Sustainability and Social Impact

Modeling of CO_2 Absorption with K_2CO_3 Diethanolamine-Piperazine Compound Using Packed Column Method

Dode Bara Septyano, Riska Dwi Sundari, Yuni Kurniati

Submitted: 20 Agustus 2023
Accepted: 24 Agustus 2023
Published: 06 Januari 2024

Keywords: Absorption, Diethanolamine, Piperazine, CO2, Packed Column

ABSTRACT

In recent years, interest in the development of carbon dioxide (CO_2) removal technology has increased due to the impact on global warming and climate change, which is mainly due to the large amount of CO_2 emissions generated from various natural activities and human activities that are leached directly into the atmosphere. Common methods often used in the chemical industry to separate CO_2 gas from process gases include absorption using chemical solvents by using a pakced column method. This study aims to obtain data on CO_2 loading and CO_2 removal in K2CO$_3$-H_2O solution with DEA-PZ promotor, and to determine the effect of concentration and temperature variables on CO_2 loading and CO_2 removal using modelling. This research was conducted with a variable temperature of 40°C-60°C, a concentration of 30% K_2CO_3, 1-3% DEA and 0.75% PZ using a packed column in atmospheric pressure. The results of the data validation obtained have an average % error of 7-12% based on previous research. The parameters obtained are the optimal temperature at 55°C and CO_2 loading and CO_2 removal increases along with the increase in the concentration of DEA-PZ promoter The effect of the PZ promoter as an additional solution has an important role in increasing the effectiveness of absorption.

INTRODUCTION

In recent years, interest in the development of carbon dioxide (CO_2) removal technology has increased due to CO_2 emissions. Reducing CO_2 emissions released into the air is an effective way to slow climate change[1]. This is one of the challenges to be able to develop and utilize renewable energy sources which are expected to reduce CO_2 emissions that are discharged directly into the atmosphere.

According to the United Nations Environment Program (UNEP), it shows that the concentration of CO_2 in the air increased by about 1% per year from 35 ppmv (part per million by volume) in 1990, and recently increased to 380 ppmv, in the next 100 years. The concentration of CO_2 in the atmosphere will increase up to two times compared to the beginning of the industrial era, which is around 580 ppm. It is predicted that the concentration of CO_2 gas will continue to increase to above 750 ppmv until 2100 if there is no effort to overcome the losses caused by CO_2 gas, so it is considered that an increase in CO_2 gas levels in the air causes climate change which results in an increase in sea water temperature and changes in extreme weather[2].

Research on the absorption of CO_2 gas with monoethanolamine (MEA) has been carried out[3] which shows that the higher the MEA concentration causes the KGa price to increase and the interfacial area of the unit packing volume also increases. Mass

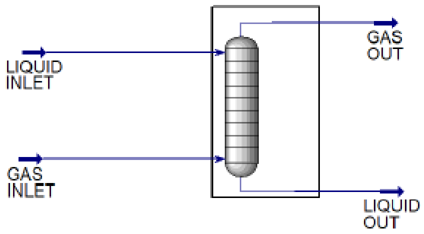

Figure 1. Packed Column Tool

transfer analysis is accompanied by a chemical reaction on CO_2 absorption with potassium carbonate solution in a packed column[4]. This research has theoretically predicted the performance of a packed column for the absorption of CO_2 gas into a K_2CO_3 solution in a packed column by taking into account the effect of heat. The results showed that increasing the absorbent flow rate from 3 to 7 liters/minute could still increase the percent removal of CO_2. Likewise, increasing the level of K_2CO_3 in the incoming absorbent from 1 to 1.5 M is still effective in increasing the percent removal of CO_2. From the predicted temperature profile in this study, it shows that the heat effect does not really affect the simulation results.

In subsequent research, Ganapathy et al.[5] studied the mass transfer of DEA and CO_2/Nitrogen (N_2) solutions and investigated the effect of CO_2 concentration on the volumetric mass transfer coefficient and the efficiency of CO_2 absorption. When the DEA concentration is low, the CO_2 concentration in the gas mixture has a more significant effect on mass transfer. Furthermore, Ganapathy et al.[6] utilized DEA solutions to absorb CO_2 from N_2 or CO_2 mixtures and investigated the effect of the inner diameter of the channel and the concentration of diethanolamine on specific surface area and mass transfer coefficients. The results show that decreasing the inner diameter of the duct can significantly increase the specific surface area and volumetric mass transfer coefficient, and the volumetric mass transfer coefficient increases with increasing solute concentration. Research conducted by Zhang et al.[7] conducted research on the absorption of CO_2 gas in MDEA solution by adding Piperazine (PZ) and DEA. The results of this study indicate the activation effect of each mixture of both DEA, PZ, and PZ + DEA in the CO_2 absorption process is generated from the variation of CO_2 rates, transport of PZ and DEA to MDEA, and regeneration rates of PZ and DEA.

The absorption of CO_2 gas using a packed column with K_2CO_3 DEA compounds still requires a promoter that functions to improve the quality of CO_2 absorption, so further research is needed, to obtain beneficial absorption of CO_2 gas due to the effectiveness and speed of its high absorption rate and low operating costs by knowing the parameters which can affect the amount of CO_2 absorption in the solution. From the existing problems, an overview is given about the variables that can affect the absorption of CO_2 gas in the K_2CO_3-H_2O compound with the addition of a DEA-PZ (Diethanolamine-Piperazine) solution promoter using the packed column method. Promoters such as piperazines, amines, arsenious acids, amine derivatives, carbonate hydrases, boric acid and amino acids have all been suggested to improve reaction kinetics. This is because amino acids have the same functional groups as amines, so they have the same reactivity to CO_2. In addition, amino acids have high resistance to oxidative degradation and low toxicity and volatility[8].

Table 1. Data variables used in simulation.

Data Variables			
% wt DEA	% wt H_2O	Pressure (kPa)	Temperature (°C)
1	98,25	10	40
2	97,25	13	50
3	96,25	16	60

EXPERIMENTAL

This experimental modeling was carried out using process simulation. The tool used in the simulation is 1 absorber. In the absorber column, CO_2 gas will enter through the bottom column (gas inlet), meanwhile, the DEA solvent will enter through the upper column (liquid inlet). Sweet gas, which is the output product from the absorber column, will come out through the top of the column (gas out) and the rich amine solution that has absorbed CO_2 gas will come out through the bottom of the absorber column (liquid out). The variables observed in this experiment, namely CO_2 loading and% CO_2 removal in the sweet gas flow.

The simulation stage begins by inputting data regarding the list of components contained in the reactants and in the product, then continued by selecting the modeling or equation that will be used in the simulation, entering the reactions that occur in the absorber column. Followed by adding one absorber column unit to the simulator and equipped with the mass flow of input and output. Then, it was continued by entering the composition data, the operating conditions of the absorber column, and also the independent variables in the form of 1-3%wt DEA concentration, 0.75% PZ concentration and 40-60˚C solution inlet temperature (temperature range 100˚C)

Table 2. Column specifications and operating conditions used in simulation.

Description	Operating Condition
Column Diameter	24 mm
Packed Height	1.40 m
CO_2 Gas Concentration	99.99%
Gas Flow Rate	48.2 $m^3/(m^2.h)$
Flow Rate Of Solution	10 $m^3/(m^2. h)$
K_2CO_3 Concentration	30 %wt
DEA Concentration	1-3 %wt
PZ Concentration	0.75 %wt
Feed Temperature	40-60 ºC
Pressure	1 atm
Packing Type	⌀3 × 3 Dixon ring

Table 3.Data validation on concentrations with CO_2 loading

Simulation Result (This Study)		
K_2CO_3 Concentratio n(%wt)	DEA-PZ Concentration (%wt)	CO_2 *Loading* (mol CO_2/mol amine)
30	(1)+(0.75)	0.0327
30	(2)+(0.75)	0.0479
30	(3)+(0.75)	0.0659
Journal Results		
K_2CO_3 Concentration (%wt)	CO_2 *loading*	% Error
30	0.0394	17.005
30	0.0492	2.642
30	0.0599	10.017
% Average Error		9.888

used in each of these. each stream. After all the related operating data is inputted into the simulator, it is followed by running with the data that has been inputted so that an equilibrium curve is obtained. The next stage is the interpretation and drawing of conclusions from the selected variables so that the CO_2 absorption process can run optimally. The conclusion of the research results is based on the research results obtained and the data analysis that has been carried out. From various variables, the best variable value is taken so as to produce the optimal absorption rate and low CO_2 concentration in the output gas.

RESULTS & DISCUSSION

Research studies on CO_2 absorption use several parameters to analyze the results of the CO_2 loading and CO_2 removal values. The parameters used were the concentration of amine and promoter, temperature and partial pressure of CO_2. These parameters will be analyzed based on the influence of each variable in the packed column using DEA solution and PZ promoter. In this case the simulation used application of using a calculation or fluid package acid gas which is specific to the amine gas treating process. In this discussion, the variable data used and the column specifications used are listed in Table 1 and Table 2.

Data Validation

The results of the data obtained from the simulation results are compared with data from references in related journals so that the desired data validation is obtained. Data validation used on temperature variables, the concentration of the main solution with the addition of a promoter compared to CO_2 loading and CO_2 removal. In Table 3. This is the data validation from the comparison of the simulation results with the results of previous studies. In this study, there was the addition of a promoter in the form of PZ as much as 0.75% wt so that the CO_2 loading results were different from previous studies. This difference can be seen in the% error which varies considerably from the range of variables used. This% error can be taken an average of 9.888%. In Table 4, it is a validation of temperature data with CO_2 removal which shows an average% error of 7.504 with a temperature variable of 40-60˚C adjusted to previous research. In this case the concentrations used in the validation of temperature data with CO_2 removal were K_2CO_3 30%, DEA 3%, PZ 0.75%. In Table 5. It can be seen that the PZ solution as an additional promoter also affects% removal compared to previous studies with an average% error of 12.408. In this condition, the temperature taken in the concentration data validation is 60˚C according to the simulation results and previous research. The results of this data validation can be classi fi ed that the% error seen is quite small so that it is still relevant in its application.

Effect of Amine Concentrations on CO_2 Loading

The CO_2 loading parameter is used to determine the appropriate loading i.e. the molar ratio of CO_2 gas absorbed compared to the moles of amine solvent (α) in the absorption column design. Low CO_2 loading results in a column with low absorption efficiency, while high loading results in excessive solvent

Table 4.Data validation at several temperatures with CO_2 removal

Simulation Result (This Study)		
Concentration (%wt)	Temperature (°C)	CO_2 Removal
K_2CO_3 (30), DEA (3) + PZ(0.75)	40	8.912
	50	18.403
	60	20.873
Journal Results		% Error
Temperature (°C)	CO_2 Removal	
40	9.322	4.398
50	17.09	7.683
60	23.304	10.432
% Average Error		7.504

Table 5.Data validation on several concentrations with CO_2 removal

Simulation Result (This Study)		
K_2CO_3 Concentration (%wt)	DEA-PZ Concentration (%wt)	CO_2 *Removal*
30	(1)+(0.75)	8.313
30	(2)+(0.75)	16.871
30	(3)+(0.75)	25.585
Journal Results		% Error
K_2CO_3 Concentration (%wt)	CO_2 *Removal*	
30	6.995	18.842
30	15.536	8.593
30	23.304	9.788
% Average Error		12.08

requirements and operating costs[9]. The reaction between amines and CO_2 is an exothermic reaction which will produce reaction heat[10]. The CO_2 loading value increases when the amine concentration increases because the DEA concentration contributes to increased diffusivity and higher mass transfer because there are more DEA molecules in the potassium carbonate, this results in more CO_2 absorption and increases CO_2 to contact and react with absorbents. The concentration of DEA in a solution of potassium carbonate (K_2CO_3) causes the CO_2 to be absorbed even more[11]. The mole ratio of CO_2 absorbed to amines (CO_2 loading) will increase when the amine concentration increases[12]. Based on the data from the analysis results in several journals, the graph shown in Figure 2 shows that the concentration of the DEA solution affects the amount of CO_2 loading in the CO_2 absorption process using the composition of the K_2CO_3 solution (30% wt) and the help of the DEA-PZ promoter (1-3 and 0.5% wt). The amount of CO_2 loading will increase with the increase in amine concentration and CO_2 removal. It can be seen that the addition of piperazine compounds is quite influential in increasing CO_2 loading so that the suitability of the mixed promoter solvent is proven to be effective.

Effect of Amine Concentration on CO_2 Removal

The addition of the amine concentration in the amine absorbent solution can affect the percent CO_2 removal. It can be seen in Figure 3. From this figure shows that the greater the amine concentration used, the higher the percent CO_2 removal with the DEA-PZ promoter range (1-3 and 0.75% wt). This shows the effect of the additional promoter mixture on potassium carbonate compounds having an impact on the% removal of CO_2. The chemical reaction between CO_2 and the solvent increases at higher concentrations due to the large number of amine molecules that can react with CO_2 in the gas phase. the increase in the amount of active amine in the liquid solution (amine) available to diffuse towards the gas-liquid interface and react with the dissociated CO_2. This condition has led to a higher chemical reaction increase factor (E) and reduced mass transfer resistance in the liquid phase[13].

Effect of Temperature on CO_2 Removal

In the CO_2 absorption process, an increase in temperature will affect the rate of amine reaction, gas solubility factor, gas-liquid diffusivity and amine concentration. The higher the temperature, the higher % CO_2 removal. Based on Figure 4, it can be seen that increasing the solvent can increase the% removal of CO_2 gas. This is because with increasing temperature there is an increase in the rate of reaction, so that the more CO_2 gas reacts with the solvent which results in an increase in the% removal of CO_2 gas. This result is positively correlated with the literature that an increase in liquid temperature above 60˚C begins to form a sloping graph showing the efficiency of CO_2 removal and KGav value due to the dominance of reversible reactions when the temperature is raised to 60°C. If the temperature is higher than 60°C, the mass transfer rate along the gas-liquid interface will decrease the vapor-liquid balance in the system. Increasing the temperature will facilitate the reaction rate and reduce the viscosity of the system, which is beneficial for the mass transfer process and maximum

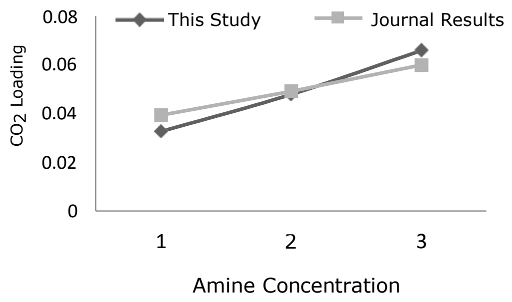

Figure 2. Effect of amine concentrations on CO_2 loading

CO_2 absorption. However, if an increase in excess temperature will decrease the solubility of the gas, which causes a decrease in the driving force, mass transfer of the gas phase. So that% CO_2 removal at a temperature of 55°C is considered the optimal condition for the CO2 absorption process[13].

CONCLUSSION

The influence on each variable has a role and function that is mutually sustainable and increases the efficiency of certain results. It is also seen that the PZ solution shows compatibility with the DEA solution which has succeeded in increasing the performance of the K2CO3 solution so that the addition of the promoter has a function in acceleration the CO2 absorption process so that it finds the effective conditions for each variable.

AUTHORS INFORMATION

First and Corresponding Author

Dode Bara Septyano – Department of Chemical Engineering, Universitas Internasional Semen Indonesia, Kompleks PT Semen Indonesia (Persero) Tbk, Gresik, Indonesia 61122
Email: dodebs01@gmail.com

Co-Authors

Riska Dwi Sundari – Department of Chemical Engineering, Universitas Internasional Semen Indonesia, Kompleks PT Semen Indonesia (Persero) Tbk, Gresik, Indonesia 61122

Yuni Kurniati – Department of Chemical Engineering, Universitas Internasional Semen Indonesia, Kompleks PT Semen Indonesia (Persero) Tbk, Gresik, Indonesia 61122
Email: yuni.kurniati@uisi.ac.id

ACKNOWLEDMENT

The author would like to thank LPPM UISI which has support facilities at the university.

REFERENCES

[1] Supitcha Rinprasertmeechai, Sumaeth Chavadej, Pramoch Rangsunvigit, S. Kulprathipanja, **2012**, DOI 10.5281/ZENODO.1332828.

[2] Juliananda, Bambang Ismuyanto, *Teknik Perlakuan Limbah Gas Hasil Bakar Industri/ Penulis, Juliananda, Bambang Ismuyanto*, UB Press, **2017**.

[3] Endang Srihari, Ricky Priambodo, Sylvia Purnomo, Hermawan Sutanto, Wentalia Widjajanti, *Jurusan Teknik Kimia* **n.d.**, *6*, 26.

[4] A. Altway, S. Susianto, K. Kuswandi, K. Kusnaryo, *JTKI* **2018**, *7*, 817.

[5] H. Ganapathy, A. Shooshtari, S. Dessiatoun, M. Alshehhi, M. Ohadi, *Applied Energy* **2014**, *119*, 43.

[6] H. Ganapathy, A. Shooshtari, S. Dessiatoun, M. M. Ohadi, M. Alshehhi, *Chemical Engineering Journal* **2015**, *266*, 258.

[7] X. Zhang, Y. Yang, C. Zhang, J. Wang, *Chinese Journal Chemical Engineering* **n.d.**, *11*, 408.

[8] H. Thee, N. J. Nicholas, K. H. Smith, G. Da Silva, S. E. Kentish, G. W. Stevens, *International Journal of Greenhouse Gas Control* **2014**, *20*, 212.

[9] Ross Edward Dugas, Carbon Dioxide Absorption, Desorption, and Diffusion in Aqueous Piperazine and Monoethanolamine, Dissertation, The University of Texas at Austin, **2009**.

[10] B. Xu, H. Gao, X. Luo, H. Liao, Z. Liang, *International Journal of Greenhouse Gas Control* **2016**, *51*, 11.

[11] J. Monde, T. Widjaja, A. Altway, *MATEC Web Conf.* **2018**, *156*, 02002.

[12] S.-J. Han, J.-H. Wee, *J. Chem. Eng. Data* **2017**, *62*, 1570.

[13] H. N. A. Halim, A. M. Shariff, M. A. Bustam, *Separation and Purification Technology* **2015**, *152*, 87.

AUTHOR CONTRIBUTIONS

Dode Bara Septyano: Conception or design of the work. Riska Dwi Sundari: Drafting the article, Data collection. Yuni Kurniati: Writing- Reviewing and Editing,

COMPETING INTERESTS

Authors have no competing interest to declare.

DATA AVAILABILITY

Data available upon request to the corresponding author.