

Even though much attention has been paid to dispersion in single-phase flow operations, very limited study has been made so far in continuous-flow two-phase operations. Mathematical solutions were developed by Miyauchi, *et al.*1) and authors2) for two-phase mass transfer accompanied by longitudinal dispersion and first order reaction with moderate rate and second order reaction with very rapid rate in continuous flow operations and the solutions were proved by authors'2) experiments of gas absorption with chemical reaction in packed columns. But the analysis has never developed for the general chemical reaction of m-th and n-th order with respect to two reactants. It was proved by Hikita, *et al.*3) that the rate of gas absorption in stagnant liquid accompanied by an irreversible chemical reaction of m-th and n-th order with respect to dissolving gas and reactant in liquid phase respectively, could be approximately derived by analogous method to the one for the rate of gas absorption with first and first order irreversible reaction with respect to dissolving gas and reactant in liquid phase.

Methods of predicting the concentration distribution necessary for evaluating the extents of chemical reaction and mass transfer and the required length of the apparatus are developed here for one-dimensional axial flow systems of two-phase

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1) T. Miyauchi, K. Nakano, K. Obata, S. Kimura : Chem. Eng. (Japan), **26**, 999 (1962).

2) Y. Miura, S. Hirota, M. Nakajima : *Ibid.*, **27**, 815 (1963).

3) H. Hikita, S. Asai : *Ibid.*, **27**, 823 (1963).

accompanying general first and first order chemical reaction with respect to two reactants respectively, mass transfer and longitudinal dispersion. General solutions for the concentration distributions are obtained numerically and the theoretical analyses developed in former part of this paper are confirmed by actual calculations through a digital electronic computer KDC-1.

Analyses of Basic Equations

It is here considered that a component A diffuses from X-phase to Y-phase and reacts irreversibly with a component B in Y-phase and each one mole of components A and B produce one mole of a product P and the reaction is first order for components A and B respectively and totally second order. The transfer rate of a component A per unit volume of the apparatus is given by Equation (1) and the relationship between the overall volumetric mass transfer coefficient and the volumetric mass transfer coefficient of individual phase is expressed by Equation (2) :

$$N_A = K_X'a[c_{AX} - (b + mc_{AY})] \tag{1}$$

$$\frac{1}{K_X'a} = \frac{1}{k_Xa} + \frac{m}{\beta k_Y a} \tag{2}$$

where β is the so-called reaction factor defined as the ratio of mass transfer coefficients with and without chemical reaction, k_Y'/k_Y, and a linear-distribution equilibrium expressed as $c_{AX}^* = b + mc_{AY}^*$ is assumed.

The theoretical expression for the reaction factor, β, for the mass transfer with second order irreversible reaction was derived by van Krevelen, *et al.*[4] on the assumption of steady state mass transfer across the stagnant fluid film at the interface as

$$\beta = \gamma\eta / \tanh(\gamma\eta) \tag{3}$$

where

$$\gamma = \sqrt{kD_{AY}c_{BY}/k_Y} \tag{4}$$

$$\eta = \sqrt{(\beta_\infty - \beta)\,/\,(\beta_\infty - 1)} \tag{5}$$

In Equation (5), β_∞ is the reaction factor for the mass transfer with second order very rapid irreversible reaction and it is expressed by the following equation based on steady state mass transfer theory[5] :

$$\beta_\infty = 1 + (D_{BY}\ c_{BY})/(D_{AY}\ c_{AY}^*) \tag{6}$$

The reaction factor based on the unsteady state mass transfer theory was derived by Hikita, *et al.*[3] But it is unimportant from the practical standpoint whether the steady state model or the unsteady state model is assumed in the derivation of the theoretical expression for β since β based on the steady state theory is practically equal to β based on the unsteady state theory.

For single-phase continuous-flow systems Damköhler[6] has given the equation of continuity,

$$\frac{\partial c_j}{\partial \theta} = -\mathrm{div}(-D_j \ \mathrm{grad}\ c_j) - \mathrm{div}(uc_j) - \psi(c_j) \tag{7}$$

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[4] D. W. van Krevelen, P. J. Hoftijzer : Rec. trav. chim., **67**, 563 (1948).
[5] S. Hatta : J. Soc. Ind. Chem. (Japan), **31**, 869 (1928).
[6] G. Damköhler : "Der Chemie-Ingenieur," A. Eucken and M. Jakob, eds., Vol. 3, Part 1, p. 366, Akademische Verlagsgesellshaft, Leipzig, 1937.

where u is the linear velocity of the fluid, c_j is the concentration of the j-th component at the point of interest, D_j is its diffusion coefficient, θ is time and $\psi(c_j)$ is a reaction-rate term. For one-dimensional steady-state flow systems in which constant velocity and constant diffusivity of the j-th component can be assumed, Damköhler's equation becomes

$$D_j\frac{d^2c_j}{dz^2}-u\frac{dc_j}{dz}-\psi(c_j)=0 \tag{8}$$

Two-phase continuous-flow systems can be treated by an extension of this equation. When the reaction rate, $\psi(c_j)$, is replaced by a rate of mass transfer linking the two phases X and Y accompanied by chemical reaction in phase Y, basic equations for concentrations of components A, B and P in phases X and Y are expressed as follows by introducing mean longitudinal dispersion coefficients analogous to diffusion coefficients and mean velocities for both phases :

$$\left.\begin{aligned}
&E_X\frac{d^2c_{AX}}{dz^2}-u_X\frac{dc_{AX}}{dz}-\frac{K_X'a}{H_X}\Big[c_{AX}-(b+mc_{AY})\Big]=0\\
&E_Y\frac{d^2c_{BY}}{dz^2}\pm u_Y\frac{dc_{BY}}{dz}-\frac{K_X'a}{H_Y}\Big[c_{AX}-(b+mc_{AY})\Big]=0\\
&E_Y\frac{d^2c_{PY}}{dz^2}\pm u_Y\frac{dc_{PY}}{dz}+\frac{K_X'a}{H_Y}\Big[c_{AX}-(b+mc_{AY})\Big]=0
\end{aligned}\right\} \tag{9}$$

In compound sign of above equations, the positive sign denotes the counter current, and the negative sign denotes the parallel current. After this, the case of the counter current is discussed. The concentration of component A in the bulk of phase Y has been assumed negligible since here the mass transfer with irreversible reaction in phase Y is discussed and rearranging above equations into dimensionless form, the following equations are obtained :

$$\left.\begin{aligned}
&\frac{d^2C_{AX}}{dZ^2}-M_X\frac{dC_{AX}}{dZ}-M_XN_{0X}C_{AX}=0\\
&\frac{d^2C_{BY}}{dZ^2}+M_Y\frac{dC_{BY}}{dZ}-M_YN_{0Y}C_{AX}=0\\
&\frac{d^2C_{PY}}{dZ^2}+M_Y\frac{dC_{PY}}{dZ}+M_YN_{0Y}C_{AX}=0
\end{aligned}\right\} \tag{10}$$

where

$$C_{AX}=\frac{c_{AX}-b}{c^0_{AX}-b}\quad C_{BY}=\frac{c_{BY}}{c^0_{AX}-b}\quad C_{PY}=\frac{c_{PY}-c_{PY}{}^1}{c^0_{AX}-b}\quad M_X=\frac{u_XL}{E_X}$$

$$M_Y=\frac{u_YL}{E_Y}\quad N_{0X}=\frac{K_X'aL}{H_Xu_X}\quad N_{0Y}=\frac{K_X'aL}{H_Yu_Y}\quad Z=\frac{z}{L}$$

The reaction factor, β, is a function of k, $c_{AY}{}^*$, c_{BY}, D_{AY}, and D_{BY}, as shown in Equations (3) to (6). Although the apparatus can be kept so that temperature might be constant and k, D_{AY} and D_{BY} might be almost constant, $c_{AY}{}^*$ and c_{BY} are changed by simultaneous mass transfer and chemical reaction and therefore the reaction factor is changed through the apparatus. Consequently N_{0X} and N_{0Y} are functions of z since N_{0X} and N_{0Y} are functions of the reaction factor, β. Therefore, Equation (10) cannot be solved analytically and must be solved numerically.

In the present reaction the reacted moles of component B are equal to the produced moles of component P and the concentration distribution of component P is obtained by that of component B. Basic differential Equations for components A and B in Equation (10) being rearranged into finite difference form with n stages, one has the following equations: for the first stage,

$$\left.\begin{aligned} C_{\mathrm{AX}2}&=\frac{1}{\alpha_{\mathrm{X}}}\left\{(1+\alpha_{\mathrm{X}}+\frac{N_{0\mathrm{X}1}}{n})C_{\mathrm{AX}1}+C^{0}_{\mathrm{AX}}\right\} \\ C_{\mathrm{BY}2}&=C_{\mathrm{BY}1}+\left(\frac{1}{1+\alpha_{\mathrm{Y}}}\right)\left(\frac{N_{0\mathrm{Y}1}}{n}\right)C_{\mathrm{AX}1} \end{aligned}\right\} \tag{11}$$

for the i-th stage,

$$\left.\begin{aligned} C_{\mathrm{AX}i+1}&=\frac{1}{\alpha_{\mathrm{X}}}\left\{(1+2\alpha_{\mathrm{X}}+\frac{N_{0\mathrm{X}i}}{n})\,C_{\mathrm{AX}i}-(1+\alpha_{\mathrm{X}})C_{\mathrm{AX}i-1}\right\} \\ C_{\mathrm{BY}i+1}&=\frac{1}{1+\alpha_{\mathrm{Y}}}\left\{(1+2\alpha_{\mathrm{Y}})\,C_{\mathrm{BY}i}+\frac{N_{0\mathrm{Y}i}}{n}C_{\mathrm{AX}i}-\alpha_{\mathrm{Y}}C_{\mathrm{BY}i-1}\right\} \end{aligned}\right\} \tag{12}$$

for the n-th stage,

$$\left.\begin{aligned} C_{\mathrm{AX}n}&=\frac{(1+\alpha_{\mathrm{X}})C_{\mathrm{AX}n-1}}{1+\alpha_{\mathrm{X}}+(N_{0\mathrm{X}n}/n)} \\ C_{\mathrm{BY}n}&=\frac{1}{(1+\alpha_{\mathrm{Y}})}\left(C_{\mathrm{BY}}{}^{1}-\frac{N_{0\mathrm{Y}n}{}'}{n}C_{\mathrm{AX}n}+\alpha_{\mathrm{Y}}C_{\mathrm{BY}n-1}\right) \end{aligned}\right\} \tag{13}$$

where

$$\alpha_{\mathrm{X}}=\frac{n}{M_{\mathrm{X}}}-\frac{1}{2} \qquad \alpha_{\mathrm{Y}}=\frac{n}{M_{\mathrm{Y}}}-\frac{1}{2}$$

$$N_{0\mathrm{X}i}=\frac{(K_{\mathrm{X}}'a)_{i}L}{H_{\mathrm{X}}u_{\mathrm{X}}} \qquad N_{0\mathrm{Y}i}=\frac{(K_{\mathrm{X}}'a)_{i}L}{H_{\mathrm{Y}}u_{\mathrm{Y}}}$$

The method for calculating the above finite difference equation is as follows: (1) assume $C_{\mathrm{AX}1}$ and $C_{\mathrm{BY}1}$ in the first stage or $C_{\mathrm{AX}n}$ and $C_{\mathrm{BY}n}$ in the n-th stage and obtain $C_{\mathrm{AX}2}$ and $C_{\mathrm{BY}2}$ by Equation (11) or $C_{\mathrm{AX}n-1}$ and $C_{\mathrm{BY}n-1}$ by Equation (13), (2) obtain successively C_{AX} and C_{BY} in the next stage by Equation (12), (3) examine if the relation of Equation (13) or (11) is satisfied, (4) assume again $C_{\mathrm{AX}1}$ and $C_{\mathrm{BY}1}$ or $C_{\mathrm{AX}n}$ and $C_{\mathrm{BY}n}$ until the relation of Equation (13) or (11) is satisfied and repeat the calculations of above (1) to (3). It takes long time to make the above-mentioned calculation without using the electronic computer.

Considering the case where the degree of longitudinal dispersion in one phase is negligible low, concentrations of components in the phase at the inlet have not to be assumed for the above-mentioned calculation of finite difference equations as shown by Miyauchi, *et al.*[1] For example, in the case where longitudinal dispersion in phase X is very low and M_{X} is converted to infinity, assuming only $C_{\mathrm{BY}1}$ make the next calculation for solving the finite difference Equations. The first assumed value of $C_{\mathrm{BY}1}$ is estimated by assuming that $C_{\mathrm{AX}1}$ is equal to C^{0}_{AX} which is dimensionless term for the concentration of reactant A in the feed of phase X, since $C_{\mathrm{AX}1}$ is very near by C^{0}_{AX} when the degree of longitudinal dispersion in phase X is very low. It gives good approximation for calculating the concentration distribution to assume that M is converted to infinity when the value of M for the phase is greater than about ten as shown in later part.

Case of High Longitudinal Dispersion or X-phase Resistance Controlling

When the degree of longitudinal dispersion is high and the value of M is small, numerical solutions close by exact solution of Equation (10) are obtained by calculating the finite difference Equations (11) to (13) with comparatively less stages because higher longitudinal dispersion makes the change of concentration less through the apparatus. The less the number of stages gets, the shorter the time for the calculation of Equations (11) to (13) gets. When longitudinal dispersion become very high and an average concentration of each component through the apparatus can be used as its representative value and the N_{0X} and N_{0Y} for the representative values of c_{AY}^* and c_{BY} can be used for calculating the concentration distribution, the Equation (10) can be solved analytically.

In the case where the resistance to mass transfer in X-phase where chemical reaction does not take place is greater than the resistance in Y-phase where chemical reaction takes place, the influences of the rates of mass transfer and chemical reaction in Y-phase on the concentration distribution decrease. For example, when the rate of chemical reaction or mass transfer in phase Y is much higher and β or $k_Y a$ is much greater and then the following relation is yielded, the influences of β and $k_Y a$ on over-

$$\frac{1}{k_X a} \gg \frac{m}{\beta k_Y a} \tag{14}$$

all mass transfer volumetric coefficient $K_X'a$ are very small. Therefore, in above-mentioned conditions, the concentration distribution can be estimated by analytical solution of Equation (10) for the representative value of the reaction factor, β, as verified in later part.

Solving Equation (10) for the representative values of N_{0X} and N_{0Y} so as to satisfy the boundary conditions suitable for the case where the rate of longitudinal dispersion in the apparatus is much higher than that in the incoming and outgoing streams away from the apparatus, one obtains the following solutions analogous to those obtained by Miyauchi, *et al.*7,8) :

$$\left.\begin{aligned} C_{AX} &\equiv \frac{c_{AX}-b}{c_{AX}^0-b} = \sum_{i=1}^{2} A_i \exp(\lambda_i z/L) \\ C_{PY} &\equiv \frac{c_{PY}-c_{PY}^1}{c_{AX}^0-b} = \sum_{i=1}^{4} B_i \exp(\delta_i z/L) \end{aligned}\right\} \tag{15}$$

where

$$A_1 = \frac{2(1-a)\exp[M_X(1-a)/2]}{(1-a)^2\exp[M_X(1-a)/2]-(1+a)^2\exp[M_X(1+a)/2]}$$

$$A_2 = \frac{2(1+a)\exp[M_X(1+a)/2]}{(1+a)^2\exp[M_X(1+a)/2]-(1-a)^2\exp[M_X(1-a)/2]}$$

$$\lambda_1 = M_X(1+a)/2, \quad \lambda_2 = M_X(1-a)/2$$

$$B_1 = -(M_Y)^{-1}[B_3\{M_X(1+a)/2+M_Y\}\exp\{M_X(1+a)/2\}+ B_4\{M_X(1-a)/2+M_Y\}\exp\{M_X(1-a)/2\}]$$

$$B_2 = \frac{M_X}{2M_Y}\left\{B_3(1+a)+B_4(1-a)\right\}, \quad B_3 = -\frac{4A_1 M_Y N_{0Y}}{M_X(1+a)\{M_X(1+a)+2M_Y\}}$$

$$B_4 = -\frac{4A_2 M_Y N_{0Y}}{M_X(1-a)\{M_X(1-a)+2M_Y\}} \quad \begin{matrix} \delta_1 = 0, & \delta_2 = -M_Y, \\ \delta_3 = \lambda_1, & \delta_4 = \lambda_2, \end{matrix}$$

$$a = \sqrt{1+4N_{0X}/M_X}$$

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7) T. Miyauchi : US-AEC-UCRL, 3911, Aug. (1957).

8) T. Miyauchi, T. Vermeulen : Ind. Eng. Chem., Fundamentals, 2, 113 (1963).

Solving Equation (10) for the representative N_{0X} and N_{0Y} so as to satisfy the boundary conditions suitable for the case where the degree of longitudinal dispersion in the apparatus is as small as outside of the apparatus, the following solutions are obtained as shown by authors in the previous paper[2) :

$$\left.\begin{aligned} C_{AX} &\equiv \frac{c_{AX}-b}{c^0_{AX}-b} = \sum_{i=1}^{2} A_i' \exp(\lambda_i z/L) \\ C_{PY} &\equiv \frac{c_{PY}-c^1_{PY}}{c^0_{AX}-b} = \sum_{i=1}^{4} B_i' \exp(\delta_i z/L) \end{aligned}\right\} \qquad (16)$$

where

$$A_1' = \frac{(1-a)\exp[M_X(1-a)/2]}{(1-a)\exp[M_X(1-a)/2]-(1+a)\exp[M_X(1+a)/2]}$$

$$A_2' = \frac{(1+a)\exp[M_X(1+a)/2]}{(1+a)\exp[M_X(1+a)/2]-(1-a)\exp[M_X(1-a)/2]}$$

$$\begin{aligned} B_1' = -(2M_Y)^{-1}[&B_3'\{M_X(1+a)\exp(-M_Y)+2M_Y\exp(M_X(1+a)/2)\}+ \\ &B_4'\{M_X(1-a)\exp(-M_Y)+2M_Y\exp(M_X(1-a)/2)\}] \end{aligned}$$

B_2', B_3', B_4', λ_i, δ_i and a are same as B_2, B_3, B_4, λ_i, δ_i, and a in Equation (15).

General Solution

Fig. 1. to 3. show some examples of numerical solution of Equation (10) which were obtained by calculating the finite difference Equations (11) to (13) with forty stages in the case where $L/u_X=0.02$[hr.], $L/u_Y=1$[hr.], $k_Xa=500$[kg-moles/(m³)(hr.) $\left(\frac{\text{kg-mole}}{\text{m}^3}\right)$], $k_Ya=20$[kg-moles/(m³)(hr.) $\left(\frac{\text{kg-mole}}{\text{m}^3}\right)$], $m=1$, $D_{BY}/D_{AY}=1$, $C^1_{BY}=200$, $\sqrt{k(c^0_{AX}-b)D_{AY}/k_Y}=1$ and $M_Y=5$.

The solutions shown in Fig. 1. to 3. indicate the influence of M_X on the concentration distributions. The influence of M_Y on the concentration distribution was similar

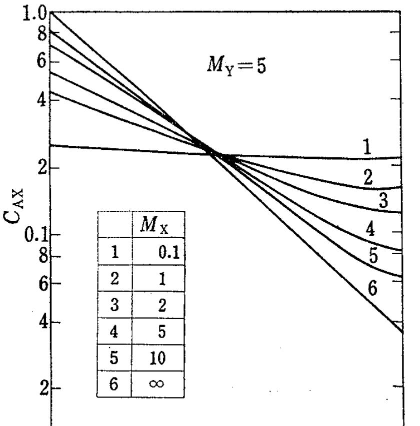

Fig. 1. General Solutions for the Concentration Distributions

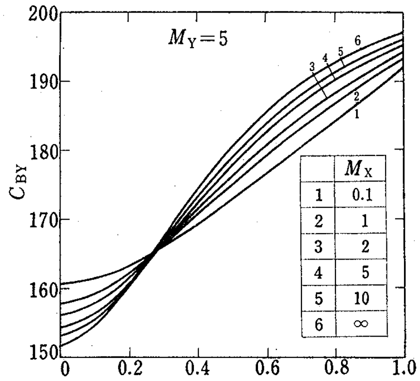

Fig. 2. General Solutions for the Concentration Distributions

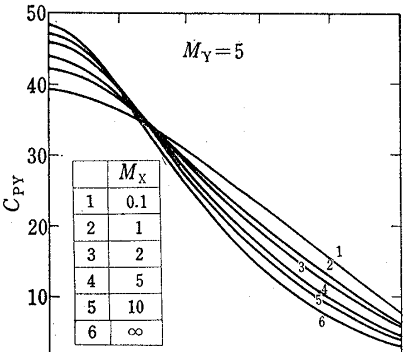

Fig. 3. General Solutions for the Concentration Distributions

to that of M_X shown in Fig. 1. to 3., although that of M_Y is not presented here. Those results show that the extent of mass transfer with chemical reaction is decreased by increase of degree of longitudinal dispersion. It is also indicated from results shown in Fig. 1. to 3., that the concentration distributions under greater M_X than about ten can be approximately estimated by calculating on the assumption of infinite M_X as predicted in above part. It diminishes the trouble of the numerical calculation for concentration distribution as shown in above part to convert the value of M in one phase to infinity.

Effect of Number of Stages in the Finite Difference Equation

The effect of number of stages in the finite difference Equations (11) to (13) on the concentration distribution is shown in Fig. 4. and 5., where the results were obtained by calculating the concentration distributions through the finite difference

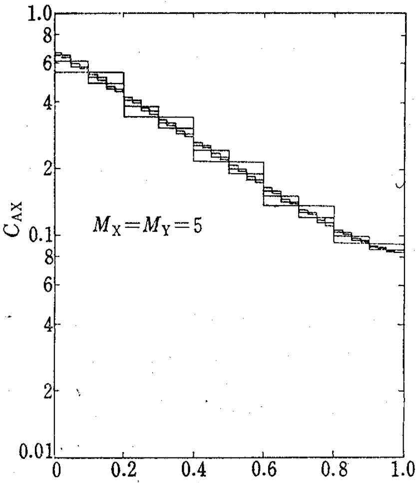

Fig. 4. Effect of Number of Stages in the Finite Difference Equation on the Concentration Distribution

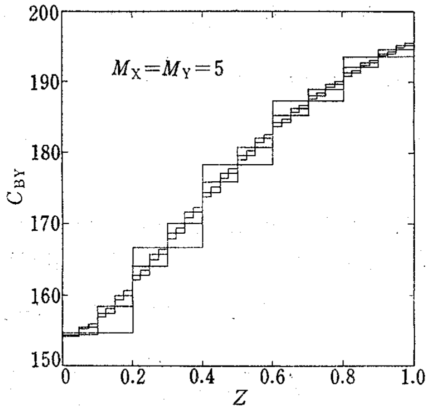

Fig. 5. Effect of Number of Stages in the Finite Difference Equation on the Concentration Distribution

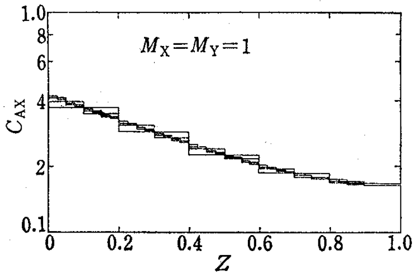

Fig. 6. Effect of Number of Stages in the Finite Difference Equation on the Concentration Distribution

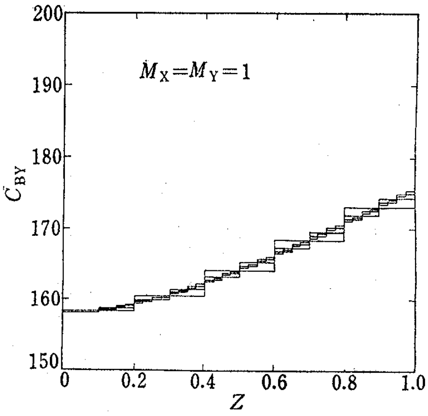

Fig. 7. Effect of Number of Stages in the Finite Difference Equation on the Concentration Distribution

Equations (11) to (13) with divisions of five, ten, twenty and forty on the condition that M_X and M_Y are equal to five and the other factors are same as shown in Fig. 1. to 3. It is found from the results shown in Fig. 4. and 5. that stages of about five give good approximation enough to obtain only the concentrations at the outlet which are necessary for evaluating total extents of mass transfer and chemical reaction. The approximation gets better as the value of M gets less as shown in Fig. 6. and 7. which indicate the concentration distributions under the condition that M_X and M_Y are equal to unity and the other factors are same as shown in Fig. 1. to 3. The above-mentioned results indicate that the less stages for calculating the concentration at the outlet and total extents of mass transfer and chemical reaction give good approximation as the degree of longitudinal dispersion increases and it shortens the time for the calculation to make the stages less.

Effect of Chemical Reaction Rate and Residence Time

Fig. 8. and 9. show the effect of chemical reaction rate on the concentration distributions, changing values of $\sqrt{k(c^0_{AX}-b)D_{AY}}/k_Y$ as 0.5, 1, 2 and 5 in the case where M_X and M_Y are infinity and five and other factors are same as shown in Fig. 1. to 3. It is obvious from Fig. 8. and 9. that the extent of mass transfer with chemical reaction is increased with higher rate of chemical reaction although that is natural.

The influences of residence time on the concentration distributions are shown in Fig. 10. and 11. where the residence times of both phases are varied as shown in tables on the same figures and the changes of the volumetric mass transfer coefficients for phases X and Y, k_Xa, k_Ya are assumed to follow to the change of residence times of both phases as shown in the same tables and values of $\sqrt{k(c^0_{AX}-b)D_{AY}}/k_Y$, M_X and M_Y are equal to five and C^1_{BY} is ten and the other factors are same as shown in Fig. 1. to 3. The results shown in Fig. 10. and 11. indicate that the extents of mass transfer with chemical reaction are increased by increasing the residence time, although that is natural.

When the resistance to mass transfer in phase X where chemical reaction does not take place is greater than that in phase Y where chemical reaction takes place, the effect of the reaction rate on the concentration distribution decrease as predicted in above part. For example, comparing the effect of reaction rate on the concentration distribution about the data of curve 3 on Fig. 10. and 11. where k_Ya is greater than k_Xa gives the results as shown in Fig. 12. which indicates that the decrease of resistance to mass transfer in phase Y gives less influence of reaction rate on the concentration distribution than that shown in Fig. 8. where k_Xa is greater than k_Ya and then the resistance to mass transfer in phase Y is greater than that in phase X. According to above comparison, it is guessed that when the volumetric mass transfer coefficient of one phase with chemical reaction is much greater than that of the other phase without chemical reaction or the reaction rate is very high and then the resistance to mass transfer in the phase without chemical reaction is controlling, the influences of the mass transfer rate in the phase with chemical reaction and the reaction rate on the concentration distribution are much less and then the concentration distribution can be obtained analytically with good approximation by using the representative values of the mass transfer coefficient and the reaction rate as predicted in above part.

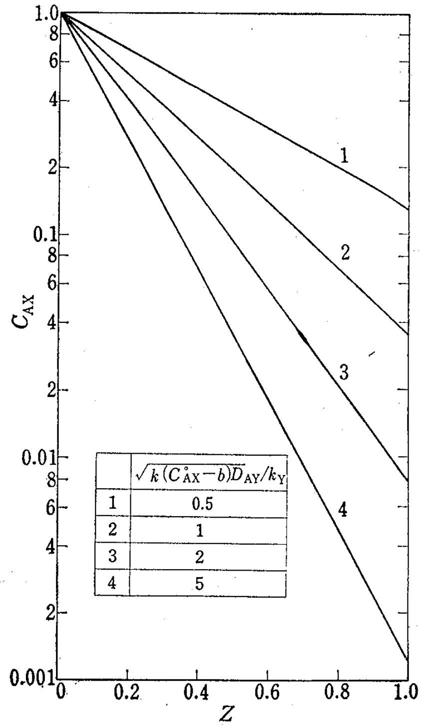

Fig. 8. Effect of Chemical Reaction Rate on the Concentration Distribution

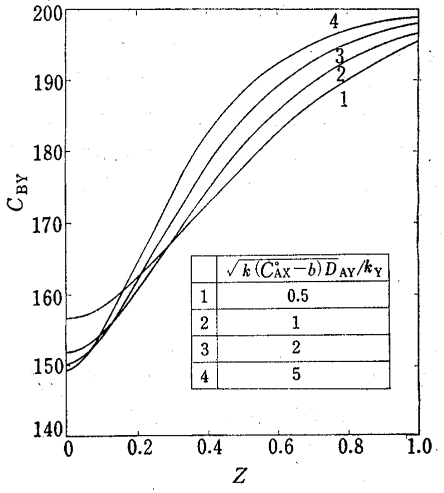

Fig. 9. Effect of Chemical Reaction Rate on the Concentration Distribution

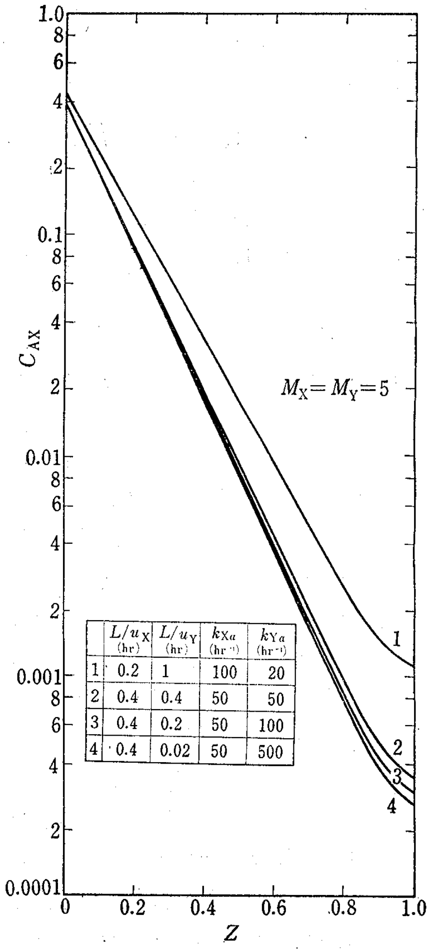

Fig. 10. Effect of Residence Time on the Concentration Distribution

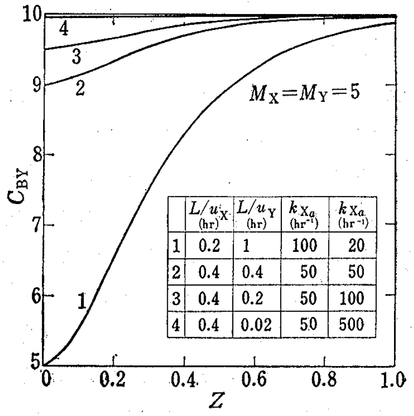

Fig. 11. Effect of Residence Time on the Concentration Distribution

Comparison between Numerical and Analytical Solutions.

Regarding the average values of N_{0X} and N_{0Y} obtained by using the arithmetical mean of outlet and inlet values of c_{AX} and c_{BY} as the representative values of N_{0X} and N_{0Y} through the apparatus, the approximate concentration distributions were evaluated by Equation (15) at M_X of one tenth to five and by Equation (16) at M_X of ten under the same conditions as those of Fig. 1. to 3. Those results are shown by full curves in Fig. 13. and 14. where the numerical solutions obtained by Equations (11) to (13) are also shown by dotted curves. The differences between the approximate solutions by Equations (15) and (16) and the numerical solutions obtained by Equations (11) to (13) get less as the degree of longitudinal dispersion is greater as shown in Fig. 13. and 14., which indicate that the concentration distribution is estimated with good approximation by the analytical solution for the case of less M than about two.

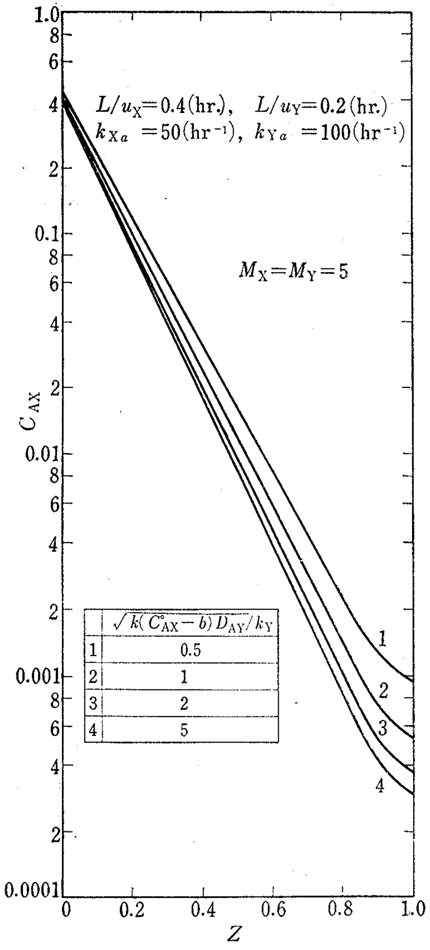

Fig. 12. Effect of Chemical Reaction Rate on the Concentration Distribution

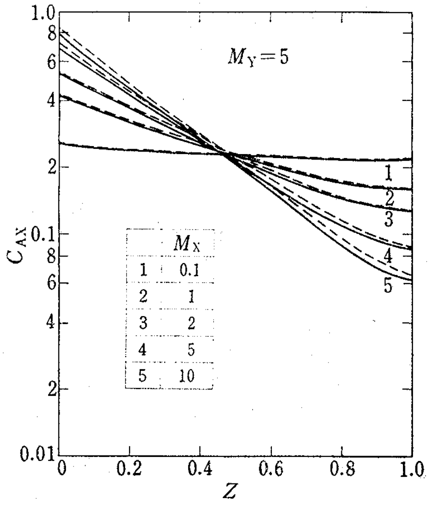

Fig. 13. Comparisons between Analytical and Numerical Solutions

Fig. 15. indicates the differences between the approximate analytical solutions shown by full curves and the numerical solutions shown by dotted curves under the same conditions as those in Fig. 12. It is verified from the comparisons shown in Fig. 15. that estimations by Equation (15) or (16) give good approximation for the concentration distributions in the case where the resistance to mass transfer in one phase with chemical reaction is much less than that in the other phase without chemical reaction as predicted in above part.

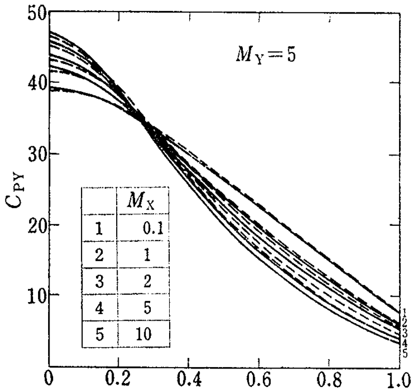

Fig. 14. Comparisons between Analytical and Numerical Solutions

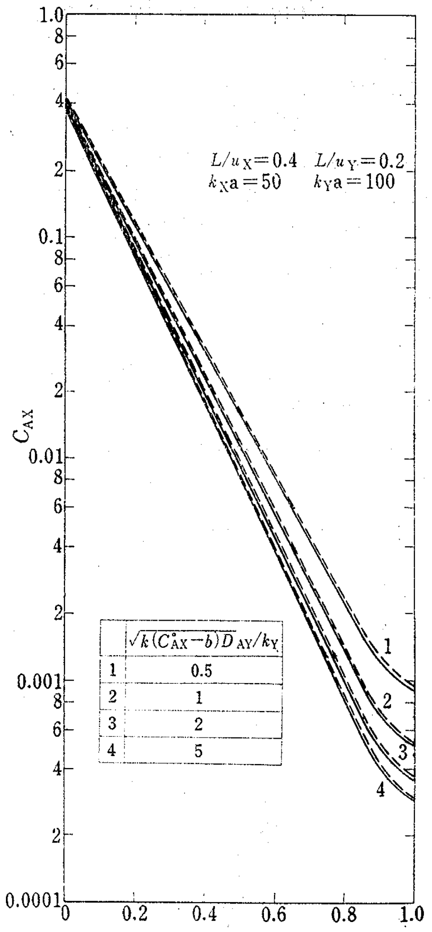

Fig. 15. Comparisons between Analytical and Numerical Solutions

Nomenclature

a : effective interfacial area per unit volume of the apparatus [m^2/m^3]
b : constant in the equilibrium distribution relation
C : dimensionless term for the concentration defined below Eqaution (10)
c : concentration [kg-moles/m^3]
D : diffusion coefficient [m^2/hr.]
div : divergence function
E : longitudinal dispersion coefficient [m^2/hr.]
exp : exponential function defined as $\exp(x)=e^x$
grad : gradient
H_X, H_Y : holdup of phases X and Y, respectively
K_X' : overall coefficient for mass transfer with chemical reaction based on phase X [m/hr.]
k_X, k_Y : mass transfer coefficients for phases X and Y, respectively [m/hr.]
k_Y' : Y-phase coefficient for mass transfer with chemical reaction [m/hr.]
k : reaction rate constant for second order reaction [m^3/(kg-mole) (hr.)]
L : total length of the apparatus [m.]
M, M_X, M_Y : dimensionless terms defined as $\frac{uL}{E}$, $\frac{u_XL}{E_X}$, and $\frac{u_YL}{E_Y}$, respectively
m : constant in the equilibrium distribution relation
N_A : rate of mass transfer with chemical reaction per unit volume of the apparatus [kg-moles/(m^3) (hr.)]
N_{OX}, N_{OY} : dimensionless terms defined as $\frac{K_X'aL}{H_Xu_X}$ and $\frac{K_X'aL}{H_Yu_Y}$, respectively
n : number of stages in the finite difference equation

u : mean linear velocity defined as L/θ 〔m/hr.〕
Z : ratio defined as z/L
z : axial distance from the inlet of phase X through the apparatus 〔m〕
α : dimensionless term defined as $(n/M)-(1/2)$
β : reaction factor defined as k_Y'/k_Y
γ : ratio defined as $\sqrt{kc_{BY}D_{AY}}/k_Y$
θ : residence time 〔hr.〕
Subscript :
A,B : refer to reactants A and B, respectively
i, n : refer to the values in the i-th and n-th stages of the finite difference equation
P : refers to product P
X, Y : refer to phase X and Y, respectively
Superscript
0 : refers to the values in the feed to one side of the apparatus, *i.e.* $Z=0$
1 : refers to the values in the feed to the other side of the apparatus, *i.e.* $Z=1$
* : refers to the values at X–Y interface