

Absorption of Chlorine into Aqueous Sodium Hydroxide System

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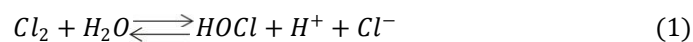
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Abstract: The absorption of chlorine into aqueous hydroxide solutions is one of the important systems having industrial importance and also is of theoretical interest. Danckwerts (1950a and 1950b), Sherwood and Pigford (1952), Brian et al. (1965), Hikita et al. (1972), Hikita et al. (1973) and Takahashi et al. (1967) have studied the gas absorption using mathematical models. In this paper, we have developed a mathematical model and analyzed the experimental data obtained by us and Hikita et al. (1973) on the basis of the penetration theory for gas absorption accompanied by a two step instantaneous chemical reaction. In this work, the rate of absorption in the jet ejector is studied by using Cl_2 aqueous $NaOH$ system at $30^{\circ}C$.

Keywords: Absorption of chlorine, Jet Ejector, Interfacial Area, Absorption rate, Mathematical Modeling, Finite Difference Method

I. INTRODUCTION

Danckwerts (1950a and 1950b) and Sherwood and Pigford (1952) showed that absorption rate could be predicted by the penetration theory for absorption accompanied by an instantaneous irreversible reaction of the type $A + B \rightarrow E$. Spalding (1962) studied the absorption rate of Cl_2 into water and aqueous solutions of H_2SO_4 and $NaOH$ using liquid-jet column. They have also established that the absorption rate of Cl_2 will be affected by the reactions (1) and/or (2):



or



depending upon the pH value of the solution.

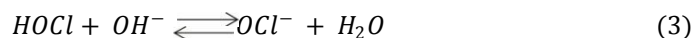
Further, they have observed that when pH value was higher than 12.6 (i.e. OH^- concentration more than 0.04 gmol/l) the forward part of reaction (2), was rate-controlling and the effect of this reaction on the absorption rate could be predicted by the penetration theory for absorption accompanied by an instantaneous irreversible reaction.

Brian et al. (1965) studied gas absorption accompanied by a two-step chemical reaction, $A + B \rightarrow C$ followed by $C + B \rightarrow E$. They have considered both steps irreversible and of finite reaction rates and presented the theoretical analysis based on both, the film theory and the penetration theory, with numerical solutions for the reaction factor, β .

Takahashi et al. (1967) used two different types of absorbers viz. liquid-jet column and a stop-cock type absorber to study the absorption rates of Cl_2 into aqueous $NaOH$ (0.05 to 0.2 gmol/l). The predicted absorption rate using penetration theory was in good agreement with experimental results.

Hikita et al. (1972) studied gas absorption of two-step chemical reaction, $A + B \xrightleftharpoons{K_1} C$ followed by $C + B \xrightleftharpoons{K_2} E$, accompanied by $A + E \rightleftharpoons 2C$. They have studied the effect of chemical equilibrium constant ratio, P (which is defined as K_1/K_2), on reaction factor, β . They have developed mathematical models for $P = 0$, finite value and ∞ , for equal diffusivity and unequal diffusivities of species on the basis of penetration theory.

Hikita et al. (1973) stated that in case of strong hydroxide solution the forward part of reaction (2) is not only reaction which governs the absorption rate of Cl_2 but the rapid reaction

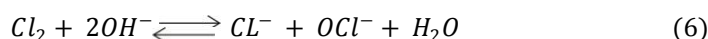
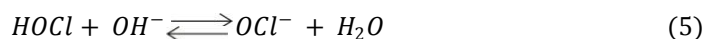


also affects the absorption rate of Cl_2 as the equilibrium constant of this reaction is very large.

II. MECHANISM OF CHEMICAL ABSORPTION

Spalding (1962) mentioned that, when OH^- concentration is more than 0.04 g mol/l the forward part of reaction (2) is rate-controlling which affects the absorption rate.

Hikita et al. (1973) stated that $HOCl$ (hypochlorous acid) formed by reaction (2) can react again with OH^- ions results in rapid reaction (3) having equilibrium constant $K = 2.2 \times 10^6 \text{ l/gmole}$. Hence considering two step mechanism of the reaction (absorption) between Cl_2 and an aqueous hydroxide solution, may be written as follows:



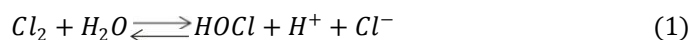
The values of the equilibrium constants of reactions (2) and (3) are K_1 and K_2 . They are stated as follows:

$$K_1 = \frac{[HOCl][Cl^-]}{[Cl_2][OH^-]}$$

$$K_2 = \frac{[OCl^-]}{[HOCl][OH^-]}$$

The values of K_1 and K_2 at $30^\circ C$ is given by 3.1×10^{10} (Connick et al., 1959) and $2.2 \times 10^6 \text{ l/gmole}$ (Morris, 1966) respectively.

The hydrolysis of dissolved Cl_2 with water takes place according to the reaction



The equilibrium constant of this reaction is given by

$$K_3 = \frac{[HOCl][H^+][Cl^-]}{[Cl_2]}$$

and having value $4.5 \times 10^{-4} (\text{gmole/l})^2$ (Connick et al., 1959) at $30^\circ C$.

The values of K_3 is very low compared to the value of K_1 , and hence reaction (1) will not have a significant contribution to the total reaction rate of Cl_2

Therefore, the absorption of Cl_2 into aqueous hydroxide solutions can be considered as an instantaneous two-step reaction, which is equivalent to say that reaction (2) followed by reaction (3) and having over all reaction (6).

III. MATHEMATICAL MODELS RELATED TO ABSORPTION

The rate of absorption of reactant A (gas) with instantaneous chemical reaction can be predicted by summing

- Amount of A diffuse away unreacted and
- Amount of reacted A (in the form of C) diffuse away from the gas-liquid interface.

Therefore,

$$-N_{A_i} = D_A \left(\frac{\partial A}{\partial x} \right)_{x=0} + \frac{1}{2} D_C \left(\frac{\partial C}{\partial x} \right)_{x=0} \quad (7)$$

The integration of equation (7) from time zero to the total exposure time t_e gives the average absorption rate and which may be written as :

$$\begin{aligned} N_A &= \frac{1}{t_e} \int_0^{t_e} N_{A_i} dt \\ &= \frac{1}{t_e} \int_0^{t_e} \left[-D_A \left(\frac{\partial A}{\partial x} \right)_{x=0} - \frac{1}{2} D_C \left(\frac{\partial C}{\partial x} \right)_{x=0} \right] dt \end{aligned} \quad (8)$$

The average absorption rate of A in absence of the chemical reaction is given by the well-known Higbie equation

$$N_A^* = 2A_i \sqrt{\frac{D_A}{\pi t}} \quad (9)$$

It is known that the reaction factor is the ratio of average rates of absorption with chemical reaction and without chemical reaction. Therefore from equation (8) and (9)

$$\beta = \frac{N_A}{N_A^*} = -\frac{1}{2A_i} \sqrt{\frac{\pi D_A}{t_e}} \int_0^{t_e} \left[\left(\frac{\partial A}{\partial x} \right)_{x=0} + \left(\frac{D_C}{D_A} \right) \left(\frac{\partial C}{\partial x} \right)_{x=0} \right] dt \quad (10)$$

Now, the rate of desorption of the $HOCl$ product is given by (Lahiri et al., 1983)

$$R_{d,HOCl} = \sqrt{\left(\frac{D_C}{\pi t} \right)} \left\{ \frac{C_{HOCl, x_1} - C_{HOCl, x=0}}{\operatorname{erf} \left[\sqrt{\left(\frac{D_A}{D_C} \right)} \sigma_1 \right]} \right\} \quad (10a)$$

Therefore, average rate of desorption over a total exposure t_e is given by

$$\begin{aligned} &= \frac{1}{t_e} \int_0^{t_e} R_{d,HOCl} dt \\ &= 2 \sqrt{\frac{D_C}{\pi t_e}} \left\{ \frac{C_{HOCl, x_1} - C_{HOCl, x=0}}{\operatorname{erf} \left[\sqrt{\left(\frac{D_A}{D_C} \right)} \sigma_1 \right]} \right\} \\ &= \underbrace{\frac{1}{\operatorname{erf} \left[\sqrt{\left(\frac{D_A}{D_C} \right)} \sigma_1 \right]}}_{\text{(Enhancement factor for desorption)}} \underbrace{2 \sqrt{\frac{D_A}{\pi t_e}} \sqrt{\frac{D_C}{D_A}}}_{\text{(The liquid mass transfer coefficient)}} (C_{HOCl, x_1} - C_{HOCl, x=0}) \\ &= \text{(Enhancement factor for desorption)} \text{(The liquid mass transfer coefficient)} \sqrt{\frac{D_C}{D_A}} (C_{HOCl, x_1} - C_{HOCl, x=0}) \end{aligned}$$

$$= \phi_{dHOCl} \cdot k_L \cdot \sqrt{\left(\frac{D_C}{D_A}\right)} (C_{HOCl, x_1} - C_{HOCl, x=0})$$

Average rate of absorption of Cl_2 is given by

$$\bar{R}_A = \beta \cdot k_L \cdot C_{Cl_2}^* \quad (10b)$$

Hikita et al. (1972) developed the model based on penetration theory for absorption with instantaneous chemical reaction and found that for $P = 0$ there exists only one reaction plane, where the over-all reaction of reactions $A + B \rightleftharpoons C$ and $C + B \rightleftharpoons E$ is $A + 2B \rightleftharpoons E$, proceeds irreversibly. The average rate of absorption of the solute gas can be calculated by following equations which were derived by Danckwerts (1950) and Sherwood and Pigford (1952).

$$N_A = \beta \left(2A_i \sqrt{\frac{D_A}{\pi t_e}} \right) \quad (11)$$

$$\beta = \frac{1}{\text{erfc}(\sigma)} \quad (12)$$

Where σ is root of the equation

$$\text{erfc} \left(\sqrt{\frac{D_A}{D_B}} \sigma \right) \exp \left[\left(\frac{D_A}{D_B} - 1 \right) \sigma^2 \right] = \sqrt{\frac{D_B}{D_A}} \frac{C_{B0}}{2A_i} \text{erf}(\sigma) \quad (13)$$

This absorption mechanism is called a “one reaction-plane model”.

Hikita et al. (1972) developed a two reaction plane model when $P = \infty$ and established the fact that two reaction planes are formed within the liquid, which are as follows:

- The reaction $A + E \rightleftharpoons 2C$ which is the sum of forward part of the first-step reaction ($A + B \rightleftharpoons C$) and the backward part of second step reaction ($C + B \rightleftharpoons E$) take place irreversibly at the first reaction plane (which is located closer to the gas-liquid interface)
- The reaction ($C + B \rightleftharpoons E$) take place irreversibly at the second reaction plane.

Further, the absorption rate may be calculated by equation (8) and following equation:

$$\beta = \frac{1}{\text{erfc}(\sigma_1)} \quad (14)$$

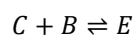
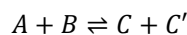
Where σ_1 is the root of following equations,

$$2\text{erfc} \left(\sqrt{\frac{D_A}{D_B}} \sigma_2 \right) \exp \left[\left(\frac{D_A}{D_C} - 1 \right) \sigma_1^2 + \left(\frac{D_A}{D_B} - \frac{D_A}{D_C} \right) \sigma_2^2 \right] = \sqrt{\frac{D_B}{D_A}} \frac{C_{B0}}{A_i} \text{erf}(\sigma_1) \quad (15)$$

$$\text{erfc} \left(\sqrt{\frac{D_A}{D_E}} \sigma_1 \right) \exp \left[\left(\frac{D_A}{D_E} - 1 \right) \sigma_1^2 \right] - 2\text{erfc} \left(\sqrt{\frac{D_A}{D_E}} \sigma_2 \right)$$

$$\exp \left[\left(\frac{D_A}{D_C} - 1 \right) \sigma_1^2 + \left(\frac{D_A}{D_E} - \frac{D_A}{D_C} \right) \sigma_2^2 \right] = \sqrt{\frac{D_E}{D_A}} \frac{C_{E0}}{A_i} \operatorname{erf}(\sigma_1) \quad (16)$$

The reaction scheme for the $Cl_2 - NaOH$ system studied in this work is similar to the work of Hikita et al. (1972). The present reaction system (Equation (4.4) and (4.5)) may be described in the form



The present system is different than the work of Hikita et al. (1972) due to presence of C' which was not present in Hikita et al. (1972). However the species C' ($NaCl$) is non-reactive. Hence the it does not effect reactive mechanism.

Since, the equilibrium constant ratio $P = K_1/K_2 = 1.4 \times 10^4 \text{ gmol/l}$, we can apply the two reaction plane model to the present system.

The diffusion of all species, based on the penetration theory is modeled by partial differential equations. The concentration profile for each species which will be derived by solving the developed model will be similar to that as shown in Figure 1.

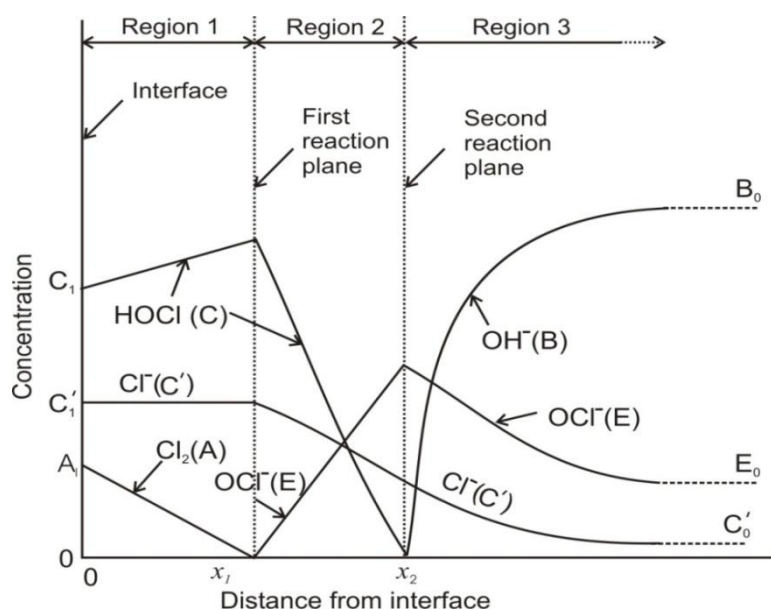


Fig. 1 Concentration profiles for absorption of Cl_2 into aqueous $NaOH$ solution

Region 1 ($0 < x < x_1$)

$$D_A \frac{\partial^2 C_A}{\partial x^2} = \frac{\partial C_A}{\partial t} + r_1 \quad (17)$$

$$D_C \frac{\partial^2 C_C}{\partial x^2} = \frac{\partial C_C}{\partial t} + r_2 \quad (18)$$

Region 2 ($x_1 < x < x_2$)

$$D_C \frac{\partial^2 C_C}{\partial x^2} = \frac{\partial C_C}{\partial t} + r_2 \quad (19)$$

$$D_E \frac{\partial^2 C_E}{\partial x^2} = \frac{\partial C_E}{\partial t} + r_3 \quad (20)$$

Region 3 ($x_2 < x < \infty$)

$$D_B \frac{\partial^2 C_B}{\partial x^2} = \frac{\partial C_B}{\partial t} + r_4 \quad (21)$$

$$D_E \frac{\partial^2 C_E}{\partial x^2} = \frac{\partial C_E}{\partial t} + r_3 \quad (22)$$

with the following initial and boundary conditions:

$$t = 0, x > 0; C_B = C_{B0}, C_E = C_{E0} \quad (23)$$

$$x = 0, t > 0; C_A = A_i, \frac{\partial C_C}{\partial x} = 0, C_C = C_{C0} \quad (24)$$

$$x = x_1, t > 0; C_A = C_E = 0, 2D_A \frac{\partial C_A}{\partial x} = 2D_E \frac{\partial C_E}{\partial x} = D_C \frac{\partial C_C}{\partial x} \quad (25)$$

$$x = x_2, t > 0, C_B = C_C = 0, D_B \frac{\partial C_B}{\partial x} = -D_C \frac{\partial C_C}{\partial x} D_E \left[\left(\frac{\partial C_E}{\partial x} \right)_2 - \left(\frac{\partial C_E}{\partial x} \right)_3 \right] \quad (26)$$

$$x = \infty, t \geq 0; C_B = C_{B0}, C_E = C_{E0} \quad (27)$$

Where x_1 and x_2 are the locations of the first and the second reaction planes, respectively, and $(\partial C_E / \partial x)_2$ and $(\partial C_E / \partial x)_3$ represent the values of $\partial C_E / \partial x$ when x approaches x_2 from region 2 and from region 3, respectively.

It is important to note that Equations (17 – 27) represents initial boundary value problem.

This Model is more general. Specifically, when $r_1, r_2, r_3,$ and r_4 are zero, the present model will reduce to Model of Hikita et al. (1973)

The analytical solution of this problem (i.e. concentration profile in the liquid) is given by Hikita et al. (1973) when and is as follows:

Region 1 ($0 < x < x_1$)

$$C_A = A_i \left[1 - \frac{\text{erfc}(x/2\sqrt{D_A t})}{\text{erfc}(\sigma_1)} \right] \quad (28)$$

$$C_B = 0 \quad (29)$$

$$C_C = C_{B0} \sqrt{\frac{D_B}{D_C}} \exp \left[\left(\frac{D_A}{D_C} - \frac{D_A}{D_B} \right) \sigma_2^2 \right] \quad (30)$$

$$\frac{\text{erf}(\sqrt{D_A/D_C} \sigma_2) - \text{erf}(\sqrt{D_A/D_C} \sigma_1)}{\text{erfc}(\sqrt{D_A/D_B} \sigma_2)}$$

$$C_E = 0 \tag{31}$$

Region 2 ($x_1 < x < x_2$)

$$C_A = 0 \tag{32}$$

$$C_B = 0 \tag{33}$$

$$C_C = C_{B0} \sqrt{\frac{D_B}{D_C}} \exp \left[\left(\frac{D_A}{D_C} - \frac{D_A}{D_B} \right) \sigma_2^2 \right] \tag{34}$$

$$\frac{\operatorname{erf}(\sqrt{D_A/D_C} \sigma_2) - \operatorname{erf}(x/2\sqrt{D_C t})}{\operatorname{erfc}(\sqrt{D_A/D_B} \sigma_2)}$$

$$C_E = A_i \sqrt{\frac{D_A}{D_E}} \exp \left[\left(\frac{D_A}{D_E} - 1 \right) \sigma_1^2 \right] \tag{35}$$

$$\frac{\operatorname{erf}(x/2\sqrt{D_E t}) - \operatorname{erf}(\sqrt{D_A/D_E} \sigma_1)}{\operatorname{erf}(\sigma_1)}$$

Region 3 ($x_2 < x < \infty$)

$$C_A = 0 \tag{36}$$

$$C_B = C_{B0} \frac{\operatorname{erf}(x/2\sqrt{D_B t}) - \operatorname{erf}(\sqrt{D_A/D_B} \sigma_2)}{\operatorname{erfc}(\sqrt{D_A/D_B} \sigma_2)} \tag{37}$$

$$C_C = 0 \tag{38}$$

$$C_E = A_i \sqrt{\frac{D_A}{D_E}} \exp \left[\left(\frac{D_A}{D_E} - 1 \right) \sigma_1^2 \right] \tag{39}$$

$$\frac{\operatorname{erf}(\sqrt{D_A/D_E} \sigma_2) - (\sqrt{D_A/D_E} \sigma_1)}{\operatorname{erf}(\sigma_1) \operatorname{erfc}(\sqrt{D_A/D_E} \sigma_2)} \times \operatorname{erfc}(x/2\sqrt{D_E t})$$

$$+ E_0 \frac{\operatorname{erf}(x/2\sqrt{D_E t}) - \operatorname{erf}(\sqrt{D_A/D_B} \sigma_2)}{\operatorname{erfc}(\sqrt{D_A/D_E} \sigma_2)}$$

A. *Present Mathematical Model I:* This model is represented by equations (17 – 27) when r_1, r_2, r_3, r_4 are non zero. We have used the numerical technique- finite difference method to solve them. The simulation have also been done using Matlab software.

B. *Present Mathematical Model II:* This model is represented by equations (17 – 22) with modifying boundary conditions and is of the form

$$t = 0, x > 0; C_B = C_{B0}, C_E = C_{E0} \tag{40}$$

$$x = 0, t > 0; C_A = A_i, \frac{\partial C_C}{\partial x} = 0, C_C = C_{C0} \tag{41}$$

$$x = x_1, t > 0; C_A = C_E = 0,$$

$$2D_A \frac{\partial C_A}{\partial x} = -2D_E \frac{\partial C_E}{\partial x} = 2D_C \frac{\partial C_C}{\partial x} = D_C \left[\left(\frac{\partial C_C}{\partial x} \right)_2 - \left(\frac{\partial C_C}{\partial x} \right)_1 \right] \quad (42)$$

$$x = x_2, t > 0, C_B = C_C = 0, D_B \frac{\partial C_B}{\partial x} = -D_C \frac{\partial C_C}{\partial x} = D_E \left[\left(\frac{\partial C_E}{\partial x} \right)_2 - \left(\frac{\partial C_E}{\partial x} \right)_3 \right] \quad (43)$$

$$x = \infty, t \geq 0; C_B = C_{B0}, C_E = C_{E0} \quad (44)$$

In present mathematical model II, we have consider the effect of jump at $x = x_1$ and $x = x_2$. The two plane model theory suggest us that at $x = x_1$ there is a instantaneous reaction between species $A(Cl_2)$ and $E(OCl^-)$ and causes jump in concentration of species $HOCl$. Similarly, at $x = x_2$ there is a sudden reaction between species $C(HOCl)$ and $B(OH^-)$ and causes jump in concentration of species $E(OCl^-)$. This jump values are defined by the last term of the Equation (42) and Equation (43) respectively.

We have used the numerical technique- finite difference method to solve them. The simulation have also been done using Matlab software. The absorption rate can be calculated by equation (8) and

$$\beta = \frac{1}{\text{erf}(\sigma_1)} \quad (45)$$

where the constant σ_1 can be determined by solving the following pair of simultaneous equations.

$$\frac{C_0}{A_i} \sqrt{\frac{D_C}{D_A}} = \frac{B_0}{A_i} \sqrt{\frac{D_B}{D_A}} \times \frac{\exp \left[\left(\frac{D_A}{D_C} - \frac{D_A}{D_B} \right) \sigma_2^2 \right] \text{erf} \left[\left(\sqrt{\frac{D_A}{D_C}} \right) \sigma_2 \right]}{\text{erfc} \left[\left(\sqrt{\frac{D_A}{D_B}} \right) \sigma_2 \right]} - \frac{2 \exp \left[\left(\frac{D_A}{D_C} - 1 \right) \sigma_1^2 \right] \text{erf} \left[\sqrt{\left(\frac{D_A}{D_C} \right)} \sigma_1 \right]}{\text{erfc}(\sigma_1)} \quad (46)$$

$$\frac{E_0}{A_i} \sqrt{\frac{D_E}{D_A}} = \frac{B_0}{A_i} \sqrt{\frac{D_B}{D_A}} \times \frac{\exp \left[\left(\frac{D_A}{D_E} - \frac{D_A}{D_B} \right) \sigma_2^2 \right] \text{erf} \left[\left(\sqrt{\frac{D_A}{D_E}} \right) \sigma_2 \right]}{\text{erfc} \left[\left(\sqrt{\frac{D_A}{D_B}} \right) \sigma_2 \right]} - \frac{2 \exp \left[\left(\frac{D_A}{D_E} - 1 \right) \sigma_1^2 \right] \text{erf} \left[\sqrt{\left(\frac{D_A}{D_E} \right)} \sigma_1 \right]}{\text{erfc}(\sigma_1)} \quad (47)$$

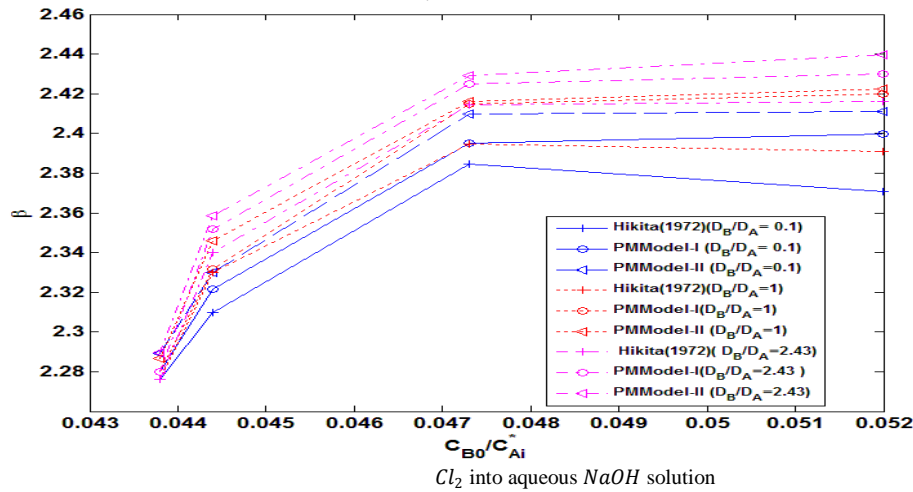
The trial and error procedure was based on Newton – Raphson technique to evaluate σ_1 and σ_2 from equations (46) and (47). In this technique the first guess values of σ_1 and σ_2 was calculated by considering equal diffusivities.

IV. RESULTS AND DISCUSSION

A. The effect of the diffusivity ratio on enhancement factor

Figure 2 shows the plot of the enhancement factor β versus the concentration ratio C_{B0}/C_{Ai}^* for different diffusivities ratio of D_B/D_A with constant D_C/D_A and D_E/D_A . The value of D_B/D_A are taken 2.43, 1 and 0.1. In this figure the plots of Hikita (1972), proposed mathematical model I [equations (17 – 27) with r_1, r_2, r_3 and r_4 are non zero] and proposed mathematical

Fig. 2 Variation in enhancement factor with respect to C_{B0}/C_{Ai}^* at different $D_B/D_A = 2.43, 1, 0.1$ and constant $D_E/D_A = 10$ and $D_C/D_A = 0.1$ for absorption of



The following results may be drawn from figure (2).

- The lines in the figure having higher D_B/D_A are at higher position for the same C_{B0}/C_{Ai}^* . This indicates that at higher ratio of diffusivities of reactants (liquid and gas), the enhancement factor is higher. It can be concluded that higher the diffusivity of liquid reactant with respect to gaseous reactant, higher is the enhancement factor. The increase in enhancement factor is due to reduction in thickness of interfacial film. The reduction in thickness in interfacial film is due to movement of reactant B (NaOH) is faster toward interface compared to movement of A (Cl_2) toward bulk of liquid.
- For same D_B/D_A plots shows that enhancement factor increases with increase in the reactant ratio (C_{B0}/C_{Ai}^*). The increase in enhancement factor is steeper at initial increase of C_{B0}/C_{Ai}^* . After that the rate of rise in enhancement factor with respect to rate of rise in reactant ratio is reducing and after certain value of C_{B0}/C_{Ai}^* , there is hardly any rise in enhancement factor with respect to reactant ratio. It can be concluded that there is increase in enhancement factor with increase in liquid reactant concentration up to certain limits. This may be taken to mean that at higher C_{B0} enhancement factor is higher. The reduction of β at higher C_{B0}/C_{Ai}^* is due to high viscosity of NaOH solution at higher C_{B0} .
- For the same ratio of C_{B0}/C_{Ai}^* the value of enhancement factor derived from proposed mathematical model II is higher than the value from proposed mathematical model I. The value derived from Hikita (1972) is the lowest. The predicted values from proposed mathematical model I and proposed mathematical model II are higher than Hikita (1972) as the effect of HOCl diffusing out have been considered.

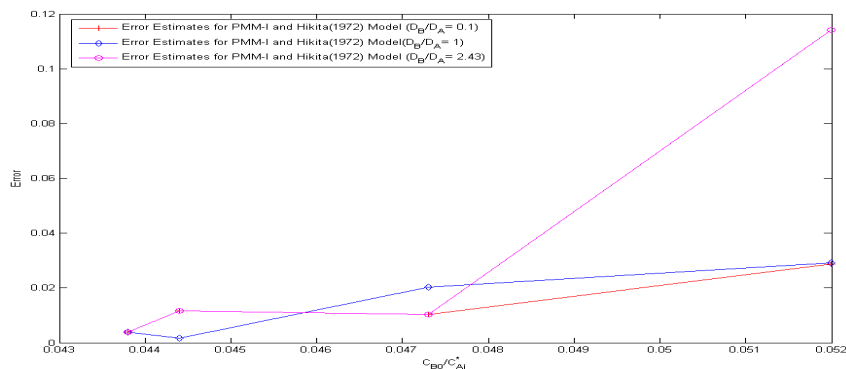


Fig 3 Error estimates between experimental data and proposed mathematical model at different $D_B/D_A = 2.43, 1, 0.1$ and constant $D_E/D_A = 10$ and $D_C/D_A = 0.1$.

The error estimates between Hikita (1972) model and proposed mathematical model I is shown in Fig. 3. The error is defined as $Error = |\beta \text{ predicted by Hikita (1972) model} - \beta \text{ predicted by proposed model I}|$ for diffusivities $D_B/D_A = 2.43, 1, 0.1$

It is observed that the lower value of D_B/D_A for different C_{B0}/C_{Ai}^* , the proposed mathematical model I and Hikita (1972) model are comparable. However, for higher values of D_B/D_A , the comparison shows that there is a numerical instability in Hikita (1972) model (higher value of error). Therefore, we conclude that the proposed model I is well-posed.

B. Comparison of experimental results with simulated results

Figure (4) is a comparison of β predicted by the simulated results of Hikita (1973), proposed mathematical model I and proposed mathematical model II with experimentally determined values (for $C_{Ag,in} = 0.602 \times 10^{-3} \text{ kmol/m}^3$) at actual value of diffusivity ratio: $D_B/D_A = 2.32, D_C/D_A = 1.04, D_{C'}/D_A = 1.4$ and $D_E/D_A = 0.786$ (Table A 3.4). It may be observed that the values obtained by experiment, Hikita (1973) model and proposed model I are comparable. Equations (17) to (22) and (45) to (50) indicate that β is a function of rate of reactions and three diffusivity (in liquid) ratios, $D_B/D_A, D_C/D_A$ and D_E/D_A . The predicted values by proposed mathematical model I are higher to some extent than Hikita (1973) model which is due to the effect of reaction on β , have been consider in mathematical model I. It may be make out that the influence of rate of reaction are marginal that may be because being instantaneous reaction diffusivity ratio of species are rate controlling.

$C_{B0}, \text{ kmol/m}^3$	0.95	0.75	0.525	0.031
Exp. value of β for $C_{Ag,in} = 0.602 \times 10^{-3} \text{ kmol/m}^3$	1.55	1.5	2.24	1.94

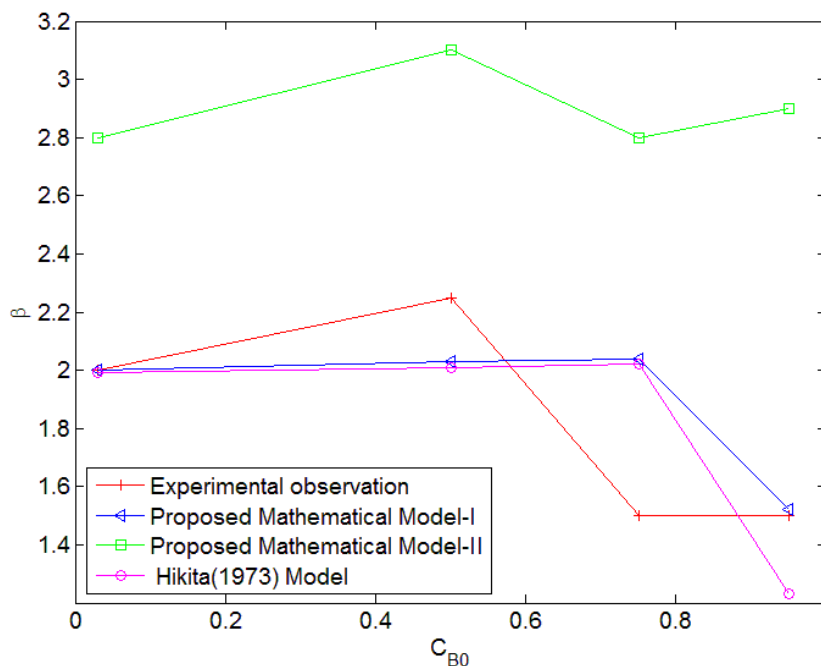


Fig. 4 Comparison of value of β determined experimentally and by proposed mathematical model for different C_{B0} at $C_{Ag,in} = 0.602 \times 10^{-3} \text{ kmol/m}^3$

The values predicted by proposed mathematical model II for β are higher than experimental values. It may be concluded that the effect of jumping in the concentration of $HOCl$ and OCl^- which have been considered in the model at the interface 1 and 2 are

not appreciable. Hence the values predicted by model II are higher. So model II is not appropriate under operating conditions of the experiment.

V. CONCLUSION

- The enhancement factor depends on the five independent dimensionless parameters i.e., three diffusivity ratios, D_B/D_A , D_C/D_A and D_E/D_A , and two concentration ratios C_{B0}/C_{Ai}^* and E_0/C_{Ai}^* .
- The enhancement factor increases as the value of D_B with respect to D_A increases.
- The value of enhancement factor increases as the value C_{B0} increases, and the effect of C_{B0}/C_{Ai}^* becomes large at low values and low at high values C_{B0}/C_{Ai}^*
- The proposed mathematical model I is more appropriate to experimental results at operating conditions i.e. at 30°C.

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NOMENCLATURE

Latin letters

A_i, A^*	physical solubility of chlorine	[kmol/m ³ or gmol/liter]
C	concentration	[kmol/m ³ or gmol/liter]
C_{B0}	concentration of B in bulk of liquid/ Initial concentration	[kmol/m ³ or gmol/liter]
D	diffusion coefficient of species indicated by subscript in the liquid phase	[m ² s ⁻¹]
H	Henry's law coefficient	[Pa m ³ mol ⁻¹]
R_A, N_A	rate of molar absorption with chemical reaction (flux)	[mol m ⁻² s ⁻¹]
N_A^*	average rate of physical absorption (flux)	[mol m ⁻² s ⁻¹]
K	equilibrium constant of reaction	[-]
k_L	liquid sided mass transfer coefficient	[m s ⁻¹]
r	chemical reaction rate of species (volumetric)	[mol m ⁻³ s ⁻¹]
t_e	exposure time	[s]
x	distance from interface	[m]

Greek letters

β	enhancement factor	[-]
σ	parameter defined by equation (1.2.13)	[-]
σ_1, σ_2	parameter defined by equation (1.2.15) & (1.2.16)	[-]

Subscripts

0	fluid bulk
A, B, \dots	component A, B, \dots
G, g	gas phase
i	interface
in	inlet
j	jet
d	desorption

Superscripts

0	fluid bulk/initial
$*$	equilibrium, physical solubility

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