GAS ABSORPTION WITH CHEMICAL REACTION IN TURBULENT FLOW

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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).
terms of Newton's law viscosity:

$$\tau_T = -(\mu + \mu_t) \frac{\partial u}{\partial y}$$  \hspace{1cm} (4)

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

$$u = \frac{\frac{y_0 - \frac{y_1}{\rho \sin \theta}}{\sqrt{\nu \tan^{-1} \left( \frac{y_0 - y}{\sqrt{\nu}} \right)}} + \frac{1}{2}}{a}$$  \hspace{1cm} (5)

where:

$$V = \frac{\mu}{\rho}, a = 7.8 \times 10^{-5} \text{Re}^{2.21}$$  \hspace{1cm} (6)

$\tau_1$ is the shear stress on liquid surface due to gas motion. (Fig. 2)

**Physical Absorption:**

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

$$-\frac{1}{\rho \sin \theta} \frac{\partial}{\partial y} (\rho u \sin \theta C y) + \frac{\partial}{\partial t} (D_T \frac{\partial C}{\partial t}) = 0$$  \hspace{1cm} (7)

And the continuity for the element gives:

$$\frac{\partial}{\partial y} (\rho u \sin \theta) = 0$$  \hspace{1cm} (8)
Rate = \(-K_r \cdot C_{CO_2} \cdot C_{MEA}\)

The rate constant for the reaction has obtained as [6]:
\[
\log_{10}(K_r) = 10.99 - 2152/T, \\
[K_r \text{ in (m}^2\text{/Kmol.sec)}, \ T \text{K}]
\]

2- Slow Chemical Reaction. CO\(_2\) absorption with MDEA solution is considered along with its reaction rate and rate constant as:
\[
CO_2(g) + MDEA(1) \rightarrow \text{Products} \\
\text{Rate} = -K_r \cdot C_{CO_2} \cdot C_{MDEA} \\
K_r = 1.02 \times 10^8 \exp\left(-4808/T\right), \ T \text{K}
\]

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:
\[
\begin{align*}
\frac{\partial C_A}{\partial \theta} + \frac{D_{TA}}{R} \frac{\partial C_A}{\partial y} &= -K_r C_A C_B = 0 \\
\frac{\partial C_B}{\partial \theta} + \frac{D_{TB}}{R} \frac{\partial C_B}{\partial y} &= -K_r C_A C_B = 0
\end{align*}
\]

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:
\[
\begin{align*}
\theta &= 0, \quad C_B = C_{B_0}, \quad 0 \leq y \leq y_o \\
y = 0, \quad \frac{\partial C_B}{\partial y} &= 0 \quad \text{nonvolatile comp.} \quad \theta_1 \leq \theta \leq \theta_2 \\
y = y_o, \quad \frac{\partial C_B}{\partial y} &= 0 \quad \text{impermeable wall} \quad \theta_1 \leq \theta \leq \theta_2
\end{align*}
\]

while for the diffusing component(A), the conditions are:
\[
\theta = \theta_1, \quad C_A = C_{A_0}, \quad 0 \leq y \leq y_o
\]
\[ y = y_o, \quad \frac{\partial C_A}{\partial y} = 0 \text{ impermeable wall } \theta_1 \leq \theta \leq \theta_2 \]
\[ y = 0, \quad C_A = C_{A_0}, \quad \theta_1 \leq \theta \leq \theta_2 \]

where, \( C_{A_0} = \frac{P_A}{H} \), \( H \) 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 \( \theta \)-direction were chosen in relation to computer capacity and sensitivity of the results.

**RESULTS AND DISCUSSION:**

**Hydrodynamics:**

Velocity distribution in the liquid film for \( \tau = 0 \) 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, turbulence is increased. Therefore, velocity gradient near gas-liquid interface is decreased.

**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.
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.

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 its 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.

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 $\theta=90$ which is confirmed by the simulation results (Fig. 8).

The simulation results also show that the increasing of turbulence 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 absorption.

Physical and Chemical Data:
- Packing radius = 0.0185 m
- Liquid viscosity = $9.825 \times 10^{-4}$ 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, K' 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$_i$ Initial gas absorption angle rad
θ$_f$ Final gas absorption angle rad
ν Kinematic viscosity m$^2$/sec
Re Reynold's number m$^2$/sec

REFERENCES: