Australian Journal of Basic and Applied Sciences, 9(32) Special 2015, Pages: 52-58

ISSN:1991-8178

Australian Journal of Basic and Applied Sciences

Journal home page: www.ajbasweb.com

Dynamic Modelling of Carbon Dioxide For Different Solvent

Faezah Isa, Haslinda Zabiri, Pravin Chandran Sigaran

Department Chemical Engineering, Universiti Teknologi PETRONAS, 32610 Bandar Seri Iskandar, Perak, Malaysia.

ARTICLE INFO

Article history:
Received 3 August 2015
Accepted 28 October 2015
Available online 31 October 2015

Keywords:
Modeling of CO_2,
MEA, NaOH

ABSTRACT

Background: Chemical absorption is a most established technology in a CO_2 removal process and many types of solvents are available. The aim of this research is to design rate based dynamic models for different types of solvent for CO_2 absorption process. Through this project, the absorption process performance for different solvent can be determined. The models are designed for two solvents, monoethanolamine (MEA) and sodium hydroxide (NaOH) in Matlab using "shooting method" with four intervals. The developed models are validated with pilot scale experimental data from Tontiwachwuthikul *et al.* (1992). The analysis of simulation results highlights that the CO_2 absorption process more likely happens at the lower segment of the absorber. Gas phase CO_2 concentration decreases along the flow of the gas from bottom to top of absorber. The overall agreement between the simulation and experimental results are good. The developed model can be used to study the performance of different types of solvent and thereby can determine the best solvent.

To Cite This Article: Faezah Isa, Haslinda Zabiri, Pravin Chandran Sigaran, Dynamic Modelling of Carbon Dioxide For Different Solvent ***Aust. J. Basic & Appl. Sci.,*** *9(32): 52-58, 2015*

INTRODUCTION

The world population is increasing yearly, thus the demand for the energy worldwide is increasing too. The source of current energy is fossil fuels combustion power plant. These power plants which produce the energy are the main source of CO_2 emissions. Four main available technical routes to capture CO_2 from fossil fuel power plants are pre-combustion, post-combustion, chemical looping combustion and oxy-fuel (Jayarathna, Lie *et al.* 2013, Mac Dowell, Samsatli *et al.* 2013).

Natural gas is the foremost alternate source of energy with lower environmental effect. Natural gas have some pollutants such as CO_2 and H_2S, which can causes excessive environmental threats when diffuse into the atmosphere and slowed down natural gas processes. CO_2 can cause process bottle necks in the pipeline and thereby reduce the plant efficiency at a low temperature and pressure. Removal of CO_2 from natural gas will ensure good environmental performance, achieve the Liquefied Natural Gas (LNG) product conditions and prevent corrosion.

Numerous gas treating processes are available for removal of CO_2 such as absorption process and membrane separation (Coyle, Durr *et al.* 2003). Chemical CO_2 absorption process is well known in the natural gas industry and post-combustion capture (PCC) (Ebenezer and Gudmunsson 2005, Rufford, Smart *et al.* 2012, Jayarathna, Lie *et al.* 2013). The absorption process for natural gas processing and PCC are using the same concept but differ in the operating conditions since natural gas contains higher CO_2 partial pressure than the flue gas.

Both process conditions available in the natural gas processing facility and post-combustion flue gas treatment may be not same. The important differences between these applications are the CO_2 partial pressure and the quantity of CO_2 to be removed. Usually the natural gases feed are at high pressures (greater than 3000 kPa) while flue gases are normally at near atmospheric pressure. Amount of CO_2 that needed to be removed from natural gas is greater than the amount for flue gas (Rufford, Smart *et al.* 2012).

There are many types of solvents being used to perform CO_2 absorption process such as chilled methanol, propylene carbonate, dimethylether of polyethylene glycol, piperazine (PZ), ammonia, potassium carbonate and ionic liquids. MEA is the most popular solvent that used in the industry of CO_2 removal. It has been established for a long time but it has a few disadvantages, MEA is not suitable to be used above 122°C because it will face degradation and corrosion (Luo, Knudsen *et al.* 2009, Kothandaraman 2010, Zhang and Guo 2013). Each solvent will have different absorption performance depending on to the operating conditions. Many

Corresponding Author: Faezah Isa, Chemical Engineering Department, Universiti Teknologi PETRONAS, 32610 Bandar Seri Iskandar, PERAK.
Tel: +605 3687625; Fax: +605 365 6176; E-mail: faezah.isa@gmail.com

studies are conducted to invent new efficient solvents to have higher the absorption efficiency. The energy requirement and capital costs of an absorption plant are be influenced by the type of solvent. There is lack of research in developing models for different type of solvents for the CO_2 absorber.

Huge amount of natural gas reserves in Malaysia are undeveloped due to high CO_2 content. The technology for CO_2 removal process for high CO_2 content natural gas is still not well-established (Tan, Shariff *et al*. 2012). Building and operating infrastructure to evaluate the process performance is a costly scheme and time consuming proposition. Simulation and modelling software provides a low cost and time saving to evaluate the CO_2 capture performance.

However there is lack in the literature on the model development of CO_2 absorber for natural gas. There are many uncertainties in the existing literature regarding on the CO_2 absorber modelling. Valid dynamic models of CO_2 absorber needed to simulate the performance of absorber by varying the parameters without disturbing the operating absorber in the plant.

This paper therefore summarizes the modelling of different solvents CO_2 absorber which can be used for natural gas processing plant.

Methodology:

First of all the detailed researched is done on the CO_2 absorber before the scope of the project is determined. Matlab is the simulation tool used in this project since it is more efficient and suitable to develop model from the sketch. Models are developed for two solvents, MEA and NaOH since the data is available to be validated.

There are plenty of methods available to run simulation in Matlab, however the best and most efficient method has to be selected in order to give a smooth and accurate results. "Shooting method" has been used in this project because it is a best method for the iteration procedure. In this method, the four intervals were used to obtain the result. This method is used to solve two-point boundary value problems and with optimisation steps. Where the total length of the absorber column is 6.55 m, so it is divided into 4 differential elements and the discretised mass and energy balance equations were assigned for each element to solve the equations.

The model is designed in such a way that can be used for different solvent. Since different solvent has different chemical properties, some parameters values have to be modified for each type solvent. However the overall developed model is valid for different types of solvent.

2.1 Model Development:

Mechanisms of the chemical absorption process have to be clearly studied and defined for developing a complete mathematical model. Treybal (1969) and Panday (1983) (Khan, Krishnamoorthi *et al*. 2011) were the one worked earlier on developing the model for the CO_2 absorption and were used as reference to developed model in this project. Fig. 1 shows the two-film theory that used to develop the mass and energy transfer model.

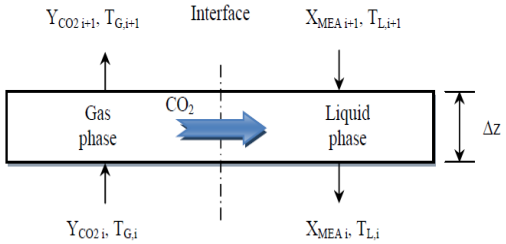

Fig. 1: Schematic two film theory

2.1.1 Material and Energy Balances:

Mass transfer rates

$$\frac{dN_{CO_2G}}{dz} = S_{CO_2} \quad (1)$$

$$N_{CO_2G_{i+1}} = N_{CO_2G_i} - S_{CO_2}\Delta z \quad (2)$$

$$N_{CO_2G} = uC_{CO_2G} = G_{air}\,Y_{CO_2} \quad (3)$$

Gas phase CO_2 concentration:

$$\frac{dC_{CO_2G}}{dz} = \frac{S_{CO_2}}{u} \quad (4)$$

$$S_{CO_2} = \frac{p_{CO_2}}{\frac{1}{k_{CO_2G}a} + \frac{H_{CO_2}}{k_{CO_2L}aE}} \quad (5)$$

Solvent concentration in the solution can be determined by:

$$X_{solvent\ i} = X_{solvent\ i+1} + \frac{(Y_{CO_2 i} + Y_{CO_2 i+1})bG_{air}}{L_{water}} \quad (6)$$

Gas phase energy balance:

$$G_{air}\, Y_{CO_2} C_{pG} \frac{dT_G}{dz} = h_G \mathrm{a}(T_G + T_L) \quad (7)$$

Liquid phase energy balance:

$$\mathrm{LC_{pL}} \frac{\mathrm{dT_L}}{\mathrm{dz}} = \mathrm{G_{air}}\, \mathrm{Y_{CO_2}}\, \mathrm{C_{pG}} \frac{\mathrm{dT_G}}{\mathrm{dz}} + \mathrm{G_{air}}\, (\mathrm{H_R} + \mathrm{H_S}) \frac{\mathrm{dY_{CO_2}}}{\mathrm{dz}} \quad (8)$$

2.1.2 Reaction Kinetics:

This is the most important and challenging part of the model development. This is because the model development for kinetics reaction will be different and vary for each solvent. Without a good understanding and detail parameters, an accurate model could not be obtained. The enhancement factor, E is one of the difficult characteristics of modeling gas absorption with chemical reaction.

$$\mathrm{E} = 1 + \frac{1}{\left[\left[\frac{1}{E_i - 1}\right]^{1.35} + \left[\frac{1}{E_1 - 1}\right]^{1.35}\right]^{1/1.35}} \quad (9)$$

$$E_i = 1 + \left[\frac{\mathrm{C}_{B,L} \mathrm{C}_D}{\mathrm{bD}_{A,L} \mathrm{C}_{A,i}}\right],\ E_1 = \left[\frac{\sqrt{\mathrm{M}}}{\tan \sqrt{\mathrm{M}}}\right] \quad (10)$$

$$M = \left[\frac{\mathrm{D}_{A,L} \mathrm{k}_2\, \mathrm{C}_{B,L}}{(\mathrm{k}_L^o)^2}\right] \quad (11)$$

$$\mathrm{D}_{CO_2,L} = \mathrm{D}_{CO_2,water} \left[\frac{\mu_{water}}{\mu_L}\right]^{0.8} \quad (12)$$

$$\mathrm{D}_{CO_2,L} = 2.35 \times 10^{-6} \left[\frac{-2119}{\mathrm{T}_L}\right]^{0.8} \quad (13)$$

$$\frac{\boldsymbol{\mu_{water}}}{\boldsymbol{\mu_L}} = \mathbf{exp}\left[\frac{(\mathbf{21.18}\boldsymbol{w}+\mathbf{2373})[\boldsymbol{\alpha}(\mathbf{0.01015}\boldsymbol{w}+\mathbf{0.0093}\boldsymbol{T}-\mathbf{2.2589})+\mathbf{1}]\boldsymbol{w}}{\mathbf{T_L}^2}\right]^{\mathbf{0.8}} \quad (14)$$

$$\mathrm{H}_{CO_2} = 10^{(5.3 - 0.035\, C_{solvent}\ - \frac{1140}{T})} \quad (15)$$

Rate constant, k_2 depends on the solvent's reaction properties. For MEA, the rate constant is second order and can be determine as shown below:

$$\log \mathrm{k}_2 = 10.99 - 2152/\mathrm{T_L} \quad (17)$$

2.1.3 Parameters:

There are many parameters used in the models that the values are taken from the literatures. The correlations are referred from the available literatures. For example the $\boldsymbol{a}.\boldsymbol{k_{CO_2 L}}$ and $\boldsymbol{k_{CO_2 L}}$ were taken from the correlations used by Onda *et al*. (1968).

RESULTS AND DISCUSSION

3.1. Model Validation:

The developed model in this project is validated with the experimental data obtained by Tontinwachwuthikul *et al*. (1992), as mention earlier. For the validation, a 6.55 m height packed absorption column with 0.1 m internal diameter was used. 12.7 mm ceramic Berl saddles were packed in the column. The operating pressure of the column is 103.15 kPa.

Fig. 2 shows the flow of the gas stream inlet and MEA solvent stream inlet conditions. NaOH solvent conditions are listed in the Table 1.

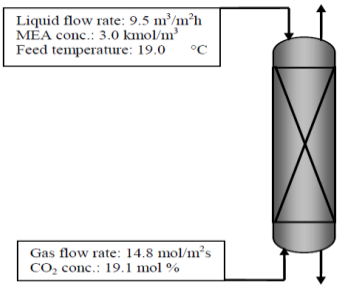

Fig. 2: Schematic of the CO_2 absorber process conditions

Table 1: NaOH solvent conditions

NaOH Inlet Stream	
NaOH feed (kmol/m^3)	2
Liquid flow rate (m^3/m^2 h)	13.5
Feed temperature (°C)	15

3.2. CO_2 Mole Fraction Profile:

Fig. 3 shows the profile of gas phase CO_2 mole fraction along the column height using MEA solvent. From the result obtained, mutual agreement had been achieved between the simulation result and the

experimental result. The mole fraction of CO_2 is slightly over-predicted around 2 to 5 meters from to bottom of column. This may be due to the minor deviations in the empirical correlations used in this project.

Fig. 4 shows the profile of gas phase CO_2 mole fraction along the column height using NaOH solvent. The simulation results shows a large deviation from experimental results due to some missing parameters of the NaOH such as heat capacity and physical liquid mass transfer coefficient of NaOH.

The CO_2 concentration in gas phase reduces along the column as the CO_2 is being continuously absorbed by the solvent. From the results, it can be concluded that the CO_2 absorption process more likely happens at the bottom of the absorber. The amount of the CO_2 being absorbed depends on the pressure of gas stream and solvent concentration and temperature.

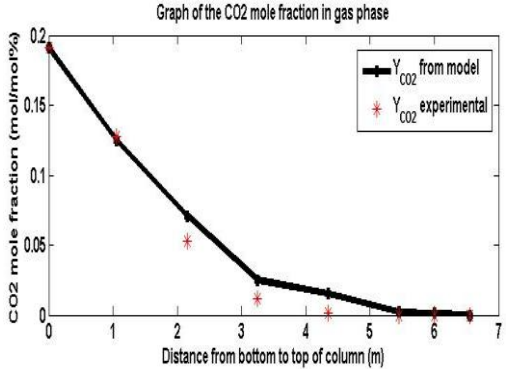

Fig. 3: Relationship between CO_2 mole fraction in gas and distance from lower segment to upper segment of column (MEA Solvent)

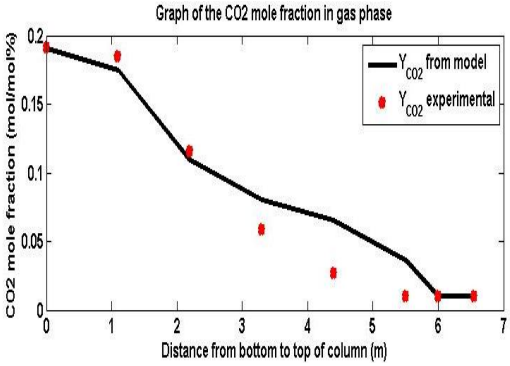

Fig. 4: Relationship between CO_2 mole fraction in gas and distance from lower segment to upper segment of column (NaOH Solvent)

3.3. Gas Temperature Profile:

Fig. 5 shows the profile of gas phase temperature across the column height using MEA solvent. Based on the graph, the agreement between the simulation results and experimental results are good.

Fig. 6 shows the profile of gas phase temperature throughout the length of the column height using NaOH solvent. The graph shows that there are discrepancies in the middle of the column. This is due to the parameter of absorption heat or reaction of NaOH-CO_2 and the heat transfer coefficient of NaOH were unable to be determined.

Based on the graphs, the temperature of inlet gas reduces along the flow from the bottom to top of absorber. This is because the heat of reaction is absorbed by the solvent solution. Thus the gas temperature profile is related and contributed to the solvent temperature profile. The results show that the enhancement factors differ significantly along the absorber. The largest changes in enhancement factors occurred at the bottom of the absorber where the chemical reaction happened vigorously.

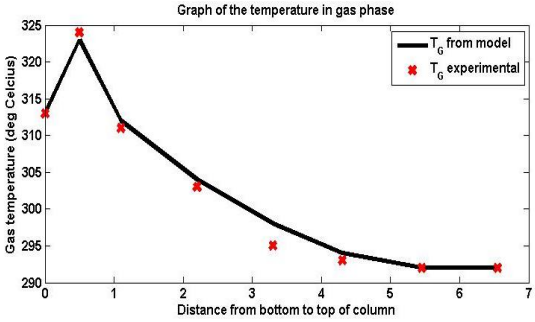

Fig. 5: Relationship between gas temperature and distance from lower segment to upper segment of column (MEA Solvent)

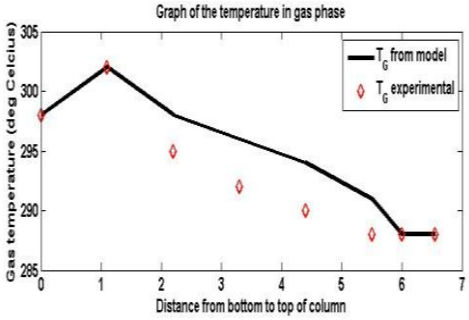

Fig. 6: Relationship between gas temperature and distance from lower segment to upper segment of column (NaOH Solvent)

3.4. Solvent Temperature Profile:

Fig. 7 shows the profile of solvent temperature throughout the length of the column height for MEA solvent. The agreement between the experimental results and simulation results are good however there are some minor variations. These variations can be reduced and eliminated by increasing the intervals in shooting method to discretize the model.

Fig. **8** shows the profile of solvent temperature throughout the length of the column height for NaOH solvent. The agreement between the simulation results and experimental results are good. The solvent temperature profile shows the temperature of solvent increases along the flow of the solvent from top of column to bottom. Since, this is exothermic reaction, the heat produced will cause the temperature increase at the lower segment of the absorber. The reaction is fairly less at top of the absorber thus the solvent temperature is almost constant or varies little. The solvent temperature profile also depend on the solubility of inlet gas

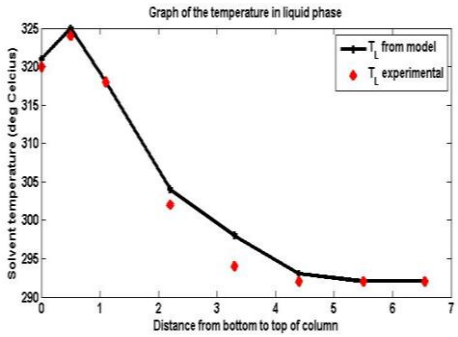

Fig. 7: Relationship between solvent temperature and distance from lower segment to upper segment of column (MEA Solvent)

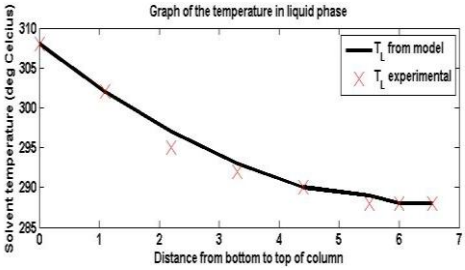

Fig. 8: Relationship between solvent temperature and distance from lower segment to upper segment of column (NaOH Solvent)

Conclusion:

From this study, mutual agreement had been found between the simulation and the pilot scale experimental data. The performance of two solvents had been successfully evaluated and compared. Specific parameters for each solvent especially the physical properties need to be thoroughly revised to emulate a better performance. Hence, this project has open up for future research on CO_2 absorption for natural gas processing plant that provides a greater challenge.

ACKNOWLEDGEMENTS

The authors would like to thank Universiti Teknologi PETRONAS for the facilities and financial support to carry out this research project

Nomenclature:

a interfacial area packing (m^2/m^3)
$\mathbf{C_{CO_2G}}$ gas phase CO_2 concentration ($kmol/m^3$)
$\mathbf{C_{pG}}$ heat capacity of gas (kJ/kmol K)
$\mathbf{C_{pL}}$ heat capacity of solution (kJ/m3 K)
$\mathbf{D_j}$ diffusivity of component j (m^2/s)
$\boldsymbol{E}$ enhancement factor
$\boldsymbol{G_{air}}$ molar flow rate of air (m^3/m^2h)
$\boldsymbol{H_{CO_2}}$ henry's law constant of CO_2 ($kmol/m^3$ kPa)
$\boldsymbol{h_G}$ heat transfer coefficient (kJ/s m^2 K)
$\mathbf{H_R}$ heat of absorption and reaction (kJ/kmol)
$\mathbf{H_S}$ heat of vaporization of solvent (kJ/kmol)
$\mathbf{k_2}$ reaction rate constant (m^3/kmol s)
$\mathbf{k_L^o}$ physical liquid mass transfer coefficient (m/s)
$\boldsymbol{k_G}$ physical gas mass transfer coefficient ($kmol/m^2$ s kPa)
L liquid flow rate, m^3/m^2 s
$\boldsymbol{N_{CO_2G}}$ molar flux of CO_2 ($kmol/m^2s$)
P total pressure, kPa
$\boldsymbol{p_{CO_2}}$ partial pressure of CO_2 (kPa)
$\boldsymbol{S_{CO_2}}$ source term representing the rate of chemical absorption of CO_2
$\mathbf{T_i}$ temperature of gas or liquid (K)
u gas velocity in the z direction along the column height (m/s)
w percentage of mass of solvent present in the solution
X Concentration of solvent ($kmol/m^3$)
$\boldsymbol{Y_{CO_2}}$ mole ratio of CO_2 in the gas phase
z distance from lower segment of packing to upper segment (m)
$\boldsymbol{\alpha}$ CO_2 loading
B Reagent in the liquid

REFERENCES

Coyle, D., *et al*., 2003. LNG: a proven stranded gas monetization option. SPE Annual Technical Conference and Exhibition, Society of Petroleum Engineers.

Ebenezer, S.A. and J. Gudmunsson, 2005. "Removal of carbon dioxide from natural gas for LNG production." carbon dioxide removal processes 21(11).

Jayarathna, S.A., *et al*., 2013. "Amine based CO2 capture plant: Dynamic modeling and simulations." International Journal of Greenhouse Gas Control., 14: 282-290.

Jayarathna, S.A., *et al*., 2013. "Dynamic modelling of the absorber of a post-combustion CO2 capture plant: Modelling and simulations." Computers & Chemical Engineering, 53: 178-189.

Khan, F., *et al*., 2011. "Modelling reactive absorption of CO 2 in packed columns for post-combustion carbon capture applications." Chemical Engineering Research and Design, 89(9): 1600-1608.

Kothandaraman, A., 2010. Carbon dioxide capture by chemical absorption: a solvent comparison study, Citeseer.

Luo, X., *et al*., 2009. "Comparison and validation of simulation codes against sixteen sets of data from four different pilot plants." Energy Procedia, 1(1): 1249-1256.

Mac Dowell, N., *et al*., 2013. "Dynamic modelling and analysis of an amine-based post-combustion CO2 capture absorption column." International Journal of Greenhouse Gas Control., 12: 247-258.

Rufford, T., *et al*., 2012. "The removal of CO 2 and N 2 from natural gas: a review of conventional and emerging process technologies." Journal of Petroleum Science and Engineering, 94: 123-154.

Tan, L.S., *et al*., 2012. "Factors affecting CO2 absorption efficiency in packed column: A review."

Journal of Industrial and Engineering Chemistry, 18(6): 1874-1883.

Zhang, M. and Y. Guo, 2013. "Rate based modeling of absorption and regeneration for CO2 capture by aqueous ammonia solution." Applied Energy, 111: 142-152.