To Study the Effect of CO$_2$ Absorption in Aqueous MEA Solution using Kent-Eisenberg Thermodynamic Model

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A R T I C L E   I N F O

A B S T R A C T

This work presents a thermodynamic investigation of CO$_2$ absorption in Mono-ethanol Amine (MEA) solution based on extensive experimental studies on this topic. Presented model can predict CO$_2$ absorption in the amine solution with high accurately. The objectives of the current research are to study the effect of CO$_2$ absorption for a wide range of gas/liquid flow rate and CO$_2$ concentration (5 -20%) in the sour gas using Kent-Eisenberg Thermodynamic Model. CO$_2$ loading in the lean gas was 0.006 mol/mol. CO$_2$ absorption in MEA was studied at 25 ºC and atmospheric pressure. In the open literature, many experimental data is available but very less work has focus on modeling and simulation of CO$_2$ absorption in MEA solution. The predicted CO$_2$ absorption trend and CO$_2$ concentration in the sweet gas is found to be in good agreement with the experimental results, which validates the simulated results forCO$_2$ mass transfer in MEA solution. Effect of Liquid and gas flow rate and concentration of CO$_2$ in flue gas are also important parameters in CO$_2$ absorption process and are discussed in detail.

INTRODUCTION

Chemical industry is producing million's of tones of CO$_2$ per year which is the main cause of increasing global warming. So removing CO$_2$ from industrial gases is of prime importance. One of the most economical and commonly used processes for CO$_2$ removal is chemical absorption/desorption technique in different amine aqueous solutions. This absorption/desorption requires a circulating solvent capable of capturing high amount of CO$_2$ at ambient temperature/pressure and release in the desorption column requiring less energy (Dechen Zhu, M.F., 2012). Selection of circulating liquid is a critical step in the absorption/desorption process. The critical issues are (1) greater capacity of CO$_2$ capture (2) degradation of the solvent at extreme conditions (Rochelle, F.C.a.G.T., 2011; Lawal, A.O.a.R.O.I., 2006) (3) efficient desorption (4) slow reaction rates for thermal and oxidation degradation (5) cheap and easily availability (Thu Nguyena, M.H., Gary Rochelle, 2011)(6) non volatility in regenerator (7) compatibility with packed bed material and phase (Fu, D.X., 2012) (8) foam ability. MEA, being a primary amine, have very fast absorption as compared to other amine solutions. It is being used as a solvent for CO$_2$ removal in most of the industries. Thermodynamic properties for MEA-H$_2$O-CO$_2$ are required to model and simulate CO$_2$ absorption process and have been reported in the literature. These properties are shown in Table 1.

Effective design for CO$_2$ absorption into amine solution, experimentally on a pilot scale absorption column has been investigated by many researchers (Patricia Mores, N.S., Sergio Mussati, 2011; Mandala, M.G.B.P., 2006; Raphael Idem, M.W., 2006; Jimmy Xiao, C.W.L., Meng-Hui Li, 2000). These pilot scale equipment are designed for specific process parameters and are expensive to build for research purpose. Process simulation and modelling have a prominent role in evaluation the process parameters and to predict the results. System optimization is also required for reducing the operational cost and develops an energy efficient process. Simulation and modelling are therefore important for both designing absorption column and to find optimum operating conditions for given process conditions.

Many of the models have been proposed for simulating the experimental absorption of CO$_2$ into MEA solution, but all of the models have limitation of one way or the other. A model based on enthalpy associated with absorption/desorption was developed to investigate amine basicity and degree of carbamate formation (Nichola McCann, M.M. and Moetaz Attalla, 2008). However, the model proposed has a 10% error in

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predicting the cyclic capacity and CO_2 absorption. In-silico amine screen was developed by (Levente, Y.E., 2011) for efficient absorption of CO_2. A reliable and robust model was also developed, but the model was able to predict the experimental data with 10 % deviation from experimental data. (Ana-Maria Cormos, J.G., 2012) developed a model using MATLAB (Anonymous,1992) to simulate CO_2 absorption in MEA solution, but simulated results shows up to 11.75 % deviation from experimental data. Another model presented includes differential equations based on mass and heat transfer of CO_2 into MEA solution with a higher concentration of MEA and simulated data is not in line with experimental data (Ugochukwu, H.F.S., 2009). Mass transfer of CO_2 into MEA solution in a packed column and proposed a model that takes into account the wetting of the packed surface, but for higher MEA concentrations (Švandová, J.M.Z., Ľ. Jelemenský, 2008). A rate based mathematical model was developed by (Patricia Mores, N.S., Sergio Mussati, 2012) to predict CO_2 absorption in MEA solution using random packing in packed column assuming that the liquid amine solution is an ideal solution and validate his data using data points from HYSYS and have considerable error in validating the model. CO_2 absorption from CO_2-CH_4 gas mixture into MEA solution was also studied by (Somnuk Boributh, W.R., 2012) using a poly-vinylidene-fluoride hollow fibre membrane contactor for higher CO_2 absorption. A mathematical model was developed, assuming that the system is steady state and gas stream is an ideal gas with no axial absorption, to validate the experimental results for estimating the wetting ratio as a function of liquid velocity. The model was proposed by (Chechet Biliyok, A.L., 2012) for CO_2 removal post combustion gases and the model was validated not only for steady state conditions but also for dynamic conditions. Again, this model was not able to predict the experimental data points.

Table 1: Thermodynamic properties for MEA-CO_2-H_2O system.

Properties	Units	Reference
Liquid density	[kg/m^3]	(Cheng, S., 1996)
Surface tension of the liquid solution	[N/m]	(Gonzalo Vazquez, E.A., 1997)
Viscosity of water	[(N s)/m^2]	(Cheng, S., 1996)
Viscosity of liquid solution	[(N s)/m^2]	(Trine, L.E., 2009; Weiland, R.H., 1998; Weiland, M.R.R.H., R.G. Rice, 1982)
Viscosity of gas	[(N s)/m^2]	(Ayyaz Muhammad, M.I.A.M., 2008; Reid, R.C., 1987)
Specific wetted area for mass and heat transfer	[m^2/m^3]	(Billet, R., M. Schultes, 1999)
Diffusion coefficient of CO_2 in liquid solution	[m^2/s]	(Peter, E.S.H., 2008; Jiun-Jie Ko, T.C.T., 2001)
Diffusion coefficient of MEA in liquid solution	[m^2/s]	(Erwin, M.J.M.t.R., 1993)
Mass transfer coefficients for gases and liquids	[m/s]	(Billet, R., M. Schultes, 1999)
Heat transfer coefficient	[W/(m^2 K)]	(Bird, R.B., 2002)
Second order reaction rate	[(m^{3}mol)/s]	(Versteeg, G.F., 1996)
Henry's law constant of CO_2 over liquid solution	[(Pa m^3)/mol]	(Wang, Y.W., 1992)
Equilibrium constant of absorption	[mol/m^3]	(Gabrielsen, J., 2007)
Heat capacity of the liquid solution	[J/(mol K)]	(Maham, Y., 1997)
Heat capacity of the gases	[J/(mol K)]	(Reid, R.C., 1987)
Heat of absorption for CO_2	[J/mol]	(Gabrielsen, J., 2007)

To make the absorption/desorption faster the gas/liquid flow rate flexibility should be there, hence this is one of the objective of this study. In the industry the CO_2 concentration varies significantly in sour gas so in current investigation, the CO_2 concentration has a wide range from 5-20 % and is the second objective of this study. In the next section, the experimental setup and test cases will be described before presenting the results with the two objectives.

Reaction mechanism and kinetics:
Many researchers have analyzed reaction mechanism for CO_2 absorption in MEA solution. Still this mechanism is not fully understood. Different reaction steps refereed by researcher for development of their mathematical models are considered in this research (Jozsef Gaspar, A.M.C., 2012; Ying Zhang, H.Q., 2011; Ahmed Aboudheir, P.T., 2003). Reactions 1-12 may occur during CO_2 absorption in amine solution.
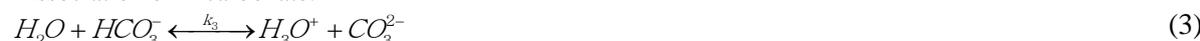Ionization of water:

$$2H_2O \xleftrightarrow{k_1} H_3O^+ + OH^- \tag{1}$$

Dissociation of dissolved CO_2 and formation of Carbonic acid:

$$2H_2O + CO_2 \xleftrightarrow{k_2,k_{21}} H_3O^+ + HCO_3^- \tag{2}$$

Dissociation of Bicarbonate:

$$H_2O + HCO_3^- \xleftrightarrow{k_3} H_3O^+ + CO_3^{2-} \tag{3}$$

Formation of Zwitter ion (CO_2 reaction with MEA):

$$CO_2 + MEA \xleftrightarrow{k_4,k_{41}} MEAH^+COO^- \tag{4}$$

Deprotonating of Zwitter ion:

$$MEAH^+COO^- + MEA \xleftrightarrow{k_5, k_{51}} MEAH^+ + MEACOO^- \tag{5}$$

$$MEAH^+COO^- + H_2O \xleftrightarrow{k_6, k_{61}} MEACOO^- + H_3O^+ \tag{6}$$

$$MEAH^+COO^- + OH^- \xleftrightarrow{k_7, k_{71}} MEACOO^- + H_2O \tag{7}$$

Bicarbonate formation:

$$MEAH + HCO_3^- \xleftrightarrow{k_8, k_{81}} H_2O + MEACOO^- \tag{8}$$

Deprotonating of MEA:

$$H_2O + MEAH^+ \xleftrightarrow{k_9, k_{91}} H_3O^+ + MEA \tag{9}$$

Bicarbonate formation:

$$CO_2 + OH^- \xleftrightarrow{k_{10}, k_{101}} HCO_3^- \tag{10}$$

Carbonates and bicarbamate:

$$MEAH^+COO^- + HCO_3^- \xleftrightarrow{k_{11}, k_{111}} H_2CO_3 + MEACOO^- \tag{11}$$

$$MEAH^+COO^- + CO_3^{2-} \xleftrightarrow{k_{12}, k_{121}} HCO_3^- + MEACOO^- \tag{12}$$

Concentration of carbamate and bicarbamates in CO_2 loaded amine solutions is considered significantly as they are the main source of CO_2 absorbed in the amine solution (Ahmed Aboudheir, P.T., 2003). Formation of Zwitter ion is one of the main contributors for CO_2 absorption in the amine solution. Reaction 5-7 shows formation of Zwitter ion containing CO_2 molecule attached with the amine solution which is deprotonated later in the desorption section to collect the absorbed CO_2 (Ahmed Aboudheir, P.T., 2003; Adisorn Aroonwilasa, A.C., 2003; Mohamed Edali, A.A., Raphael Idem, 2009).

CO_2 absorption in MEA solution is exothermic and have high reaction rate. Temperature of the system rises when CO_2 comes in contact with the amine solution and detail of temperature profile in absorption column is discussed in detail, in this research. Reaction rate reported by different researcher is tabulated along with temperature range, experimental technique and MEA concentration in Table 2.

Table 2: Reaction rate for CO_2 absorption in MEA solution*.

[MEA] (mol/dm^3)	Experimental Technique	T (K)	k (dm^3/mol s)	Reference
0.25 –2.0	Laminar jet absorber	294.5	5400	(Astarita, G., 1961)
1.6–4.8	Laminar jet absorber	298	7500	(Clarke, J.K.A., 1964)
1	Laminar jet absorber	303	9700	(Sharma, M.M., 1965)
1	Laminar jet absorber	308	13,000	(Danckwerts, P.V., M.M. Sharma, 1966)
--	Stirred cell reactor	353	90,400	(Alper, E., 1990)
0.02–0.18	Rapid mixing method	278.6–308.4	$9.77 \times 10^{10}\exp(-4955/T)$	(Hikita, H., 1979)
0–0.06	Stopped flow method	278–303	$1.23 \times 10^{11}\exp(-5078/T)$	(Penny, D.E., T.J. Ritter, 1983)
0–0.45	Stopped flow method	278–298	$8.51 \times 10^{11}\exp(-5617/T)$	(Alper, E., 1990)
0.1– 0.4	Wetted wall column	303	4774	(Jimmy Xiao, C.W.L., Meng-Hui Li, 2000)
0.1– 0.5	Wetted wall column	303–313	$3.014 \times 10^{11}\exp(-5376.2/T)$	(Li, S.Y.H.a.M.H., 2002)
1-10	Laminar jet absorber	293-333	$4.61 \times 10^9\exp(-4412/T)$	(Ahmed Aboudheir, P.T., 2003)

*Abbreviation for table 2

k	Reaction rate for CO_2 absorption in MEA (dm^3/mol s)
T	Temperature (K)
[MEA]	Concentration of Mono-Ethanol Amine

Experimental setup and test cases:

Figure 1 shows the systematic diagram of the absorption column used in the simulation of the experiment reported by (David deMontigny, A.A., 2004). In the experiment concentration of CO_2 on each of the stages is measured and is recorded in the controller to know about CO_2concentration in the gas phase on each stage of the absorption column (David deMontigny, A.A., 2004). Sour gas enters into the column from the bottom of the column and sweet gas, after the removal of CO_2, leaves the column from the top. Lean solution enters into the column from the top, interacts counter currently with the gas, and leaves the column from the bottom, when rich with CO_2. The equipment mainly consists of an absorption column, 40 packed elements containing Sulzer DX structured packing. Packed column design details are shown in table 3 and are taken as a base case for this study.

Absorption data from bench scale laboratory experiment is used as the basis of this study and to validate the results shown in this study (David deMontigny, A.A., 2004). In the experiment, gas stream consists of a mixture

of air and CO_2, where the concentration of CO_2 varied from 5-20 % mol/mol. Lean amine solution is an aqueous solution of MEA, where the concentration of MEA is between 1 - 3 kmol m^{-3}. Sour gas flow rate is in the range of 5.4 - 12.6 m^3 m^{-2} h^{-1} and the flow rate for lean amine solution was 30.9 kmol m^{-2} h^{-1}. List of test cases studied in this study is given in table 2. Experimental results for this experimentation are taken from the work of (David deMontigny, A.A., 2004). The model presented in this study is not good enough to predict the results of the experiment at low liquid flow rates and low amine concentration in lean solution.

Table 3: Packet column Internals and Packing Design used for CO_2 absorption in amine solution.

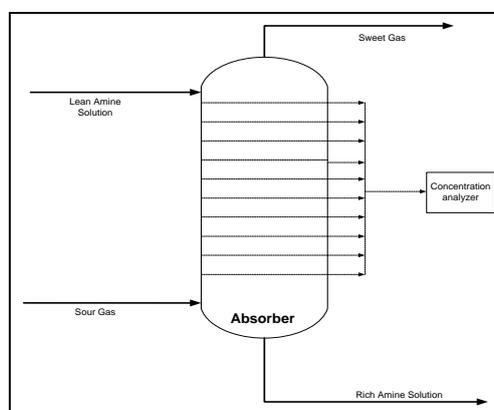| Description	Sulzer DX
Packing Data	
Surface area	900 m^2/m^3
Crimp height	2.9 mm
Corrugation base	6.4 mm
Crimp angle	60^0
Void fraction	0.775
Packed column data	
Diameter	0.028 m
Number of packing elements	40
Element length	0.054
Total packing height	2.16 m
Total available surface area	1.20 m^2

Fig. 1: Process flow diagram for CO_2 absorption.

Table 4 and Table 5 show test cases for studying the effect of initial CO_2 concentration in the sour gas. The concentration of CO_2 in sour gas was varied in the range of 5 -20 mol %. Temperature and pressure for all the test cases were at 25°C and one atm as same operating conditions were considered in the experiments performed by (David deMontigny, A.A., 2004). Similarly, MEA concentration in the amine solution was also kept constant at 2.0 kmol/kmol. Kent-Eisenberg vapor liquid equilibrium model is used in this package to calculate CO_2 absorption in the amine solution (Kent, R., B. Eisenberg, 1976). Non-Ideal vapor phase model is used in this study because CO_2 diffusion in the gas phase and at gas liquid inter-phase has high resistance especially at low CO_2 concentration in the gas stream.

Table 4: Validation Test Cases for CO_2 absorption in MEA solution in a Sulzer DX Packed Column.

Description	TC-1	TC-2	TC-3
Sour gas flow rate (m^3 m^{-2} h^{-1})	30.9	30.9	30.9
Lean amine solution flow rate (kmol m^{-2} h^{-1})	5.4	6.7	8.4
MEA Concentration (kmol/m^3)	2.0	2.0	2.0
CO_2 concentration in the sour gas (mol/mol)	14.23	14.35	14.38

*Abbreviation for table 4

TC-1	Test Case-1
TC-2	Test Case-2
TC-3	Test Case-3
MEA	Mono-Ethanol Amine

Table 5: Validation Test Cases for CO_2 absorption in MEA solution in a Sulzer DX Packed Column.

Description	TC-4	TC-5	TC-6
Sour gas flow rate (m^3 m^{-2} h^{-1})	30.9	30.9	30.9
Lean amine solution flow rate (kmol m^{-2} h^{-1})	5.4	5.4	5.4
MEA Concentration (kmol/m^3)	2.0	2.0	2.0
CO_2 concentration in the sour gas (mol/mol)	5	10	18

[*]Abbreviation for table 5

TC-4	Test Case-4
TC-5	Test Case-5
TC-6	Test Case-6
MEA	Mono-Ethanol Amine

RESULTS AND DISCUSSION

Table 4 shows three different validation cases for the experimental absorption of CO_2 into aqueous amine solution (Figure 2) (David deMontigny, A.A., 2006). Results obtained from this study and the study are shown in Figure 2 (a) along with the simulated results other researchers for some experimental data (TC-1) (David deMontigny, A.A., 2006; Henriques de Brito, U.v.S.M., 1994). Sulzer DX structured packing is used as packing material in the absorption column as Sulzer DX structured packing was used in the experimental study of CO_2 absorption, in MEA solution. Figure 2 (a) is a height vs. CO_2 concentration in gas phase profile, for different plate efficiencies and experimental data as mentioned in table 4. For all cases, initial CO_2 concentration in flue gas was 14.23 mol %. Flue gas enters the column from the bottom of the column and moves upwards in the column. When the flue gas comes in contact with lean solution, CO_2 in the gas stream starts to react with MEA present in the amine solution. Reaction rate for CO_2 absorption in MEA is fast (Gibbins, J., H. Chalmers, 2008). So, concentration of CO_2 in the flue gas readily decreases as more CO_2 in absorbed in the amine solution. CO_2 concentration in the gas stream reduces to almost zero before it exits to the atmosphere, from the top of the column. When the concentration of CO_2 in sour gas is less than ~ 2%, CO_2 mass transfer into the amine solution becomes very low and the slope of CO_2 absorption curve for all the cases becomes steeper (Ashleigh Cousins, L.T.W., 2011; Maceiras, R., 2008). This trend can be explained on the basis of high reaction rate for CO_2 absorption in amine solution and gas / liquid film resistance (Joseph, D.E.G., 1961; Inna Kim, C.M.J., 2011).

When flue gas enters in the absorption column from the bottom of the column, it contains relatively high CO_2 concentration. Similarly, lean amine solution entering from the top of the column also contains high free MEA concentration. When gas and liquid stream interact with each other in the absorption column, there is a high mass transfer of CO_2 from the gas stream into the amine solution. As the gas moves upward in the column CO_2 concentration in the amine solution decreases as most of the CO_2 is already absorbed in the amine solution. Now, CO_2 from the gas stream have to move from the gas stream to the gas film and then have to pass from the gas film into the liquid film, where it can react with any free MEA solution. For this reason, more stages are required to remove the remaining portion of CO_2 in the amine solution. This increase in gas/liquid film resistance is not very much high as eventually all of the CO_2 from the gas stream is absorbed into the amine solution and CO_2 free flue gas exits from the top of the column.

Plate efficiency has a vital role in CO_2 absorption process, as it will decide the efficiency of the column. Many plate efficiencies for have been studied for different operating conditions and only two plate efficiencies are reported in this research. In TC-1 (test case-1) two plate efficiencies have been studied for CO_2 absorption study. It can be seen from Figure 2 (a) that for 20% plate efficiency, the simulated curve is closer to the experimental data than for 15% plate efficiency. For 15% efficiency, simulated curve is showing less CO_2 absorption and simulates curve is away from the experimental data. This shows that for these operating conditions, the packing efficiency of the column was 20%. Packing efficiency is a function of gas and liquid flow rates and diameter of the column.

Simulated results for TC-2 are shown in Figure 2 (b). Details of operating conditions for TC-2 are given in Table 4. In TC-2, there is an increase in CO_2 absorption process as the curve for simulation is steeper as compared to TC-1. However, gas liquid film resistance decreases with a relative increase in liquid flow rate. This also increases the process of CO_2 absorption at high liquid flow rates. Simulated curve for 20% plate efficiency is much close to the experimental results for TC-2. Figure 2 (c) shows the simulated and experimental results for TC-3 (Table 4). TC-3 has the highest liquid flow rate as compared to other test cases. With an increase in liquid flow rate, CO_2 absorbtion is also increased and complete removal is achieved with fewer stages of the absorption column. This is due to a reduced amount of gas and liquid film resistance and high absorption rates for CO_2 and MEA solution. This shows that packing efficiency for high liquid flow rate (8.4 kmol m^{-2} h^{-1}) is higher than other liquid flow rates.

Effect of CO_2 concentration in the flue gas on overall absorption process is shown in Figure 3. Details of process parameters and operating conditions are enlisted in Table 5. This Figure 3 shows CO_2 removal from the flue gas along the height of the packed column for different CO_2 concentrations in flue gas. Overall height of the column required for CO_2 absorption is shown in Figure 3. This shows overall height of the column required for processes where the concentration of CO_2 varies in the gas stream. CO_2 concentration in the flue gas for this study was in the range of 5 - 18 mol % in sour gas. In all the cases, the overall efficiency of packing elements was set to 20 %. There are four curves in Figure 3 for TC-1, TC-4, TC-5 and TC-6. All other process parameters such as MEA concentration in the amine solution, flow rate for lean amine solution and sour gas stream were kept constant to observe the trend of CO_2 mass transfer from the flue gas (containing different concentrations

CO_2) into the amine solution. Low transfer rates for flue gas containing less CO_2 mol % is because with low CO_2 concentration there is less chance of CO_2 interaction with free MEA molecule in the amine solution. This is because there are more inter gas molecules to interact the CO_2 molecule and this decreases the chance of CO_2 collusion with the amine molecule. More packing stages are required to remove low CO_2 concentration from the flue gas which reduces the overall efficiency of the process. For all the cases, the gas has to travel up to the middle of the column for total absorption into the amine solution. Reactions rates are same for all CO_2 molecules and free MEA.
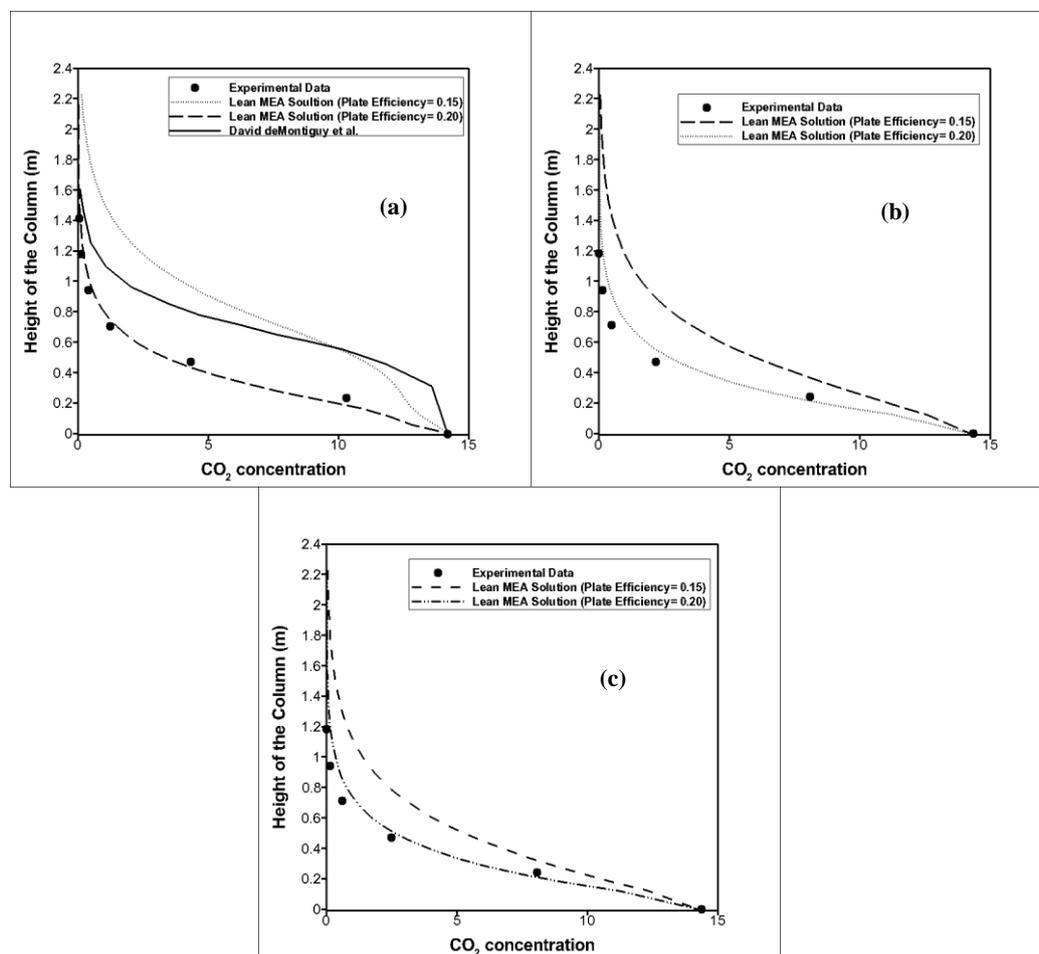
Fig. 2: Validation cases for CO_2 absorption in MEA solution. (a) Simulation result for TC-1, (b) Simulation result for TC-2 and (c) Simulation result for TC-3.
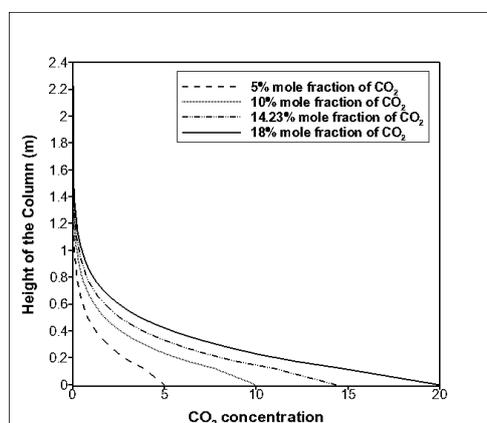
Fig. 3: Effect of CO_2 mole fraction in flue gas on overall CO_2 removal from sour gas.

Effect of gas flow rate and liquid flow rate on CO_2 loading in the amine solution is shown in Figure 4 and Figure 5. Figure 4 is a function of gas / liquid flow rate for different gas flow rates while keeping the liquid flow rate constant as for TC-1. Increase in gas flow rate reduces the contact time available for Gas / Liquid Interaction and can reduce CO_2 capture efficiency if it is increased to very high values. However, in this study there is an increase in gas flow rate in a very small range and results obtain are different than the results achieved for a typical gas / liquid absorption process. Figure 5 shows a plot for CO_2 loading in the amine solution for different amine solution flow rates. This shows that there is a decrease in the absorption process with increase in amine solution flow rate. This can be attributed to low contact time available for gas / liquid interaction at high amine flow rates.
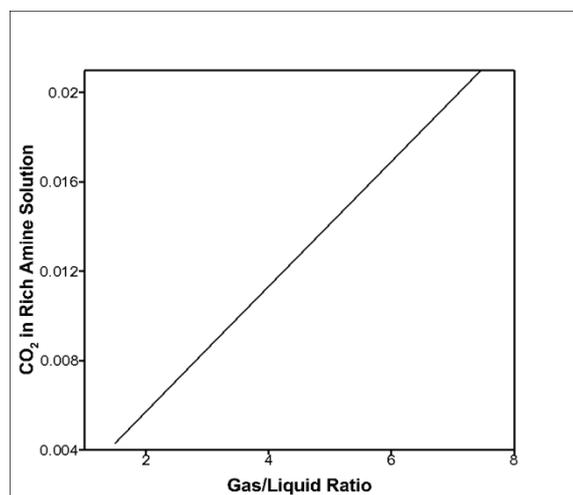

Fig. 4: Effect of Gas flow rate on overall CO_2 loading in Rich Amine Solution.
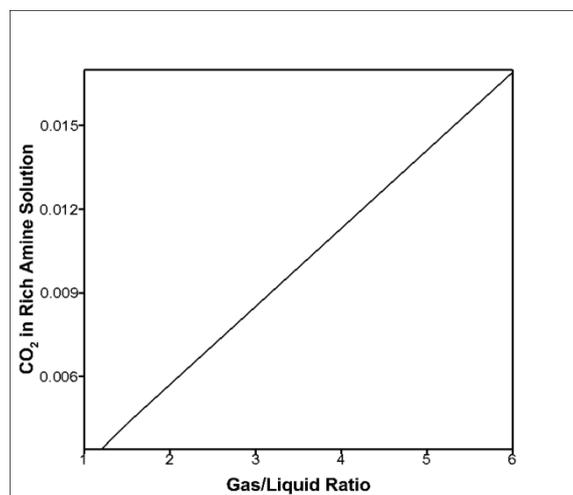

Fig. 5: Effect of Liquid flow rate on overall CO_2 loading in Rich Amine Solution.

Conclusion:

CO_2 absorption into aqueous MEA solution was simulated and compared for a lean amine solution flow rate in the range of 5.4 to 8.4 kmol m^{-2} h^{-1} and gas flow rate was kept constant at 30.9 m^3 m^{-2} h^{-1} in a simulated absorption column filled with Sulzer DX as a packing. Wetting of the packing element is very important for CO_2 absorption so the process was simulated for different plate efficiencies. It was observed that the simulated results do perfectly match with experimental data. It is noticed in this research that CO_2 mass transfer into the amine solution is much higher when flue gas has high CO_2 concentration. However, more stages are required to remove the remaining small amount from the flue gas. It is also noticed that the absorption process increases with steady increase in gas flow rate while it decreases with increase in amine solution flow rate. It is concluded that there should be a balance in gas and liquid flow rate as low flow rate can reduce the wetting efficiency of the packing and very high flow rates can reduce the contact time gas gas-liquid interaction.

ACKNOWLEDGMENTS

Appendix A:

Mass Balance in liquid phase:

Equation of continuity for one phase is given as:

$$\frac{\P r}{\P t} + Ñ(r.\vec{u}) = 0 \tag{13}$$

Where, u represents velocity of fluid and ρ is density of the fluid. Multiplying equation 13 with a factor v_z. S on both sides:

$$\frac{\P (r.v_z.S)}{\P t} + Ñ(r.\vec{u}.v_z.S) = 0 \tag{14}$$

Now introducing flow rate in equation 14 *as F=ρ.v_z.S*:

$$\frac{\P (F)}{\P t} + Ñ(F.\vec{u}) = 0 \tag{15}$$

This is continuity equation in 3D. For, 1D equation and for liquid phase, 15 can be written as

$$\frac{\P (F_L)}{\P t} + \frac{\P}{\P z}(F_L.v_{z,L}) = 0 \tag{16}$$

Equation 16 represents continuity equation with only one phase. However, there is a phase change for all the components in CO_2 absorption process. A new factor is introduced in equation 16 to modify continuity equation and to incorporate the phase change during CO_2 absorption process.

$$\frac{\P (F_L)}{\P t} + \frac{\P}{\P z}(F_L.v_{z,L}) = source \tag{17}$$

The source term in equation 17 should have the same unit as for other terms in the equation ($kg/m^3.s$). However, phase change occurs at the interface. So, interfacial area is to be considered in calculation of source term. Similarly, how much mass of each component is transferred from liquid to gas phase per unit time. Therefore, N ($mol/m^3.s$) gives rate of change in liquid phase per unit time. The source term will also depend upon the molecular weight of the component, M and density ρ_L. Therefore, expression for source term can be given as:

$$source = \frac{v_L.S.(N.M)}{r_L} \tag{18}$$

However, there are many components in the system with different physical properties so equation 18 is modified as:

$$source = \frac{v_L.S.å(N_i.M_i)}{r_L} \tag{19}$$

Putting the value of source in equation 17:

$$\frac{\P (F_L)}{\P t} + \frac{\P}{\P z}(F_L.v_z) = \frac{v_L.S.å(N_i.M_i)}{r_L} \tag{20}$$

This is the expression for mass balance for CO_2 absorption process in liquid phase.

Mass balance for gas phase in CO_2 absorption process

Mass balance expression for gas phase is obtained from continuity and can be given by modifying equation 20 as:

$$\frac{\P\,(F_G)}{\P\,t} + \frac{\P}{\P\,z}(F_G.v_z) = \frac{v_G.S.\mathring{a}\,\left(N_i.M_i\right)}{r_G}$$

(21)

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