Modeling of Acid Gas Absorption in MDEA Solution in Liquid Ring Compressors Extending Film Theory

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ABSTRACT
A theoretical study is represented to discuss a novel approach for modeling the total amount of mass transfer in liquid ring compressor of a gas-sweetening unit for the first time. Accordingly, concentration distribution and mass transfer of a single bubble obtained based on the definition of film theory. Bubble size distribution calculated with the method of maximum entropy formalism (MEF) used in accompanied with probability density function curve to calculate the total amount of mass transfer. Partial pressure of CO₂ and H₂S in outlet stream were in good agreement with operating curve of commercial compressors.

Keywords: Liquid Ring Compressor; Bubble Size Distribution; Amine Unit; Mass Transfer; Film Theory
1. Introduction

Carbon dioxide is one of the most significant sources of greenhouse gases. There exist an inexorable trend toward limiting anthropogenic emissions of carbon dioxide and other gases suspected of causing global climate change. Hydrogen sulfide is such a toxic and corrosive gas and major source of acid rains upon combustion (Keshavarz et al., 2008); as a result, its elimination is of paramount importance from HSE, corrosion and catalyst poisoning viewpoints (Gerc et. al., 2008). The level of H$_2$S should meet standard restrictions. Moreover, hydrogen sulfide is extremely toxic to the living organisms and plants (Alexander and Winnick, 1994)

Due to existence of these toxic compounds in many industrial gases, the direct use of them is prohibiting. Simultaneous removal of CO$_2$ and H$_2$S increase the amount of chemicals required during the removal step, and therefore is not desired. Many processes have developed to remove H$_2$S from gas streams (Maat et. al., 2005) see e.g. Kohl and Nielsen (Kohl and Nielsen, 1997).

In recent years, more studies have been implemented on removal of H$_2$S at elevated temperatures. Different methods such as chemical absorption by alkanolamines (Furhacker et. al., 2003), bioscrubber (Potivichayanon et. al., 2006) and oxidation of H$_2$S in iron-chelate process (Iliuta and Larachi, 2003) have been studied over years. One conventional method for H$_2$S removal is using scrubbers. Alkanolamines and their aqueous solutions absorb H$_2$S and CO$_2$ at low temperatures. Methyl-di-ethanolamine selectively removes H$_2$S from natural gas streams (Furhacker et. al., 2003). Another method is injection of sorbent into gasifier. In situ desulphurization is also done using generable metal oxides (Elseviers and Verelst, 1999). Clinoptilolite is another method for H$_2$S removal at lower temperatures; however, its major drawback is discharging solid wastes.

Among these, absorption methods of purification are extremely used in commercial plants. It is the first choice among different separation techniques. Amines have high ability to absorb acid gases because chemical reactions between the alkanolamines and these gases create a good driving force. Since these chemical reactions are reversible, alkanolamines are easily recovered (Baniadam et. al., 2009).

A number of purification processes exist based on physical dissolution of gases in liquids or dissolution combined with chemical reaction in liquid phase. The cost of purifying a gaseous mixture is generally very high. As a result, the processes of CO$_2$ and H$_2$S absorption are highly interested (Pohorecki and Mozenski, 1998).

Aqueous di-ethanolamine (DEA) is commonly used as an absorbent in refineries for removal of hydrogen sulfide from off gases (Kohl and Nielsen, 1997). Aqueous MDEA is selectively removing H$_2$S (Mandal et. al., 2004). Besides MDEA, di-isopropanolamine (DIPA) has been also reported to have higher selectivity for H$_2$S over CO$_2$ than either MEA or DEA. Over the past two decades, aqueous amine solvent technology has evolved from total acid gas removal processes for removing acid gas into selectively removing processes by using complex blended amine solvents. These results in higher CO$_2$ reaction rates of the primary or secondary amine with higher CO$_2$ loading capacity of the tertiary amine and lower solvent circulation rates compared to a single amine solvent (Mandal and Bandyopadhyay, 2005).
Simultaneous absorption of H$_2$S and CO$_2$ into diethanolamine is modeled using penetration theory (Haimour and Sandall, 1983). Say used hindered amine as the promoter of hot carbonate solutions for simultaneous absorption of H$_2$S and CO$_2$ (Say et al., 1984). Rascol interpreted a numerical solution for the case of simultaneous mass transfer of H$_2$S and CO$_2$ into aqueous blends of MDEA and DEA (Rascol et al., 1997). They used approximate film theories to describe mass transfer within the liquid phase. Rinker accomplished a theoretical and experimental study on simultaneous absorption of H$_2$S and CO$_2$ into aqueous blends of MDEA and DEA (Rinker).

Recently, amine modified adsorbents was studied for H$_2$S removal (Wang et al., 2007; Wang et al., 2008). It is found that removal of H$_2$S on the adsorbent is diffusion-limited. Group of Sayari (Belmabkhout et al., 2009) studied serial adsorbents of conventional and pore-expanded MCM-41 modified with amines. Some advantages of high adsorption capacity of MDEA-modified SBA-15 was shown and positive effects of moisture on adsorption capacity was also reported (Xue and Liu, 2011). A promising adsorbent for H$_2$S removal of minor concentration for gas purification was prepared by synthesizing and modifying the mesoporous molecular silica of SBA-15 with methyl-diethyl-amine (MDEA) (Xue and Liu, 2011).

In the present study, the amount of mass transfer in liquid ring compressors at gas and liquid interface is calculated based on definition of falling film theory, considering the bubble size distribution in the chamber. This equipment can be used as a substitution for absorption columns in sweetening units. This study aims at improving the interest on these processes, which are more effective, economically and technologically.

2. Liquid Ring Compressors

Liquid ring compressors belong to positive displacement machines in which the delivery of gas to be sucked is achieved by a circulating liquid. The working principle and simple design of LRC has resulted in its vast use in different industries. In this machine, the compression element instead of metal and iron piston is composed of a liquid with definite shape in casing. Through compression, a chemical reaction is performed between amine as the operating liquid and CO$_2$ or H$_2$S to sweeten the gas. Working fluid would be water, sulfuric acid, crude oil, gasoline or any other liquid non-reacting with gas feed. This feature eliminates metal parts and keeps the efficiency of machine constant for a long time with low maintenance cost (Bannwarth, 2005).

2.1 Working Principle

As shown in fig. 1, rotor is in the center of casing. System is filled with service liquid up to the centerline. Gas is discharged to compressor via fixed distribution cone. When the machine starts, service liquid distributes evenly on the walls of double lobe casing due to centrifugal force. The cone has two gas inlets and two gas outlets. In the first phase, impeller moves the gas towards the large section of the casing. In the second phase, gas is pushed towards the narrow part of the casing, totally occupied by service liquid that compresses the gas in the second outlet (Garo company website).
The most important Features of this process are:

- **Safety**: The recovered gas can directly be used as fuel even in case of unscheduled shutdown of fuel gas absorber.
- **Flexibility of the process**: There could be placed a final clean up section by a small column on top of the separator to stand sudden and wide variations of CO₂ content in the gas, fed to compressor.
- **Reliability of the process**: The nature of the system presents the buildup of ammonium salts in the service liquid and scale formation inside the compressor. This allows a virtually unlimited compressor working life.

3. Model Development

A mathematical model is developed to describe the absorption of CO₂ from a gas stream using MDEA aqueous solution in liquid ring compressors. To do this, bubble size distribution in the chamber obtained using maximum entropy formalism. Then the total amount of mass transfer was calculated by probability density function curve vs. dimensionless diameter. The gas stream enters the chamber with flow rate of 150 m³/h and CO₂ volume content of 9.9%.

3.1 Bubble size distribution functions

As mentioned before, gas bubbles are distrusted in compressor chamber. There are some established correlations for droplet size distribution, often called probability density functions (PDF), such as Rossin-Rammler and Nukiyama-Tanasawa distribution. However, these may suffer from lack of theoretical foundations (Brodkey, 1967).

Through the last 15 years, there has been vast usage of maximum entropy formalism (MEF). The advantage of MEF approach is that it avoids the detailed modeling of the process. However, its disadvantage is that there is no priori justification for the choice of constraints in MEF approach.

In simplified models, besides the mass conservation and normalized constraint, a few more constraints are considered. Ahmadi and Sellens used conservation of surface energy with
additional “partition of surface energy” constraints without conservation of kinetic energy of the released liquid (Ahmadi and Sellens, 1993). From engineering point of view, some simplified MEF models, which have less constraint, may be used.

3.1.1 A Model for PDF of Droplet Size Based on Maximum Entropy Formalism

Maximum entropy formalism is a method of statistical interface that provides the least biased estimate of a probability distribution. The resultant PDF is obtained by maximizing Shannon’s Entropy (Chen and Yapa, 2007). Physical conservation principles are used in a set of constraint equations that carry sufficient information to compute a good droplet size distribution. Following the model developed by Li and Tankin (Li and Tankin, 1992), the following constraint equations are considered in the continuous integral form. $f$ is the joint PDF, with functionality of, $f = f(\delta^*, u^*)$ in which, $\delta^* = \delta / \delta_0$ is the non-dimensional droplet diameter; $u^* = u / U_0$ is non-dimensional droplet velocity and $U_0$ is the jet release velocity.

- Normalization constraint:

$$\int \int f \, d\delta^* \, du^* = 1 \tag{1}$$

- Conservation of mass:

$$\int \int f \, \delta^*^3 \, d\delta^* \, du^* = 1 + S_m \tag{2}$$

- Conservation of momentum:

$$\int \int f \, \delta^*^3 \, u^* \, d\delta^* \, du^* = 1 + S_{mV} \tag{3}$$

- Conservation of kinetic and surface energy:

$$\int \int f \, (\delta^*^3 \, u^*^2 + \delta^*^2 \, \beta) = d \, \delta^* \, du^* = 1 + S. \tag{4}$$

$$\beta = \frac{2S}{\sigma}, s = \text{shape factor}$$

By maximizing Shannon’s entropy, subject to above constraints:
\[
f = 3\delta^{2}\exp\left[-\lambda_0 - \lambda_1\delta^3 - \lambda_2\delta^3u^* - \lambda_3\left(\delta^3u^* + \delta^2\beta\right)\right], \tag{5}\]

The Lagrangian multipliers (\(\lambda_i\)) are evaluated by solving the set of nonlinear constraint equations.

### 3.2 Simplified Maximum Entropy Formalism-Based Model

The MEF model described was solved analytically using constraint equations. The solution of number-based PDF is as follows:

\[
f_N = \frac{dN}{d\delta^*} = 3\delta^{2}\exp\left(-\delta^3\right) \tag{6}\]

In which, \(\lambda_1 = 1, \lambda_0 = 0\). In terms of Sauter mean diameter, this equation may be expressed as:

\[
f_N = \frac{dN}{d\bar{\delta}} = 3C_1\bar{\delta}^2\exp\left(-C_2\bar{\delta}^3\right) \tag{7}\]

Where,

\[
\delta_{32} = A\delta_{30}, \quad \bar{\delta} = \frac{\delta}{\delta_{32}}
\]

With \(A\) as a constant, \(C_2 = A^3, C_1 = A^2, \delta^* = A\bar{\delta}\)

This simplified distribution is actually a number-based Nukiyama-Tanasawa distribution, which is to be used in the modeling.
Following Zwitterions’ mechanism for reaction of CO\(_2\) with MDEA, we have:

\[ r_{CO_2-MDEA} = \frac{C_{CO_2} C_{R,R,R,N} - C_{HCO_3}^{-}}{C_{HCO_3}^{-}} \left( k_{I}^{-1} \left( k_{I-H_2O}^{-1} C_{R,R,R,N}^{+} + k_{I-OH}^{-1} C_{R,R,R,N}^{OH^{-}} \right) \left( k_{I-H_2O}^{-1} C_{H_2O}^{+} + k_{I-OH}^{-1} C_{OH^{-}} \right) \right) \]  

(8)

Finding the rate constants and substituting them in the above equation, we have:

\[ K_{CO_2-OH}^{-} = \frac{K_{HCO_3}^{-}}{K_{H_2O}} \]  

(9)

\[ K_{I-OH}^{-1} = \frac{K_{I}^{-1} K_{I-H_2O}^{-1}}{k_{I}^{-1} K_{H_2O}^{-}} \]  

(10)

\[ r_{CO_2-MDEA} = \frac{K_{I} C_{R,R,R,N} \left( C_{CO_2} - \frac{C_{HCO_3}^{-}}{k_{HCO_3}^{-} C_{OH^{-}}} \right)}{1 + \frac{k_{I}^{-1}}{k_{I} \left( k_{I-H_2O}^{-1} C_{H_2O}^{+} + k_{I-OH}^{-1} C_{OH^{-}} \right)}} \]  

(11)

This is a general rate expression for reaction of CO\(_2\) with MDEA or any other tertiary amine. Depending on the magnitude of the second term in denominator, one can obtain two limiting forms:

1. Rate expression in this case is reduced to:

\[ r_{CO_2-MDEA} = K_{I} C_{R,R,R,N} \left( C_{CO_2} - \frac{C_{HCO_3}^{-}}{k_{HCO_3}^{-} C_{OH^{-}}} \right) \]  

(12)
The rate constant of the reaction is given as a function of temperature by:

\[ K_I = K_I^0 \exp \left[ -\frac{E}{RT} \left( \frac{1}{T} - \frac{1}{298.15} \right) \right] \]  

(13)

2. In this case, the rate expression is given by:

\[ -r_{CO_2-MDEA} = (K_{MDEA-H_2O} C_{H_2O} + K_{MDEA-OH} C_{OH^-}) C_{R_3R_4N} \left( C_{CO_2} - \frac{C_{HCO_3^-}}{k_{HCO_3^-} C_{OH^-}} \right) \]  

(14)

Glasscock showed that this form reconciled the published rate data better (Glasscock et. al., 1991). In this article, the rate constant of Critchfield is used as:

\[ K_I = 2.5 \exp \left[ -6894.81 \left( \frac{1}{T} - \frac{1}{298.15} \right) \right] \]  

(15)

5. Mathematical Implementation and Method of Solution

Using the second order reaction for CO₂ and MDEA, the resulted nonlinear differential equation was solved numerically. Boll’s equation for calculating bubble’s mean diameter is defined as (Emanuele and Francesca, 2004):

\[ 32 = \frac{4.22 \times 10^{-2} + 5.77 \times 10^{-3}(1000Q_L)}{V_r^{1.602} \left( \frac{1000Q_L}{Q_g} \right)^{1.932}} \]  

(16)

With substitution of parameters in Boll’s relation, mean diameter and probability density function are obtained:

\[ D_{32}=7 \text{ mm} \]
Bubble size distribution curve is plotted in fig. 2. To obtain the concentration distribution, dimensions of a compressor belong to Nash Company, Model SB1/SB2-30-75 were used. Residence time is calculated at a defined flow rate. The effective volume of chamber is 0.4 m$^3$, obtained by subtracting the space between impellers and rotor from overall chamber volume. The calculated residence time is 9.6 seconds. On the other hand, with calculating the length of arch swiped by bubbles based on appendix 2 as well as using kinetic data (Lemoine et. al., 2000; Chunix and Furst, 2000) and operating parameters of the commercial plant stated in table 1 using concentration distribution equation derived in appendix 1, which its method is expressed in compressors for the first time, we have:

$$Z=2.1 \, \text{m}$$

$$K=5.3$$

$$D_{AB}=1.39 \, \text{m}^2/\text{s}$$

$$\frac{C}{C_0} = \frac{1}{2} \exp(-\frac{x}{D_{AB}}) \text{erfc}(\frac{x}{2\sqrt{S/l_{exp}}}) - \frac{(A+B)}{D_{AB}z} \text{erfc}(\frac{x}{2\sqrt{S/l_{exp}}}) + \frac{(A+B)x}{S/l_{exp}z} \frac{(A+B)}{D_{AB}z} \text{erfc}(\frac{x}{2\sqrt{S/l_{exp}}})$$

(18)
This equation solved numerically and the result is plotted in fig. 3. Mass transfer rate is obtained using the slope of curve at x=0 in mass flux equation:

\[ N_A = -D \frac{\partial C}{\partial x} \]  \hspace{1cm} (19)

Table 1 - Data of CO\(_2\) sweetening unit (Emanuele and Francesca, 2004)

<table>
<thead>
<tr>
<th>Gas flow (m(^3)/hr)</th>
<th>Liquid temp. (°C)</th>
<th>Liquid circ. Flow (m(^3)/hr)</th>
<th>CO(_2) in (%vol)</th>
<th>CO(_2) out (%vol)</th>
<th>Pressure (bar)</th>
</tr>
</thead>
<tbody>
<tr>
<td>150</td>
<td>35</td>
<td>2</td>
<td>9.9</td>
<td>1.08</td>
<td>3</td>
</tr>
</tbody>
</table>

The probability density function curve was divided into five intervals in which the above calculations were conducted for each as shown in fig. 2. The total amount of mass transfer was then obtained by multiplying mass transfer flux in number and mean area of bubbles in each section and finally adding them up.
5.1 Estimating the Number of Bubbles in Each District

The volume of inlet gas with residence time of 9.6 seconds was about 0.4 m$^3$. The total number of bubbles was estimated for subsequent calculations. Mean diameter and volume of bubbles were calculated for each interval based on probability density function. Using the normalized bubble size distribution and dividing it into different districts based on bubbles’ radius, the area of each section was found and by multiplication total number of bubbles to the area of each section, the number of bubbles in that area was obtained. Mean radius and number of bubbles in each interval are stated in subsequent equations.

\[
\begin{align*}
\bar{r}_1 &= 0.875mm \\
\bar{r}_2 &= 2.625mm \\
\bar{r}_3 &= 4.375mm \\
\bar{r}_4 &= 6.125mm \\
\bar{r}_5 &= 7.8875mm
\end{align*}
\]
Total volume of bubbles obtained by multiplying the total number of bubbles in their mean volume should be equal to inlet gas volume as follows:

\[
\begin{align*}
I) \ & 2.2e + 6 \times 0.1175 = 0.26e + 6 \\
II) \ & 2.2e + 6 \times 0.61 = 1.34e + 6 \\
III) \ & 2.2e + 6 \times 0.3 = 0.66e + 6 \\
IV) \ & 2.2e + 6 \times 0.0336 = 0.074e + 6 \\
III) \ & 2.2e + 6 \times 0.00028 = 0.0061e + 6
\end{align*}
\]

\[
(21)
\]

The total volume of bubbles is less than inlet gas volume. For the second estimation, the total number of bubbles was assumed, 2.5e+6.

5.2 Calculation of Total Amount of Mass Transfer in Compressor

To calculate the total amount of mass transfer, the number of bubbles in each interval was multiplied by the mean area of bubbles in that interval and finally the results were added up.

\[
\begin{align*}
I) \ & 9.6e - 6 \times 0.29e + 6 \times 0.00009 = 0.00025 \ (kg/s) \\
II) \ & 8.6e - 5 \times 1.52e + 6 \times 0.00009 = 0.01176 (kg/s) \\
III) \ & 2.4e - 4 \times 0.75e + 6 \times 0.00009 = 0.0162\ (kg/s) \\
IV) \ & 4.7e - 4 \times 0.084e + 6 \times 0.00009 = 0.00355\ (kg/s) \\
V) \ & 7.7e - 4 \times 0.0007e + 6 \times 0.00009 = 0.00005\ (kg/s)
\end{align*}
\]

\[
(23)
\]
\[ \sum N_i = 0.031 \text{ kg/s} \]  

5.3 Results and Discussion

At mean diameter of 0.007 m and solubility of 300 ppm, based on total number of bubbles, the concentration of unreacted gas and percentage of absorbed CO\textsubscript{2} were obtained.

In acid load of 0.22 in gas, the concentration of CO\textsubscript{2} in outlet stream was 1 percent, which by considering the outlet pressure of compressor, it would be 33.3 ppm.

Also in acid load of 0.1 with assumption of 90% absorption, the partial pressure of acid gas reached to 20 ppm. The plot of acid gas load Vs. partial pressure is plotted in fig. 4.

As can be seen in fig. 4, the results were in good agreement with operative curve of LRCs for Garo Company. Using the same data for H\textsubscript{2}S elimination in two different temperatures and repeating the same procedure, the results of table 2 and operative curve plotted in fig. 5 are obtained.

![Fig. 4. Resulted partial pressure curve](image)
As expected, increasing the operating temperature and changing the gas solubility in constant molar ratio of H$_2$S to amine, causes the partial pressure of gas to increase. Moreover, with increasing this ratio in a constant temperature, partial pressure of H$_2$S increases linearly.

### Table 2 Data of H$_2$S sweetening

<table>
<thead>
<tr>
<th>$K_{eq}$</th>
<th>$D_{AB}$(m$^2$/s)</th>
<th>Z(m)</th>
<th>$N_A$ (kg/m$^2$s)</th>
<th>Total number of bubbles</th>
<th>$N_A$(kg/s)</th>
<th>Output (bar)pressure</th>
<th>Mean diameter of bubbles (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>23.5</td>
<td>1.8e-9</td>
<td>2.1</td>
<td>0.000</td>
<td>257142</td>
<td>0.22</td>
<td>6</td>
<td>0.003</td>
</tr>
<tr>
<td>7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
6. Conclusion

In this article, in the meantime of introducing LRCs as an appropriate substitution for absorption columns in gas sweetening units, a novel approach for modeling the total mass transfer in the casing based on film theory was introduced. Using MEF model, distribution of the bubbles in the chamber was obtained. To calculate the total mass transfer, the mean surface of bubbles in each region was multiplied by the amount of mass transfer and the number of bubbles in that region and finally the results added up. Based on the data available from gas sweetening unit, the operating curve of compressor was obtained which was in good agreement with commercial case. These calculations can be used as a basic design for process engineers.

7. Appendix A

A.1. Mass Flux Calculation in Compressor Based on Falling Film Theory

A wetted wall column is used to model the absorption of gas $A$. The gas is consumed in liquid phase by first order reaction. Developing the expression gives absorption rate and effective penetration depth as a function of distance from liquid inlet.

\[ -v \frac{\partial c}{\partial z} + D \frac{\partial^2 c}{\partial x^2} = Kc \]  

(A-1)

Using Laplace transform, we have:

\[ -Sc - D \frac{\partial^2 c}{\partial x^2} = Kc \]  

(A-2)

\[ \therefore D \frac{d^2 c}{dx^2} - (K + S)v c = 0 \]  

(A-3)

For our model:

\[ D \frac{d^2 c}{dx^2} - (A + \frac{B}{T} + Sv_T) c = 0 \]  

(A-4)
Solving the second order reaction, we have:

\[ \frac{-c}{c} = A \exp[x \sqrt{\frac{K + Sv}{D}}] + B \exp[-x \sqrt{\frac{K + Sv}{D}}] \]  
(A-5)

\[ \frac{-c}{c} = \frac{c_0}{s} \exp[-x \sqrt{\frac{K + Sv}{D}}] \]  
(A-6)

Using the Laplace transform and shifting theorem:

\[ \ell[\frac{x}{2} \sqrt{\frac{v}{D\pi z^3}} \exp(-\frac{x^2 v}{4Dz}) \exp(-\frac{Kz}{v})] = \exp[-x \sqrt{\frac{v}{D}} (S + \frac{K}{v})] \]  
(A-7)

Inverting the equation gives:

\[ c = c_0 \int_0^x \frac{x}{2} \sqrt{\frac{v}{D\pi z^3}} \exp(-\frac{x^2 v}{4Dz}) \exp(-\frac{Kz}{v}) dz \]  
(A-8)

With Substitution of:

\[ \alpha^2 = \frac{x^2 v}{4D} \]  
(A-9)

\[ \beta^2 = \frac{K}{v} \]  
(A-9)

\[ r = \frac{\alpha}{\sqrt{z}} - \beta \sqrt{z} \]  
(A-10)
\[ dr = (-\frac{\alpha}{2z^{3/2}} - \frac{\beta}{2z^{1/2}})dz \]  

(A-11)

With substitution in equation we have;

\[ \frac{1}{2} \exp(-x\frac{k}{D}) \text{erfc}(\frac{x}{\sqrt{v_r}}) - \frac{1}{2} \exp(x\frac{k}{D}) \text{erfc}(\frac{x}{\sqrt{v_r}}) + \frac{1}{2} \frac{K_z}{\sqrt{v_r}} \]  

(A-12)

Substitution of screw velocity equation in concentration profile in LRC compressor:

\[ c = c_o e^{-\frac{\alpha^2}{z^2}} \text{erfc}\left(\frac{\alpha}{\sqrt{z}} + \beta\sqrt{z}\right) + c_o \beta \int_0^z \exp\left(-\frac{\alpha^2}{z^2} - \beta^2 z\right)dz \]  

(A-13)

When a cylinder with radius ‘a’ perpendicular to XY plane is swiped by screw M, if M is proportional to θ:

\[ z = h\theta + z_o \]

\[ at.\theta = 0 \rightarrow z = 0 \]

\[ \Rightarrow z_o = 0 \]  

(A-14)

\[ x = a \cos \theta \]

\[ y = a \sin \theta \]  

(A-15)

\[ z = h \theta \]
Velocity vector is obtained by:

\[ \vec{v}(\theta) = -a \sin(\theta) \hat{i} + a \cos(\theta) \hat{j} + h \hat{k} \] (A-16)

\[ \text{A.2. Arch length function} \]

If \( r(t) \) is a defined curve, the arch length function is as follow:

\[ S(t) = \int_{r_0}^t \| r'(u) \| du \]

\[ dS^2 = dx^2 + dy^2 + dz^2 = (a^2 + h^2)d\theta^2 \]

\[ dS = \sqrt{a^2 + h^2} d\theta \]

\[ \Rightarrow S = \sqrt{a^2 + h^2} \theta \] (A-17)

With considering the length of swiped arch equivalent to tube length, at a defined residence time in the chamber, the resulted velocity is substituted in falling film equation to give:

\[ S = \mathbf{V} t_{\text{exp}} \]

\[ \mathbf{V} = \frac{S}{t_{\text{exp}}} \] (A-18)

The concentration profile obtained as follow:

\[ c = \frac{1}{c_o} \left[ \exp\left(-x \sqrt{\frac{k}{D}} \right) \text{erfc}\left(\frac{x}{2 \sqrt{Dz}} - \frac{Kz}{v_r}\right) + \frac{1}{2} \exp\left(x \sqrt{\frac{k}{D}} \right) \text{erfc}\left(\frac{x}{2 \sqrt{Dz}} + \frac{Kz}{v_r}\right) \right] \] (A-19)
With substitution of the screw velocity and the residence time in equation:

\[
\frac{C}{C_0} = \frac{1}{2} \exp\left(-\frac{x}{D_{AB}}\right) \text{erfc}\left(\frac{x}{2D_{AB}z}\right) \sqrt{\frac{S/t_{exp}}{D_{AB}z}} - \frac{(A + \frac{B}{T})z}{S/t_{exp}} \\
+ \frac{1}{2} \exp\left(\frac{x}{D_{AB}}\right) \text{erfc}\left(\frac{x}{2D_{AB}z}\right) \sqrt{\frac{S/t_{exp}}{D_{AB}z}} + \frac{(A + \frac{B}{T})z}{S/t_{exp}}
\]  

(A-20)

The above results are used to determine the amount of H\(_2\)S absorbed from the first order reaction.

**Nomenclature**

- \(u^*\) nondimensional droplet velocity
- \(\delta_{s2}\) Sauter mean diameter (m)
- \(\delta_{30}\) mass mean volume-equivalent diameter (m)
- \(\delta^*\) Nondimensional droplet diameter
- \(S\) Shape factor
- \(V_p\) Volume (\(m^3\))
- \(A_p\) Surface area
- \(D\) Diffusion coefficient (\(m^2\))
- \(N_A\) Mass flux (\(\frac{kg}{m^2.s}\))
- \(Z\) distance from the liquid inlet (m)
- \(x\) coordinate measured inward from the surface of the film (m)
- \(C\) Concentration of gas (ppm)
K       Reaction constant (m⁴/mol·s)

sₘ       source term for mass conservation

tₑₓᵖ       Exposure time (s)

T       Temperature (K)

References


Li, X. and Tankin, R. S. (1992), On the prediction of droplet size and velocity distributions in sprays through maximum entropy principle, Particle particle system characterization, 9, 195–201.


