Gas Absorption Accompanied by Instantaneous Bimolecular Reaction in Turbulent Liquids

Gas absorption accompanied by instantaneous bimolecular reaction in turbulent liquids ($Re > 1200$) is treated in terms of an eddy diffusion model. The species balance equations are integrated for the eddy diffusivity varying as the square of the distance from the free surface. Experimental mass transfer coefficients were measured in a wetted-wall column for the absorption of carbon dioxide in aqueous sodium hydroxide solutions. Experimental results were obtained for carbon dioxide partial pressures of 1.0 and 1.5 atm. and for sodium hydroxide concentrations varying between 0.020 and 0.220N over the Reynolds number range 1400 to 5400. The experimental data showed good agreement with the theoretical calculations, the mean deviation being 8.2%.

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SCOPE

For absorption accompanied by chemical reaction, concurrent operation is desirable since in this case the driving force advantages of countercurrent operation are not applicable. Since there are no flooding limitations for concurrent flow in packed columns, the flow in the liquid film will be turbulent under usual operating conditions.

In the work reported here, gas absorption accompanied by an instantaneous bimolecular reaction is treated. The turbulent transport is modeled using a previously proposed eddy diffusivity expression. Physical absorption experiments by Lamourelle and Sandall (1972) in a long wetted-wall column gave an expression for the liquid phase eddy diffusivity variation in the region near the free gas-liquid interface.

$$\epsilon = ay^2 \tag{1}$$

Equation (1) is used to integrate the conservation equation for each component under the boundary condition of an instantaneous bimolecular reaction with stoichiometry given by

$$mA + nB \rightarrow A_mB_n \tag{2}$$

The theoretical predictions are compared with experimental mass transfer coefficients measured in a long wetted-wall column. The particular system chosen for the experiments is the absorption of carbon dioxide in aqueous sodium hydroxide solutions.

CONCLUSIONS AND SIGNIFICANCE

The theoretical results give the enhancement factor for the absorption of gas A expressed as

$$\phi = \pi/2\tan^{-1}\beta \tag{3}$$

β is the dimensionless distance from the free surface to the reaction plane ($\beta \equiv y_r\sqrt{a/D_A}$) and is determined from a solution of the nonlinear equation

$$\frac{\pi}{2} - \tan^{-1}\beta\sqrt{D_A/D_B} = \frac{nC_{Bb}}{mC_{As}}\sqrt{D_B/D_A}\tan^{-1}\beta \tag{4}$$

Asymptotic solutions to Equation (4) are obtained for large and small values of the parameter $nC_{Bb}/mC_{As}\sqrt{D_B/D_A}$.

As a check on the experimental procedure, physical and chemical absorption runs were carried out for laminar flow with a surfactant added to eliminate ripples and give well-defined hydrodynamics. These laminar flow experiments agreed well with the predictions of penetration theory.

Experimental results were obtained for turbulent liquid films for the sodium hydroxide concentration range 0.020 to 0.220N, for Reynolds numbers varying between 1400 and 5400 and for carbon dioxide partial pressures of 1 and 1.5 atm. The experimental results agree well with the theoretical calculations (mean deviation = 8.2%), thus confirming the validity of the eddy diffusion model for the case of gas absorption accompanied by an instantaneous bimolecular reaction.

The theoretical results obtained in this work should be applicable to gas absorption equipment in which the film lengths are long enough so that the concentration profiles become fully developed, provided that the eddy diffusivity varies as the square of the distance from the free surface.

It is often the case for gas absorption that the controlling resistance to mass transfer lies in the liquid phase. In order to reduce the liquid mass transfer resistance and also to increase the capacity of the liquid to absorb, it is frequently desirable to use a liquid in which the absorbing gas will chemically react. In the work reported here, a previously proposed eddy diffusivity expression is used to analyze gas absorption accompanied by instantaneous bimolecular reaction in turbulent liquid films ($Re >$ 1200).

Liquid-phase mass transfer across a free gas-liquid interface has been treated in terms of an eddy diffusivity by Lamourelle and Sandall (1972). These authors experimentally determined the behavior of the liquid-phase eddy diffusivity near the free surface, in the absence of surface shear, from gas absorption measurements in a long wetted-wall column. They found that the eddy diffusivity varies as the square of the distance from the free surface.

$$\epsilon = ay^2 \tag{5}$$

For water at 25°C, a was found to be

$$a = 7.90 \times 10^{-5} Re^{1.678} \tag{6}$$

Equation (5) is valid for the region adjacent to the free surface. Since the major resistance to mass transfer occurs close to the free surface because of the low molecular diffusivity normally encountered in liquids, it is important to know the eddy diffusivity accurately only in this region.

Equation (5) has been used by Mills and Chung (1973) to correlate heat transfer rates across turbulent liquid films. Menez and Sandall (1974) have used Equation (5) to describe gas absorption with first-order reaction at long exposure times. Sandall (1974) and Kayihan and Sandall (1974) have integrated the diffusion equation for short exposure times under conditions of physical absorption and absorption accompanied by first-order chemical reaction, respectively, using Equation (5) to describe the turbulent transport.

For our work, the eddy diffusivity given by Equation (5) is used to integrate the species balance equations for the case of absorption accompanied by instantaneous bimolecular reaction. The theoretical predictions are compared to experimental results obtained for turbulent flow in a wetted-wall column. The specific system chosen for the experimental work is the absorption of carbon dioxide into sodium hydroxide solutions. This particular reaction was chosen because of its industrial importance and because the kinetics of this reaction are well understood. The fundamental global reaction which describes the process is

$$CO_2 + 2OH^- \rightarrow CO_3^= + H_2O$$

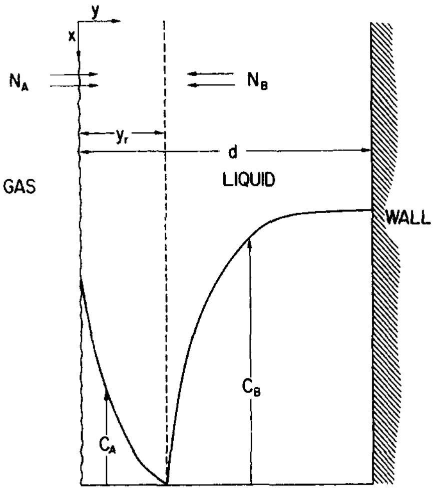

Fig. 1. Concentration profiles for instantaneous bimolecular reaction.

Information regarding the kinetics of this reaction can be found in the book by Astarita (1967) and the paper of Danckwerts and Sharma (1966).

THEORY

Consider a reaction of the form

$$mA + nB \rightarrow A_mB_n \tag{7}$$

where A is the absorbing gas and B the reactant in the liquid phase. Under conditions of an instantaneous, second-order, irreversible reaction both species A and B diffuse toward each other and meet in a plane where the reaction takes place. This situation is illustrated in Figure 1. The concentration of both reactants is zero at the reaction plane because the reaction is taken to be instantaneous.

The condition for the reaction to be considered instantaneous has been given by Astarita (1967) by comparing the penetration theory solutions for fast reactions and for instantaneous reactions. The criterion for the reaction to be considered instantaneous is expressed as

$$\sqrt{\frac{t_D}{t_R}} > \frac{nC_{Bb}}{mC_{As}} \tag{8}$$

The diffusion time t_D is defined as

$$t_D = \frac{D_A}{k_c^{\circ 2}} \tag{9}$$

and the reaction time t_R is defined as

$$t_R = \frac{C_{As}}{r} \tag{10}$$

where the reaction rate r is evaluated under the maximum possible driving force

$$r = kC_{As}C_{Bb} \tag{11}$$

To analyze the rate of absorption under the condition of an instantaneous reaction in a turbulent liquid, it is assumed that the depletion of B is slow enough so that y_r, the distance to the reaction plane, is not a function of x. Under these conditions if we are sufficiently far downstream from the entrance, then $\partial C_A/\partial x = 0$. The differential equation governing the diffusion of the gas being absorbed A may be written in terms of an eddy diffusivity as

$$\frac{d}{dy}\left\{ (D_A + \epsilon(y)) \frac{dC_A}{dy} \right\} = 0 \tag{12}$$

The boundary conditions for A may be expressed as

$$\begin{aligned} &\text{(i)} \quad y = 0, \quad C_A = C_{As} \\ &\text{(ii)} \quad y = y_r, \quad C_A = 0 \end{aligned} \tag{13}$$

Equation (12) neglects axial transport and assumes no diffusion-induced velocity, these assumptions are generally valid for liquids. Solution of Equation (12) and (13) with the eddy diffusivity given by Equation (5) gives an expression for the concentration of A.

$$C_A = C_{As}\{1 - \tan^{-1} y\sqrt{a/D_A}/\tan^{-1} y_r\sqrt{a/D_A}\} \tag{14}$$

The differential equation describing the diffusion of reactant B may be written with the same assumptions as for Equation (12) as

$$u\frac{\partial C_B}{\partial x} = \frac{\partial}{\partial y}\left\{ (D_B + \epsilon(y))\frac{\partial C_B}{\partial y} \right\} \tag{15}$$

The boundary conditions for B may be expressed as

$$\begin{aligned} &\text{(i)} \quad y = y_r, \quad C_B = 0 \\ &\text{(ii)} \quad y = d, \quad \frac{\partial C_B}{\partial y} = 0 \end{aligned} \tag{16}$$

If we are sufficiently far downstream the concentration profile for B becomes fully developed. This may be expressed as

$$\frac{\partial}{\partial x}\left(\frac{C_B}{C_{Bb}}\right) = 0 \tag{17}$$

A material balance relates dC_{Bb}/dx to the mass transfer coefficient

$$\frac{dC_{Bb}}{dx} = -\frac{m}{n}\frac{k_c C_{As}}{q} \tag{18}$$

Substitution of Equations (17) and (18) into Equation (15) and expressing C_B in dimensionless form gives

$$\frac{d}{dy}\left\{ (D_B + \epsilon(y))\frac{d\theta}{dy} \right\} + u\theta\frac{m}{n}\frac{k_c C_{As}}{q C_{Bb}} = 0 \tag{19}$$

Equation (19) may be integrated twice, applying both boundary conditions, and the resulting expression for θ may be substituted into the definition of the bulk concentration to give on rearrangement

$$\frac{1}{k_c}\frac{mC_{As}}{nC_{Bb}} = \frac{1}{q^2}\int_{v=y_r}^{d} u(v)\int_{t=y_r}^{v}\frac{1}{D_B + \epsilon(t)}\int_{s=t}^{d} u(s)\theta(s)\,ds\,dt\,dv \tag{20}$$

Changing the order of integration for the second and third integrals in Equation (20) results in

$$\begin{aligned} \frac{1}{k_c}\frac{mC_{As}}{nC_{Bb}} &= \int_{t=y_r}^{d}\frac{dt}{D_B + \epsilon(t)} - \frac{1}{q}\int_{t=y_r}^{d}\frac{1}{D_B + \epsilon(t)}\int_{v=0}^{y} u(v)\,dv\,dt \\ &\quad - \frac{1}{q^2}\int_{t=y_r}^{d}\frac{1}{D_B + \epsilon(t)}\int_{v=t}^{d} u(v)\int_{s=0}^{y} u(s)\theta(s)\,ds\,dv\,dt \end{aligned} \tag{21}$$

Equation (21) is a general expression relating the mass transfer coefficient to y_r, the eddy diffusivity, and the velocity and concentration profiles. Since the velocity and concentration distributions are not known, the second and third integrals can not be evaluated exactly. However, these integrals are very small compared to the first integral and may be neglected. This is the case since y_r will be very small and because ϵ goes to zero at the free surface. Thus for small D_B, as is the case for liquids, the major contribution to these integrals occurs near $y = y_r$ and the first integral dominates the second and third integrals. Therefore, to a good approximation Equation (21) may be represented as

$$\frac{1}{k_c}\left(\frac{mC_{As}}{nC_{Bb}}\right) = \int_{t=y_r}^{\infty}\frac{dt}{D_B + \epsilon(t)} \tag{22}$$

Equation (22) may be integrated for the eddy diffusivity expressed by Equation (5) to give

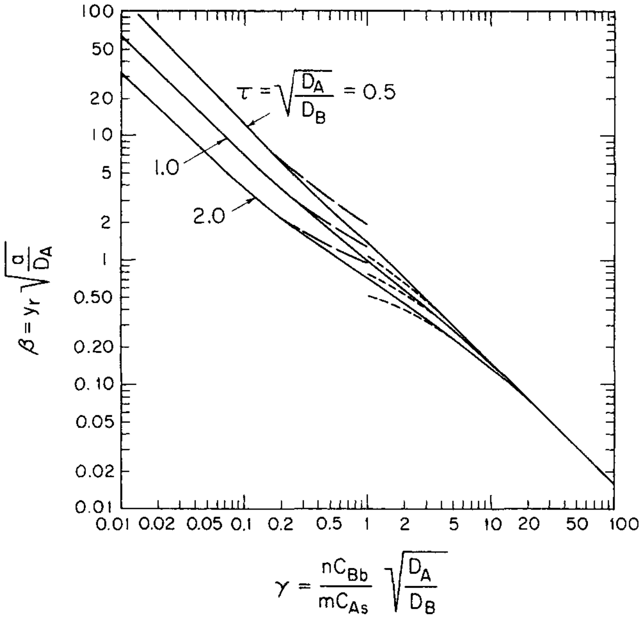

Fig. 2. Dimensionless reaction plane distance as a function of γ and τ.

$$\frac{1}{k_c}\left(\frac{mC_{As}}{nC_{Bb}}\right) = \frac{1}{\sqrt{aD_B}}\left(\frac{\pi}{2} - \tan^{-1} y_r\sqrt{a/D_B}\right) \tag{23}$$

An equation for the mass transfer coefficient may also be obtained by differentiating Equation (14)

$$k_c = \sqrt{a\,D_A}/\tan^{-1} y_r\sqrt{a/D_A} \tag{24}$$

The mass transfer coefficient, given by Equation (24), is expressed in terms of y_r, the distance to the reaction plane. A relationship for y_r is obtained by solving Equation (23) for k_c and equating to Equation (24).

$$\frac{\pi}{2} - \tan^{-1}\beta\tau = \gamma\tan^{-1}\beta \tag{25}$$

Asymptotic solutions for β can be obtained from Equation (25) for the limiting cases of large and small γ. In the limit of $\gamma \rightarrow 0$, Equation (25) gives the small γ asymptote for β as

$$\beta = 2(1 + \gamma\tau)/\pi\gamma\tau \tag{26}$$

The asymptotic solution to Equation (25) for large γ gives

$$\beta = \pi/2(\gamma + \tau) \tag{27}$$

Equation (25) was solved for β using the Newton method and the results are shown in Figure 2. The small and large γ asymptotes are also shown in Figure 2. For γ less than about 0.1, Equation (26) represents β with good accuracy for $0.1 < \tau < 10$. For γ greater 10, Equation (27) shows good agreement with the exact results over the same range in τ.

It is of interest to consider the ratio of the mass transfer coefficient with chemical reaction to the mass transfer coefficient without chemical reaction since this ratio may have a more general application than the mass transfer coefficient alone. The expression for the mass transfer coefficient for physical absorption is given by Lamourelle and Sandall (1972).

$$k_c^0 = \frac{2}{\pi}\sqrt{aD_A} \tag{28}$$

The enhancement factor is obtained from Equations (24) and (28).

$$\phi = \pi/2\tan^{-1}\beta \qquad (29)$$

The magnitude of the errors incurred due to the assumptions made in deriving Equation (23) may be estimated. For the conditions of our experiments and for $\beta = 1$ and $Re = 3000$, the sum of the neglected integrals in Equation (17) is estimated to represent a maximum of less than 3.8% of the retained term. This estimate was obtained by taking $u = 1.2u_b$ and $\theta = 1$ and evaluating these integrals analytically. The change in y_r over a film length of 75 cm, as is the case for our experiments, is calculated to be 3.5% and the error incurred by changing the upper limit to infinity in Equation (22) may also be estimated and is found to be extremely small. Thus the assumptions made in arriving at Equation (19) would appear to be justifiable.

It is interesting to note that for equal diffusion coefficients for the gas and liquid phase reactants, $\tau = 1$, Equation (25) can be solved exactly for β. In this case Equation (29) reduces to $\phi = 1 + \gamma$. This may be compared to the film theory result $\phi = 1 + \gamma/\tau$ and the penetration theory prediction, $\phi = \tau + \gamma$ (Astarita, 1967). Thus for $\tau = 1$ all three theories give equivalent results.

EXPERIMENTAL APPARATUS AND PROCEDURE

The wetted-wall column apparatus of Lamourelle and Sandall (1972) was used for the experiments. A schematic drawing of the apparatus is shown in Figure 3. The liquid film was formed on the outside of a ⅝-in. diameter stainless steel tube enclosed in a 3.0-in. diameter glass pipe. The liquid was distributed on the outside wall of the tube through a distributor cap having an annular width of 0.054 in. The column length could be varied by adjusting the height of the liquid receiver at the bottom of the column. This receiver consisted of a 2.0-in. diameter plexiglass pipe concentric to the wetted-wall column.

A desorption column was provided, since the water flow rates used for the physical absorption studies were such that it was necessary to recycle the water. The desorption column was a disk and a doughnut baffle tower and was operated at absolute pressures of about 300 mmHg. Water flow rates were measured with rotameters. The viscosity of all solutions was determined at 25°C with a falling ball viscometer. Liquid temperatures were measured in the outlet stream with a chromel-alumel thermocouple.

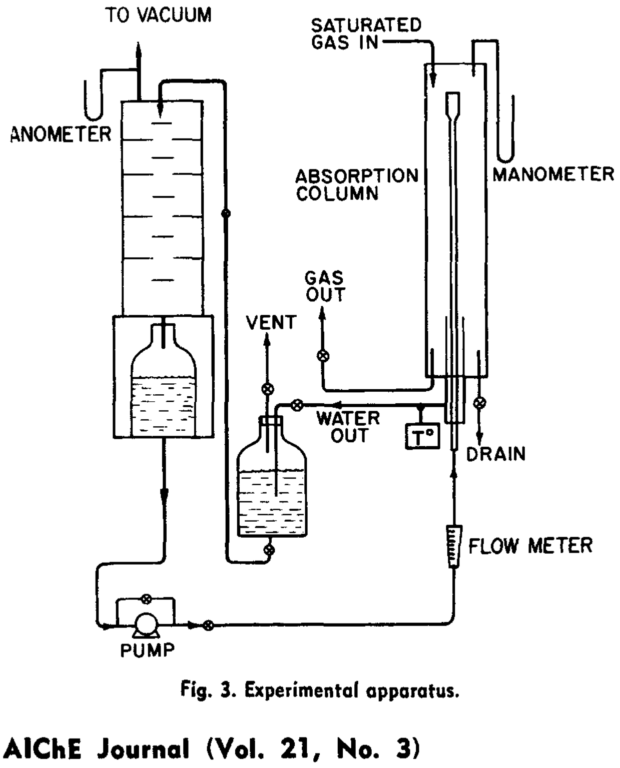

Fig. 3. Experimental apparatus.

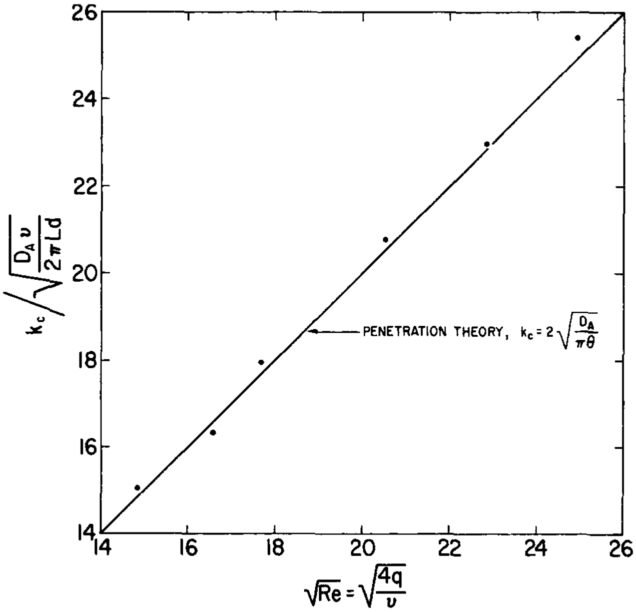

Fig. 4. Physical absorption of carbon dioxide in water for laminar flow. $L = 20$ cm.

For the physical absorption experiments 50-ml samples were collected at the inlet and the outlet of the column and were analyzed for carbon dioxide by precipitating the carbon dioxide as barium carbonate from a solution of barium chloride and sodium hydroxide, and the excess sodium hydroxide was titrated to a phenolphthalein end point with hydrochloric acid.

For the chemical absorption experiments the desorption column was not used since there was no free carbon dioxide in the sodium hydroxide solutions. At the beginning of each run, make-up sodium hydroxide was added in order to maintain a fairly uniform hydroxide concentration through a series of runs. Three samples were taken in the case of chemical absorption. In addition to samples withdrawn from the inlet and outlet of the wetted-wall column, a third one was taken at the beginning of each run before introducing carbon dioxide into the column. This was done in order to determine the carbonate and sodium hydroxide concentrations before starting the run. Samples were analyzed for total alkalinity by titration with hydrochloric acid using methyl orange indicator. The sodium hydroxide concentration was determined by titrating with hydrochloric acid using phenolphthalein indicator after the carbonate present had been precipitated as barium carbonate by the addition of an excess of barium chloride. Further details of the experiment may be found in the original thesis (Méndez, 1973).

EXPERIMENTAL RESULTS AND DISCUSSION

Physical Absorption

Several initial runs were made for the physical absorption of carbon dioxide in water as a check on the experimental procedure. These runs were made for both laminar and turbulent flow. Mass transfer coefficients for these runs were calculated from an integrated material balance equation

$$k_c = \frac{q}{L}\left[\frac{R}{R+d}\right]\ln\left[\frac{C_{As}{}^0 - C_{A1}}{C_{As}{}^0 - C_{A2}}\right] \qquad (30)$$

In Equation (30), q, R, L, C_{A1}, and C_{A2} were measured. The solubility of carbon dioxide in water $C_{As}{}^0$ was taken from Perry et al. (1963) and is expressed by Henry's law

$$C_{As}{}^0 = p_A/H \qquad (31)$$

For turbulent films, the film thickness d was obtained from the correlation of Brötz (1954)

$$d = 0.0672\ (\nu^2/g)^{1/3}Re^{2/3} \qquad (32)$$

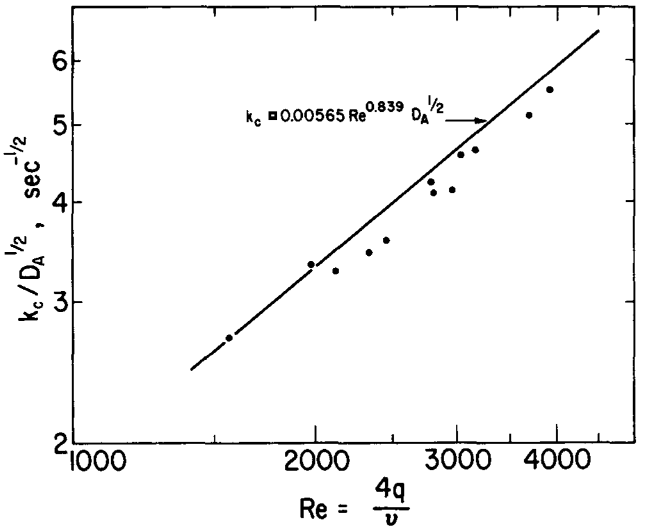

Fig. 5. Physical absorption of carbon dioxide in water for turbulent flow.

For laminar films the film thickness is given by the Nusselt relationship

$$d = (3\nu q/g)^{1/3} \tag{33}$$

The laminar flow physical absorption data for carbon dioxide over the Reynolds number range 220 to 620 are compared to the Higbie (1935) penetration theory in Figure 5. The mass transfer coefficient from penetration theory may be expressed

$$k_c{}^0 = \sqrt{D_A \nu / 2\pi L d} \cdot \sqrt{Re} \tag{34}$$

The data show good agreement with penetration theory, the mean deviation being 1.25%. The mean deviation is defined as

mean deviation =

$$\frac{1}{N}\sum_{i=1}^{N} \left| \frac{\text{experimental value} - \text{theoretical value}}{\text{theoretical value}} \right|_i \tag{36}$$

The diffusivity for the carbon dioxide-water system which is needed for this comparison was taken from Vivian and King (1964). Diffusivities were corrected for small temperature deviations from 25°C by using the Stokes-Einstein relationship.

$$D_A \mu / T = \text{a constant} \tag{37}$$

For the laminar flow runs the film length was adjusted to 20.0 cm and 0.30 wt. % of a surface active agent, Petrowet R, was added to suppress ripples and to give well-defined hydrodynamics. The column length and concentration of surfactant were similar to that used by Perez and Sandall (1973) and by Lynn et al. (1955). These authors found agreement with the Higbie penetration theory for wetted-wall column gas absorption experiments.

The turbulent flow physical absorption data are compared to Equation (28) in Figure 5. The Reynolds number was varied from 1550 to 3960 for these experiments. The data agree with the predictions of Equation (28) to within a mean deviation of 6.1%. The film length for the turbulent flow experiments was adjusted to 75 cm.

Chemical Absorption

Chemical absorption runs were made for both laminar and turbulent flow for the absorption of carbon dioxide into aqueous sodium hydroxide solutions. The laminar flow experiments were conducted as a further test of the experimental procedure and as a check on the various physical properties used. An integrated material balance for the case of an instantaneous irreversible reaction gives an equation for the mass transfer coefficient.

$$k_c = \frac{q}{2L}\left(\frac{R}{R+d}\right)\left(\frac{C_{OH^-,1} - C_{OH^-,2}}{C_{As}}\right) \tag{38}$$

In this case the surface equilibrium concentration C_{As} must be corrected due to the presence of the salts in solution. The correlation of Nijsing and Kramers (1957) was used for this purpose.

$$\log \frac{C_{As}}{C_{As}{}^0} = -0.088I \tag{39}$$

I is the ionic strength, defined as half the sum of the concentrations of the various ions multiplied by the square of the corresponding electrical charge.

Figure 6 shows the laminar flow chemical absorption data compared to the predictions of penetration theory.

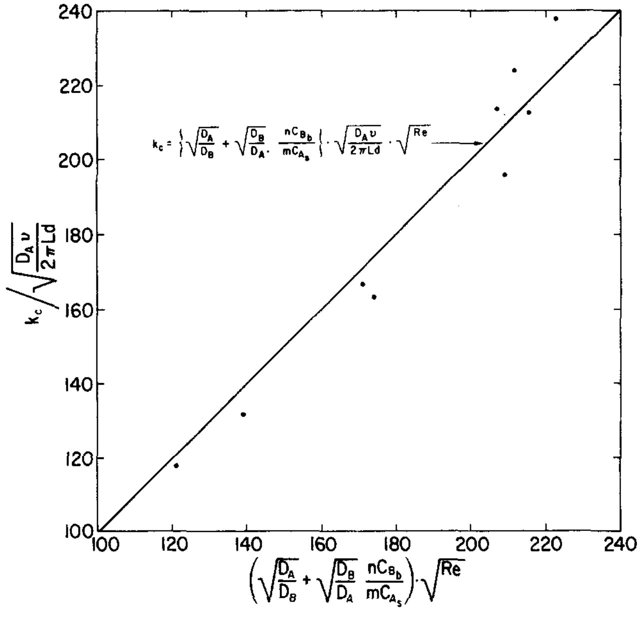

Fig. 6. Laminar flow absorption accompanied by instantaneous reaction, carbon dioxide absorption in aqueous sodium hydroxide solution. L = 20 cm.

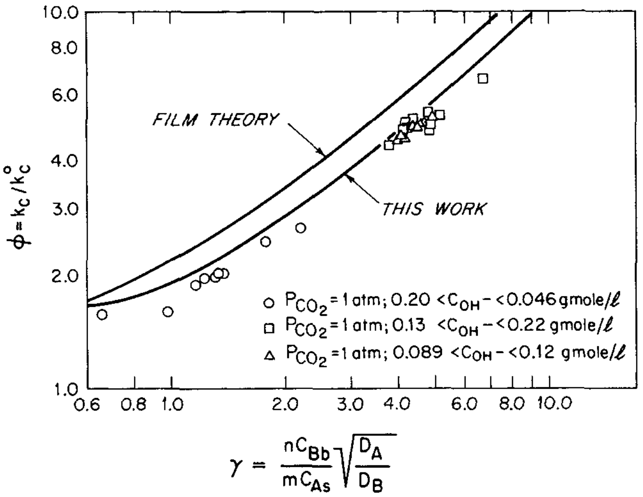

Fig. 7. Turbulent flow absorption accompanied by instantaneous reaction: carbon dioxide absorption in aqueous sodium hydroxide.

For an instantaneous bimolecular reaction in a laminar film the penetration theory result is given by Astarita (1967) as

$$k_c = \left\{ \sqrt{\frac{D_A}{D_B}} + \sqrt{\frac{D_B}{D_A}}\,\frac{nC_{Bb}}{mC_{As}} \right\} \sqrt{\frac{D_A \nu}{2\pi L d}} \cdot \sqrt{Re} \qquad (40)$$

The data agree with Equation (40) within a mean deviation of 4.4%. The value for the diffusion coefficient of hydroxide ions D_B at infinite dilution and 20°C was obtained from Astarita (1967) as 2.84×10^{-5} cm²/s. D_B was corrected for temperature using Equation (37). Through use of Equation (37), both D_A and D_B were corrected for the effects of ions in solution by measuring the viscosities of the various solutions.

For these laminar flow chemical absorption experiments, the film length and surfactant concentration were the same as for the laminar flow physical absorption experiments. The Reynolds number was varied between 140 and 560 and the sodium hydroxide concentration was maintained at approximately 0.36 g moles/l.

The experimental results for chemical absorption in turbulent liquid films are shown in Figure 7 as the enhancement factor versus γ, the dimensionless distance to the reaction plane. The data are compared to the theoretical expression, Equation (29), in Figure 7. It is seen that the experimental results are generally lower than theory predicts; however the agreement is fairly close, the mean deviation being 8.2%. This compares with an estimated maximum experimental error in the enhancement factor of 8.0%. For these experiments the Reynolds number varied between 1380 and 5360. The sodium hydroxide concentration ranged from 0.020 to 0.220 g mole/l; the partial pressure of carbon dioxide was held at 1.0 or 1.5 atmospheres.

The enhancement factor from film theory is also shown in Figure 7. It is seen that the data deviate significantly more from the film theory prediction than from the results of this work. On the scale of Figure 7 the penetration theory curve cannot be distinguished from the results of this work. It should be noted that in plotting the data shown in Figure 7, the experimental mass transfer coefficient for chemical absorption is divided by the physical absorption mass transfer coefficient obtained from the eddy diffusion model [Equation (28)].

SUMMARY

The species balance equations have been integrated for the case of gas absorption accompanied by an instantaneous bimolecular reaction in a turbulent liquid. The turbulent transport was modeled using an eddy diffusivity which varies as the square of the distance from the free surface. The results, as expressed by Equation (29), show that the enhancement factor is a function only of the dimensionless distance to the reaction plane β. The experimental results obtained for $0.21 < \beta < 1.56$ are in good agreement with the theoretical calculations, showing a mean deviation of 8.2%.

NOTATION

a = turbulence parameter in eddy diffusivity expression, s^{-1}
C_A = concentration of A, g mole/cm³
C_{As} = concentration of A at gas-liquid interface, g-mole/cm³
C_{As}^0 = concentration of A at gas-liquid interface for pure water, g-mole/cm³
C_{A1} = bulk concentration of A in inlet sample, g-mole/cm³
C_{A2} = bulk concentration of A in outlet sample, g-mole/cm³
C_B = concentration of B, g moles/cm³
C_{Bb} = bulk concentration of $B = \frac{1}{q}\int_0^d uC_B dy$, g mole/cm³
$C_{OH^-,1}$ = sodium hydroxide concentration in inlet sample, g mole/cm³
$C_{OH^-,2}$ = sodium hydroxide concentration in outlet sample, g mole/cm³
d = film thickness, cm
D_A = diffusion coefficient for A, cm²/s
D_B = diffusion coefficient for B, cm²/s
g = acceleration of gravity, cm/s²
H = Henry's coefficient, atm cm³/g mole
I = ionic strength
k = reaction rate constant, cm³/g moles s
k_c = mass transfer coefficient, cm/s
k_c^0 = mass transfer coefficient without chemical reaction, cm/s
L = film length
N = number of data points
N_A = molar flux of A, g moles/cm²s
N_B = molar flux of B, g moles/cm²s
p_A = partial pressure of carbon dioxide, atm
q = liquid flow rate per wetted perimeter, cm²/s
r = rate of reaction, g moles/cm³s
R = radius of wetted-wall column, cm
Re = Reynolds number = $4q/\nu$
s = dummy variable for y
t = dummy variable for y
t_D = diffusion time, s
t_R = reaction time, s
T = temperature, °K
u = velocity, cm/s
u_b = bulk velocity, cm/s
v = dummy variable for y
x = distance in direction of flow, cm
y = distance into liquid film, cm
y_r = distance to reaction plane, cm

Greek Letters

β = dimensionless parameter = $y_r\sqrt{a/D_A}$
γ = dimensionless parameter = $nC_{Bb}/mC_{As}\sqrt{D_B/D_A}$
ϵ = turbulent eddy diffusivity, cm²/s
θ = dimensionless concentration of $B = C_B/C_{Bb}$
μ = absolute viscosity, g/cm s
ν = kinematic viscosity, cm²/s
τ = dimensionless parameter, $\sqrt{D_A/D_B}$
ϕ = enhancement factor = k_c/k_c^0

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The Behavior of a Power-Law Fluid Flowing Through a Sudden Expansion:

Part I. A Numerical Solution

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A numerical solution for the axisymmetric flow of an inelastic power-law fluid through an abrupt circular expansion is presented. The equations of motion were solved using an Alternating Direction Implicit method. Both a stream tube-real tube and a real tube-real tube model were investigated and the conditions for significant upstream diffusion of momentum were specified. Secondary flow characteristics and the bulk flow field development are predicted as a function of the flow behavior index (n) and of the Reynolds number. Some results are presented to show the influence of the expansion ratio.

SCOPE

The flow of inelastic power-law fluids through sudden circular expansions is not a problem of great commercial significance in its own right, but this flow field must be understood before the flow of the more complex viscoelastic fluid can be examined. The viscoelastic fluid in abruptly expanding flow fields is of considerable importance in polymer melt processing.

Only one numerical solution, which is confined to Newtonian fluids, is available in the literature. No experimental data for inelastic or viscoelastic fluids are available. The object of this work is to present an experimentally verified numerical solution of the equations of motion for flow of inelastic power-law fluids in abrupt circular expansions.

The numerical solution was obtained using an Alternating Direction Implicit method. Both a stream tube-real tube and a real tube-real tube model were investigated. The conditions for significant diffusion of momentum upstream of the plane of expansion are specified. Eddy characteristics and flow field development are predicted as functions of the flow behavior index n and of the Reynolds number. Some results showing the influence of the expansion ratio are presented. Experimental data are presented to verify the numerical model. Streak photography was used for recording flow patterns and a multiple flash technique was used for point velocity measurement. Fluid properties were determined with an R16 Weissenberg Rheogoniometer. The measured reattachment lengths, the recorded flow patterns, and the developing axial velocity field all show excellent agreement with the numerical predictions.

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