GAS ABSORPTION WITH CHEMICAL REACTION IN TURBULENT FLOW

Jahanmiri, Abdol Hossein *
Eghbalpoor, Akbar
Department of Chemical Engineering, Shiraz University, Shiraz, Iran.

(Received : May 17th 1993 , Accepted : Jan. 17th 1994)

ABSTRACT : *In order to increase the rate of gas absorption, chemical reaction in the liquid phase is considered. The purpose of this paper was to simulate gas absorption process by a liquid film over a spherical packing incorporating eddy viscosity and diffusivity. Second order chemical reaction for two different cases (fast and slow) were considered. The system of partial differential equations obtained was solved by the use of finite difference method. In this study absorption of CO_2 by mono- ethanol amine (MEA) and methyl di- ethanol amine (MDEA) were considered, and velocity and concentration profiles in the liquid film were obtained. The simulation results revealed that, increasing of turbulence in the liquid film, increases the rate of gas absorption while decreases the thickness of the reaction zone.*

KEY WORDS : *Mass Transfer, Turbulent flow, Gas Absorption, Chemical Reaction, CO_2, Monoethanol Amine, Methyl-Di-Ethanol Amine.*

INTRODUCTION :

Liquid flow on spherical packing has been analyzed by several investigators [1,2]. Their results are in good agreement with experimental data, only for small flow rates and in the absence of shear stress on the surface of liquid film (Fig. 1).

* Corresponding author

1021-9986/93/2/85 6 / $ /2.60

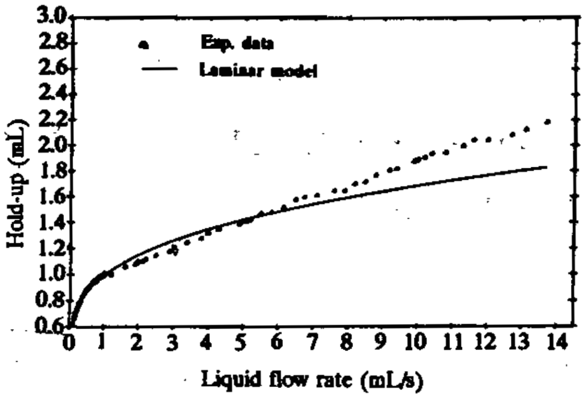

Fig. 1 : Predicted and measured hold-up for one sphere [2]

By using the two- film theory of *Lewis* and *Witman* (1924) concentration profiles for the two components- diffusing (A) and reacting (B)- have been obtained in laminar flow and in a wide range of reaction rates [3].

In turbulent flow, since the momentum and mass transfer are mostly affected by eddies, eddy viscosity and diffusivity are encountered. *Lamourelle* and *Sandall* [4] treated mass transfer near a free surface in term of eddy diffusivity for gas absorption of different gases in a wetted wall column. They found that the eddy diffusivity in the vicinity of the free surface may be expressed as:

$$D_t = 7.9 \times 10^{-5}\, Re^{1.678}\, (y_o - y)^2 \qquad (1)$$

Jahanmiri [5] analyzed liquid film flow over sphere and by measuring the liquid hold- up he found that the eddy viscosity is given by:

$$\nu_t = 7.8 \times 10^{-5}\, Re^{2.21} (y_o - y)^2 \qquad (2)$$

Where :

$$Re = \frac{4Q}{2\pi R \nu \sin\theta} \qquad (3)$$

Hydrodynamics :

If we consider similar and parallel processes for momentum transfer between molecules and eddies, the total shear stress may be written in terms of *Newton's* law viscosity:

$$\tau_T = -(\mu + \mu_t)\frac{\partial u}{\partial y} \qquad (4)$$

The turbulent viscosity is the main difficulty, μ_t, in such studies. Solving the momentum equation by using Eq. (2) the velocity distribution is obtained as:

$$u = \frac{g\sin\theta}{a}\left[\frac{y_o - \frac{\tau_i}{\rho g \sin\theta}}{\sqrt{\frac{\nu}{a}}}\tan^{-1}\left(\frac{y_o - y}{\sqrt{\frac{\nu}{a}}}\right) + \frac{1}{2}\, Ln\left(\frac{\frac{\nu}{a}}{\frac{\nu}{a} + (y_o - y)^2}\right)\right] \qquad (5)$$

where :

$$V = \frac{\mu}{\rho} \quad , a = 7.8 \times 10^{-5}\, Re^{2.21} \qquad (6)$$

τ_i is the shear stress on liquid surface due to gas motion. (Fig. 2)

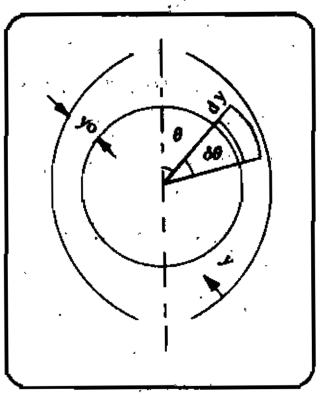

Fig. 2 : Liquid flow on a sphere

Physical Absorption :

Considering an element of the liquid film between two streamlines, the species, mass balance gives ($R >> y_o$): (Fig. 3)

$$-\frac{1}{R\sin\theta\partial y}\frac{\partial}{\partial\theta}(u\sin\theta C\partial y) + \frac{\partial}{\partial r}\left(D_T\frac{\partial C}{\partial r}\right) = 0 \qquad (7)$$

And the continuity for the element gives :

$$\frac{\partial}{\partial\theta}(u\sin\theta\partial y) = 0 \qquad (8)$$

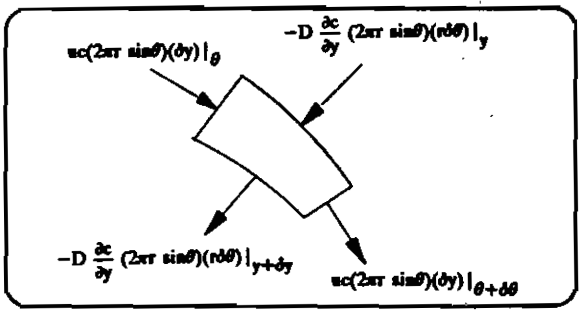

Fig. 3 : Representation of a liquid element

Then :

$$-\frac{u}{R}\frac{\partial C}{\partial \theta}+\frac{\partial}{\partial y}(D_T\frac{\partial C}{\partial y})=0 \qquad (9)$$

Where C is the concentration of the desired component and D_T is the total diffusivity. The basic assumptions are:

1- Steady state condition.

2- Neglecting molecular diffusion compared to convection in the flow direction.

3- Liquid film thickness is small compared to radius of sphere. ($y_o << R$)

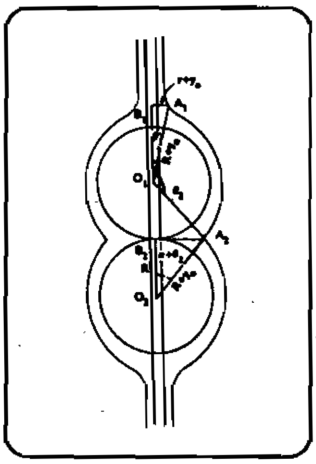

Fig. 4 : Liquid flow on a packing of spherical particles

Chemical Absorption :

Two cases are considered:

1- Fast Chemical Reaction. CO_2 absorption with MEA is considered. The reaction is [6]:

$$CO_2(g) + MEA(1) \dashrightarrow Products$$

Considering a second order reaction,

$$Rate = -K_r \cdot C_{CO_2} \cdot C_{MEA}$$

The rate constant for the reaction has obtained as [6]:

$Log_{10}(K_r) = 10.99 - 2152/T$,
$[K_r$ in $(m^3/Kmol.sec)]$, T°K

2- Slow Chemical Reaction. CO_2 absorption with MDEA solution is considered along with its reaction rate and rate constant as:

$$CO_2(g) + MDEA(1) \dashrightarrow Products$$
$$Rate = -K_r \cdot C_{CO_2} \cdot C_{MDEA}$$
$$K'_r = 1.02\times10^8 \exp(-4808/T) \text{ , T°K}$$

By using species mass, balance for the diffusing and reacting components on a liquid element (Fig. 3) together with the continuity equation, the following partial differential equations are obtained:

$$-\frac{U}{R}\frac{\partial C_A}{\partial \theta}+\frac{\partial}{\partial y}(D_{T_A}\frac{\partial C_A}{\partial y})-K_rC_AC_B=0 \qquad (10)$$

$$-\frac{u}{R}\frac{\partial C_B}{\partial \theta}+\frac{\partial}{\partial y}(D_{T_B}\frac{\partial C_B}{\partial y})-K_rC_AC_b=0 \qquad (11)$$

If the concentration of components(A) and (B) are assumed to be small, then the average values of C_A and C_B (Time-Smoothing Values) may be used [7].

Boundary Conditions :

The initial and boundary conditions for the reacting component (B) are:

$$\theta=\theta_1 \text{ , } C_B=C_{B_o} \text{ , } 0\le y\le y_o$$

$$y=0 \text{ , } \frac{\partial C_B}{\partial y}=0 \text{ nonvolatile comp. } \theta_1\le\theta\le\theta_2$$

$$y=y_o \text{ , } \frac{\partial C_B}{\partial y}=0 \text{ impermeable wall } \theta_1\le\theta\le\theta_2$$

while for the diffusing component(A), the conditions are:

$$\theta=\theta_1 \quad C_A=C_{A_o} \quad 0\le y\le y_o$$

$y=y_o$, $\frac{\partial C_A}{\partial y} = 0$ impermeable wall $\theta_1 \le \theta \le \theta_2$

$$y=0\ ,\ C_A = C_{A_i}\ ,\ \theta_1 \le \theta \le \theta_2$$

where, $C_{A_i} = \frac{P_A}{H}$, H Henry's constant, P_A Gas pressure

Solution of Differential Equations :

In order to find concentration profiles of the components A and B in liquid film and the rate of gas absorption, the system of partial differential Eqs. (10) and (11) must simultaneously be solved. Finite difference method with an iteration procedure have been used. Number of nodes in y and θ- direction were choosen in relation to computer capacity and sensitivity of the results.

RESULTS AND DISCUSSION :

Hydrodynamics :

Velocity distribution in the liquid film for $\tau_i=0$ at two different angles are shown in Figs. 5 and 6. Note that velocity is zero on surface of sphere and is maximum in gas- liquid interface. Generally, when Reynold's number rises, turbulency is increased. Therefore, velocity gradient near gas- liquid interface is decreased.

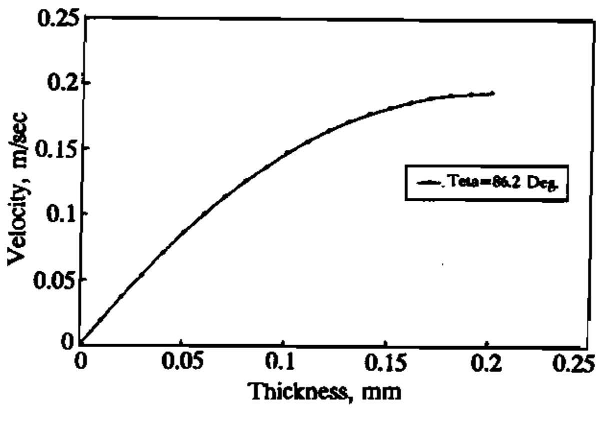

Fig. 5 : Velocity profile in liquid film for Q=3 mL/sec

Mass Transfer :

In case of physical absorption, Eq. (9) can be solved for the diffusing component (A). Fig. 7 shows the steady state concentration profile of diffusing component. Note that maximum concentration is at gas- liquid interface.

When reaction occurs in liquid film, rate of gas absorption is much more than that of pure absorption. Fig. 8 shows a comparison of results for these two cases for a second order chemical reaction.

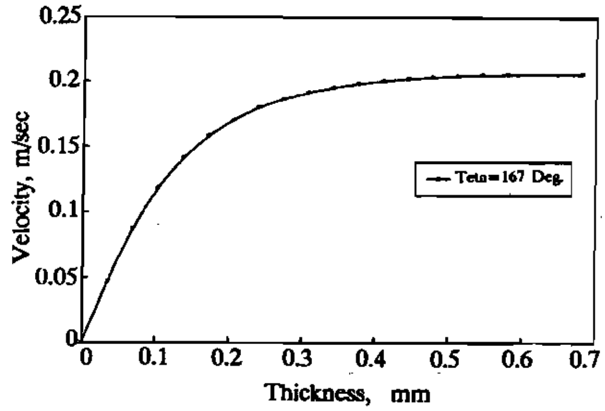

Fig. 6 : Velocity profile in liquid film for Q=3 mL/sec

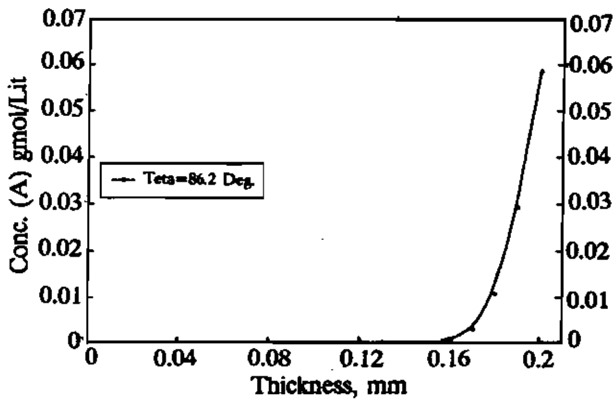

Fig. 7 : Concentration profile for diffusing component in pure gas absorption for Q=3 mL/sec

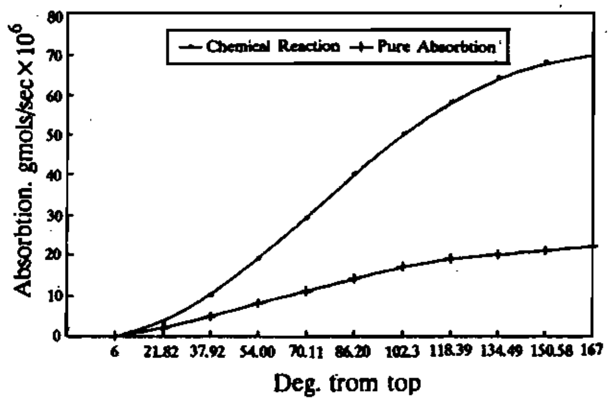

Fig. 8 : Physical and chemical absorption in flow direction for Q=3 mL/sec

Concentration profiles of components (A)and (B) in the liquid film at different angles from top of sphere for fast and slow reactions, are shown in the Figs. 9, 10 and 11.

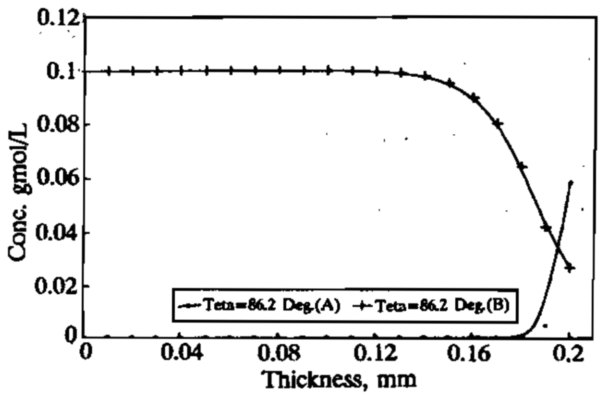

Fig. 9 : Concentration profiles for (A) and (B) for fast second order reaction for Q=3 mL/sec

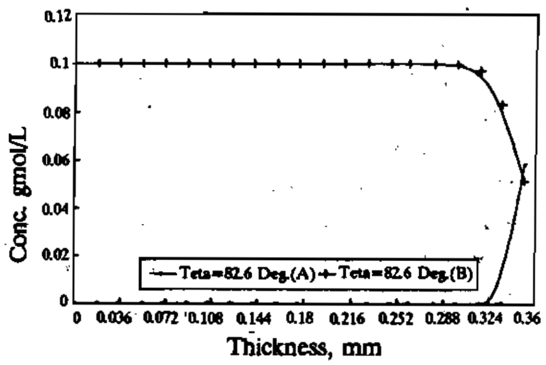

Fig. 10 : Concentration profiles for (A) and (B) for fast second order reaction for Q=12 mL/sec

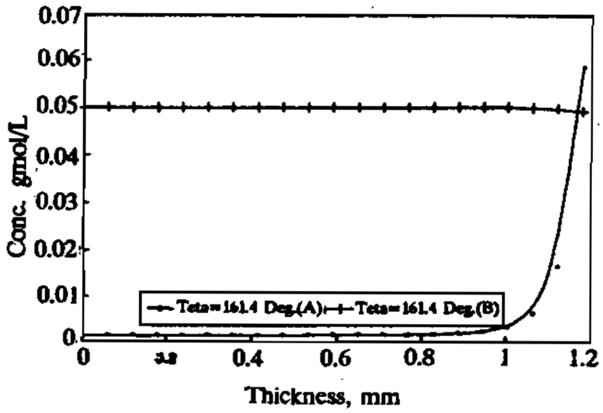

Fig. 11 : Concentration profiles for (A) and (B) for slow second order reaction for Q=10 mL/sec

When liquid with initial concentration of C_{BO} is poured from top of series of spheres, and is contacted with an absorbing gas (A), the gas is absorbed gradually and it's concentration is increased in liquid film from top to bottom of each sphere. The reaction causes a decrease in the concentration of "B" simultaneously. Fig. 12 shows the amount of gas (A) absorbed and reactant (B) consumed with respect to number of spheres.

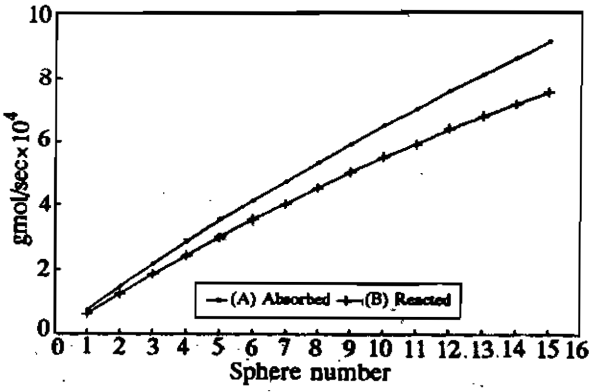

Fig. 12 : Amount of (A) absorbed and amount of (B) consumed with respect to number of spheres for Q=12mL/sec and for fast second order reaction.

CONCLUSIONS :

In absorption by a packing of spherical particles, the area of the liquid film increases from top to equator and decreases to bottom of each sphere, then the rate of gas absorption shows a peak at θ=90 which is confirmed by the simulation results (Fig. 8).

The simulation results also show that the increasing of turbulency in the liquid film, increases the rate of gas absorption, which causes a thinner reaction zone near the liquid surface (Figs. 9 and 10). Therefore, the higher the radial mixing in the liquid film, the higher the rate of gas absorpion.

Physical and Chemical Data :

Packing radius =	0.0185 m
Liquid viscosity =	9.825×10^{-4} Kg/m.sec
Liquid density =	1000 Kg/m^3

Gas pressure = 1.009 atm
Henry's constant for CO_2 = 17.263 atm.m^3/Kmol
Rod radius = 0.0015 m
Temperature = 10 °C
Diffusion coef. for (A) = 1.46×10^{-9} m^2/sec
Diffusion coef. for MEA = 4.92×10^{-9} m^2/sec
Diffusion coef. for MDEA = 7.04×10^{-10} m^2/sec
Rate constant for CO_2, MEA = 2430.86 m^3/Kmol.sec
Rate constant for CO_2, MDEA = 4.2677 m^3/Kmol.sec
Initial condition for fast reaction
Initial cond. of (B) = 0.1 mols/Lit
Initial condition for slow reaction
Initial conc. of (B) = 0.05 mols/Lit
Initial conc. of (A) = 0.0015 mols/Lit
Number of nodes in r- direction : 201
Number of nodes in θ- direction : 601

Nomenclatures :

C	Concentration in liquid phase	mols/Lit
D	Diffusion coefficient	m^2/sec
g	Gravity acceleration	9.81 m^2/sec
H	Henry's constant	atm.m^3/Kmol
K_r,K'_r	Rate constant	m^3/Kmol.sec
P_A	Pressure of absorbing gas	atm
Q	Liquid volumetric flow rate	m^3/sec
r	Distance to sphere centre in liquid film	m
R	Packing radius	m
u	Velocity	m/sec
θ	Angle from top	rad
y	Distance to free surface	m
y_o	Liquid film thickness	m
δ	Liquid density	Kg/m^3
μ	Liquid viscosity	Kg/m.sec
θ_1	Initial gas absorption angle	rad
θ_2	Final gas absorption angle	rad
ν^2	Kinematic viscosity	m^2/sec
Re	Reynold's number	m^2/sec

REFERENCES :

[1] Lynn, S., Stroatemeier, J.R., and Kramers, H., *Chem. Eng. Sci.*, **4**, 63(1955).

[2] Davidson, J.R., et al., *Trans. Instn. Chem. Eng.*, **37**, 122 (1959).

[3] Levenspiel, O., "*Chemical Reaction Engineering*" Wiley, 2nd Ed (1972).

[4] Lamourelle, A.P., and Sandall, O.C., *Chem. Eng. Sic.*, **27**, 1035(1972).

[5] Jahanmiri, A., "*Ph.D. Thesis*", UMIST University of Manchester (1990).

[6] Hikita, H.S., Asai, Ishikowa, H., and Handa, M., *Chem. Eng. J.*, **13**, 7(1977).

[7] Bird, R.B., Stewart, W.E., and Lightfoot, E.N., "*Transport Phenomena*", Wiley, New York (1960).