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Modeling and Analysis

GREENHOUSE GASES SCIENCE AND TECHNOLOGY

Performance study on mixed solvent for post-combustion carbon capture using rotating packed bed technology

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Abstract: Modeling of CO_2 removal in a rotating packed bed using a mixed amine solution of piperazine and methyldiethanolamine with various molar concentration ratios was done with Aspen Plus® and dynamically linked with Intel® Visual Fortran. In addition to the mass and energy balances, all the necessary correlations for the rotating packed bed were written in Intel® Visual Fortran. The developed model was validated, and the result showed good agreement with a percentage error of less than 10%. The model was scaled-up to absorb CO_2 from the flue gas composition of a typical 6.4 MWe biomass power plant with the goal of producing net negative CO_2 emissions. The effect of process parameters such as temperature, rotation speed, liquid-gas ratio, methyl diethanolamine concentration, and piperazine concentration on capture efficiency and regeneration energy was investigated. It was discovered that increasing the rotational speed results in an improvement in the separation efficiency. Increasing the temperature of the lean solvent causes a decrease in separation efficiency, which is due to a decrease in solubility as the temperature increases. Increasing the liquid-to-gas ratio leads to an increase in CO_2 absorption efficiency because more hydroxide ions are present to react with the CO_2. Piperazine is a reactive compound and increasing its concentration in the mixed solvent leads to an increase in CO_2 absorption efficiency. Finally, the results of the study demonstrated that a solvent mixture consisting of piperazine and methyldiethanolamine has the potential to be utilized in post-combustion CO_2 capture using rotating packed bed technology. © 2024 Society of Chemical Industry and John Wiley & Sons, Ltd.

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Keywords: post-combustion carbon capture; methyldiethanolamine; piperazine; rotating packed bed; process intensification

Introduction

At a global level, efforts are being made to reduce greenhouse gas emissions in many different industries and countries. Studies have shown that the use of renewable energy sources, such as wind energy, can make a significant contribution to reducing CO_2 emissions in the transport and industrial sectors.[1] In addition, it is worth noting that developing countries such as Brazil, China, and India have unintentionally mitigated the increase in their emissions by adopting strategies to increase industrial efficiency, diversify energy sources, and address local environmental concerns.[2] According to the International Energy Agency, despite these obvious efforts, carbon dioxide emissions are gradually increasing until they reached an all-time high in the year 2022.[3] Carbon capture and storage is believed to be one of the options that has the potential of mitigating the emission of CO_2 by almost 20%.[4] Pre-combustion, oxy-fuel combustion, post-combustion, and direct air capture are the technological possibilities for CO_2 capture. The most mature technological option is post-combustion CO_2 capture (PCC) via chemical absorption with amines, since it has already reached industrial implementation. Despite PCC's advancement to industrial scale, its capital and operating costs are too high for global acceptance by the business community for commercial implementation.

The use of monoethanolamine (MEA) for carbon dioxide capture is undergoing change with more effective solvents due to its corrosive nature, toxicity, and high heat of reaction with CO_2 which consequently needs substantial amount of energy for solvent regeneration.[5] Methyldiethanolamine (MDEA) has several advantageous characteristics in comparison to MEA, including a reduced energy requirement (lower heat of reaction with CO_2), enhanced absorption capacity, and higher thermal stability. However, it should be noted that MDEA does exhibit a slower reaction rate.[6] The concentrated solution of piperazine (PZ) has the potential to increase the reaction rate, but it has some limitations, including limited solubility in water and higher volatility compared to MEA.[7] PZ is a solvent containing diamine molecules, where one of the amine groups interacts rapidly with carbon dioxide, leading to the formation of carbamate. At the same time, the other amine group readily absorbs the proton formed during this process. As a result, researchers have become interested in the potential of PZ as a promoter to enhance the CO_2 absorption rate in solutions containing carbonate and tertiary amines. According to Liu *et al.*,[8] it is advisable to use a solvent that has an increased absorption capacity and a fast reaction rate in rotating packed bed (RPB) because its residence time is 10% shorter than that of the conventional column.

Process intensification using rotating packed bed has been reported by many researchers to have the potential of reducing both capital and operating costs.[9–13] Joel *et al.*'s [11,14] studies showed that there is significant size reduction of about 12 times and 9.63 times for the absorber and stripper compared to conventional columns, respectively. This indicates a decrease in the capital cost of the columns.

In this research, a rotating packed bed absorber and stripper were used to absorb CO_2 from a typical 6.4 MWe biomass power plant using a mixed solvent of PZ and MDEA to obtain an ideal chemical solvent that has high reactivity to CO_2, low heat of reaction with CO_2, low circulation rate, high thermal and chemical degradation resistance, and low cost. The performance of the intensified PCC process was studied by looking at the effect of process parameters on CO_2 capture efficiency and regeneration energy.

Model development

Currently, there is no readily available model for an RPB absorber/stripper in any of the publicly accessible model libraries. To facilitate the simulation of an intensified absorber/stripper using the rate-based model in Aspen Plus®, existing mass/heat transfer correlations which were affected by centrifugal force were replaced with customized subroutines coded using Intel® Visual FORTRAN.

In our study, we considered several correlations, including the liquid-phase mass transfer coefficient proposed by Chen *et al.*,[15] the gas-phase mass transfer coefficient suggested by Chen,[16] the estimated interfacial correlation provided by Luo *et al.*,[17] and the liquid-hold-up correlation presented by Burns *et al.*[18]

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To account for the combined effects of drag and centrifugal forces, gas-solid sliding, and radial acceleration, we incorporated the dry pressure drop expression proposed by Llerena-Chavez & Larachi.[19]

Gas and liquid phase material balances

According to Eqns (1) and (2), the material balances in the RPB were defined for both the gas and the liquid phase under the assumption of steady state. A numerical discretization in the radial direction was used to create the equations for the mass balances. This was done considering the flow pattern in the RPB. In addition, the tangential area was denoted by the term $2\pi rH$, which changes radially from section to section.

Material balances for gas phase[20]:

$$0 = \frac{1}{2\pi rH}\frac{\delta\left(G^m y_i\right)}{\delta r} - aN_i \quad (1)$$

Material balances for liquid phase[20]:

$$0 = -\frac{1}{2\pi rH}\frac{\delta\left(L^m x_i\right)}{\delta r} + aN_i + \in_L rxn_i \quad (2)$$

The molar fluxes at the interfaces (aNi), the derivative terms across each radial segment per tangential area and liquid phase reaction rate ($\in_L rxn_i$) represent the component molar flow balances. With this assumption, the reactions only take place in the liquid film, and for this purpose the ionic components only exist in the liquid phase.

Gas and liquid phase energy balances

Kang *et al.*[20] correlations were used to calculate energy balances for gas and liquid phase which were given by Eqns (3) and (4), respectively.

Gas phase energy balances:

$$0 = \frac{1}{2\pi rH}\frac{\delta\left(G^m h_G\right)}{\delta r} - ah_{\frac{g}{l}}\left(T_l - T_g\right) - Q_G^{\text{loss}} \quad (3)$$

Liquid phase energy balances:

$$0 = -\frac{1}{2\pi rH}\frac{\delta\left(L^m h_L\right)}{\delta r} - a\left(h_{\frac{g}{l}}\left(T_l - T_g\right) - \Delta H_r N_{CO_2} - \Delta H_{\text{vap}} N_{\text{H}_2\text{o}}\right) - Q_l^{\text{loss}} \quad (4)$$

The term $h_{g/l}(T_l - T_g)$ represents interfacial heat transfer, $\Delta H_r N_{\text{CO}_2}$ for the heat released by CO_2 desorption from the loaded MEA solvent. The heat emitted and absorbed by the condensation or evaporation of H_2O is represented by the term ($\Delta H_{\text{vap}} N_{\text{H}_2\text{o}}$). The heat loss due to relative temperature difference between the stripper temperature and ambient condition were represented by the terms (Q_l^{loss} and Q_G^{loss}).

Thermodynamic and kinetic models

The use of the electrolyte non-random two-liquid (ElecNRTL) activity coefficient model in the Aspen Plus® software results in a more accurate calculation of the vapor–liquid equilibrium, chemical equilibrium, and physical properties of the system. Calculating the standard change in Gibbs free energy, equilibrium constants for reactions 5 through 9 were found, assuming that the equilibrium reactions occur within the liquid layer. The equations and values used to describe the kinetic processes were from AspenTech.[21]

$$2H_2O \leftrightarrow H_3O^+ + OH^- \quad (5)$$

$$HCO_3^- + H_2O \leftrightarrow CO_3^{2-} + H_3O^+ \quad (6)$$

$$PZH^+ + H_2O \leftrightarrow PZ + H_3O^+ \quad (7)$$

$$HPZCOO + H_2O \leftrightarrow PZCOO^- + H_3O^+ \quad (8)$$

$$MDEAH^+ + H_2O \leftrightarrow MDEA + H_3O^+ \quad (9)$$

$$CO_2 + OH^- \rightarrow HCO_3^- \quad (10)$$

$$HCO_3^- \rightarrow CO_2 + OH^- \quad (11)$$

$$PZ + CO_2 + H_2O \rightarrow PZCOO^- + H_3O^+ \quad (12)$$

$$PZCOO^- + H_3O^+ \rightarrow PZ + CO_2 + H_2O \quad (13)$$

$$PZCOO^- + CO_2 + H_2O \rightarrow PZ(COO^-)_2 + H_3O^+ \quad (14)$$

$$PZ(COO^-)_2 + H_3O^+ \rightarrow PZCOO^- + CO_2 + H_2O \quad (15)$$

$$MDEA + CO_2 + H_2O \rightarrow MDEAH^+ + HCO_3^- \quad (16)$$

$$MDEAH^+ + HCO_3^- \rightarrow MDEA + CO_2 + H_2O \quad (17)$$

The power law expressions used for the rate-controlled reactions (10 – 17) are shown in Eqn (18). The kinetic parameters for the reactions in equations 10 – 17 are listed in Table 1.

$$r_j = k_j^o\, exp\left(-\frac{E_j}{R_c}\left[\frac{1}{T} - \frac{1}{298.15}\right]\right)\prod_{i=1}^{N} a_i^{\alpha_{ij}} \quad (18)$$

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Table 1. Kinetic parameters of CO_2 absorption by PZ-MDEA-H_2O.[21]

Reaction No.	k_j^o	E_j, kJ/mol
10	1.33 e^{+17}	55.4709
11	6.63 e^{+16}	107.4165
12	1.7 e^{+10}	1.3356
13	3.4 e^{+23}	59.2851
14	1.04 e^{+14}	33.6548
15	3.20 e^{+20}	36.3917
16	6.85 e^{+10}	37.8026
17	6.22 e^{+17}	92.6581

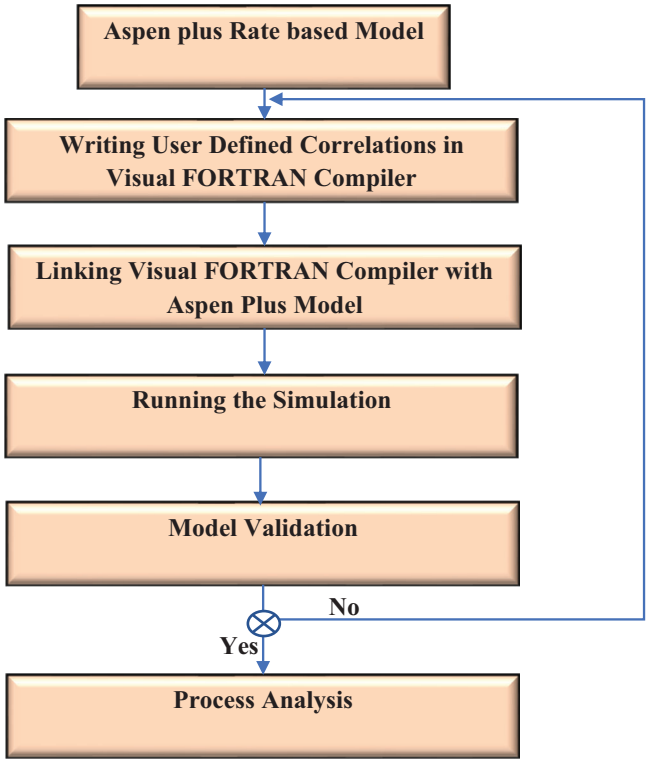


Figure 1. Modeling implementation procedure.[11]

The process of carbon capture with RPB was modeled and validated using experimental data. Aspen Plus® and Intel® Visual Fortran software was used to develop the model for RPB, and the step-by-step procedure used is shown in Fig. 1.

Transport properties

Transport properties were calculated using transport property correlations as summarized in Table 2.

Table 2. Some of the models in Aspen plus® that were used for transport properties

Property	Gas phase	Liquid phase
Density	COSTALD model by Hankinson and Thomson	Clarke density model
Viscosity	Chapman–Enskog model with Wilke approximation	Jones–Dole model
Surface Tension	Not applicable	Onsager–Samaras model
Thermal conductivity	Stiel–Thodos model with Wassiljewa–Mason–Saxena mixing rule	Reidel model
Binary diffusivity	Chapman–Enskog Wilke–Lee model	Nernst–Hartley model

Mass and heat transfer correlations suitable for rotating packed beds

Appropriate mass correlations for RPB were used to calculate the liquid and gas phase mass transfer coefficient, the effective interfacial area, pressure drop and the liquid holdup. A summary of the correlations can be found in Table 3.

Aspen Plus® model

The post-combustion carbon capture model for a 6.4 MWe power plant using the input conditions developed in Aspen Plus® is shown in Fig. 2.

Model validation

The experimental data for model validation were taken from Zhan *et al.*[22] The input parameters for model validation are listed in Table 4.

The validation of the RPB absorber model with a PZ+MDEA mixture as solvent was done based on CO_2 capture efficiency. Equation 19 was used to calculate the absorption efficiency, while Eqn 20 was used to determine the percentage error. Figure 3 shows that the percentage error in capture efficiency is less than 10% when using the input conditions in Table 4. The model was applied to a typical 6.4 MWe power plant, and then a process analysis was performed to evaluate the impact of some process variables on the performance of the RPB model, as the prediction error of the model

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Table 3. Sets of correlations for mass transfer calculations

Model	References
Liquid phase mass transfer coefficient $\frac{k_L a d_p}{D_L a_t}(1-0.93\frac{V_o}{V_i}-1.13\frac{V_i}{V_t}) = 0.35 Sc_L^{0.5} Re_L^{0.17} Gr_L^{0.3} We_L^{0.3} (\frac{a_t}{a_p'})^{-0.5} (\frac{\sigma_c}{\sigma_w})^{0.14}$	15
Gas phase mass transfer coefficient $\frac{k_G a}{D_G a_t^2}(1-0.9\frac{V_o}{V_t}) = 0.023 Re_G^{1.13} Re_L^{0.14} Gr_G^{0.31} We_L^{0.07} (\frac{a_t}{a_p})^{1.4}$	16
Liquid holdup $\in_L = 0.039(\frac{g_c}{g_o})^{-0.5}(\frac{U}{U_o})^{0.6}(\frac{\nu_L}{\nu_o})^{0.22}$ where, $g_o = 100\ m\ s^{-2},\ U_o = 1\ cm\ s^{-1},\ \nu_o = 1\ cS = 10^{-6}\ m^2\ s^{-1}$ $U = \frac{Q_L}{2\pi r H}$	18
Effective interfacial area $\frac{a}{a_t} = 66510 Re_L^{-1.41} Fr_L^{-0.12} We_L^{1.21} \varphi^{-0.74}$	17
Dry pressure drop expression $\Delta P_{RPB} = \frac{150(1-\varepsilon)^2\mu}{d^2\varepsilon^3}(\frac{G}{2\pi H})\ln\frac{r_o}{r_i} + \frac{1.75(1-\varepsilon)\rho}{d\varepsilon^3}(\frac{G}{2\pi H})^2(\frac{1}{r_i}-\frac{1}{r_o}) + \frac{1}{2}\rho\omega^2(r_o^2-r_i^2) + F_c$ where, $F_c = \varepsilon(a - G + (b+\omega^c)G^2)$ a, b, and c are fitting parameters given as: $a = -0.08\ m^3/s\ b = 2000(rpm)^c\ c = 1.22$	19

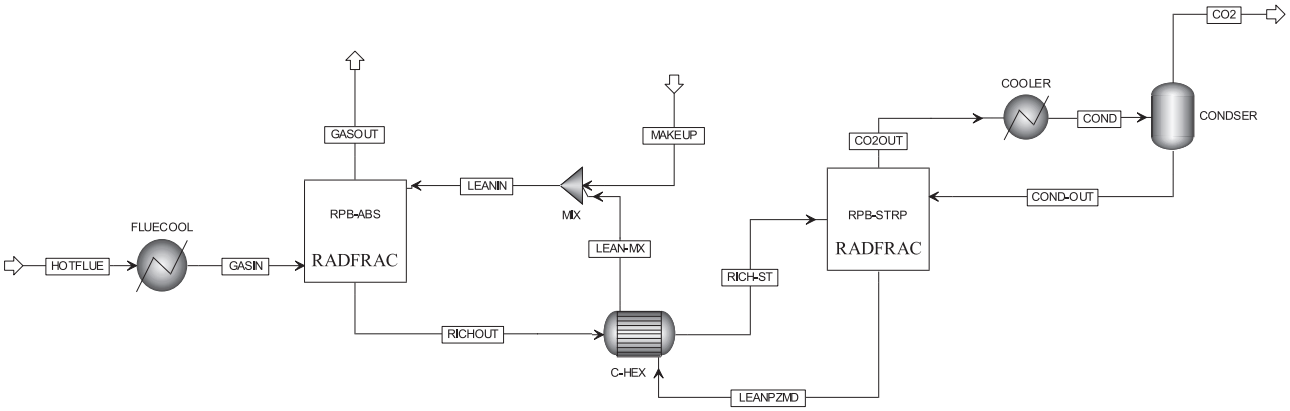


Figure 2. Aspen Plus® model of post-combustion carbon capture for a 6.4 Mwe power plant.

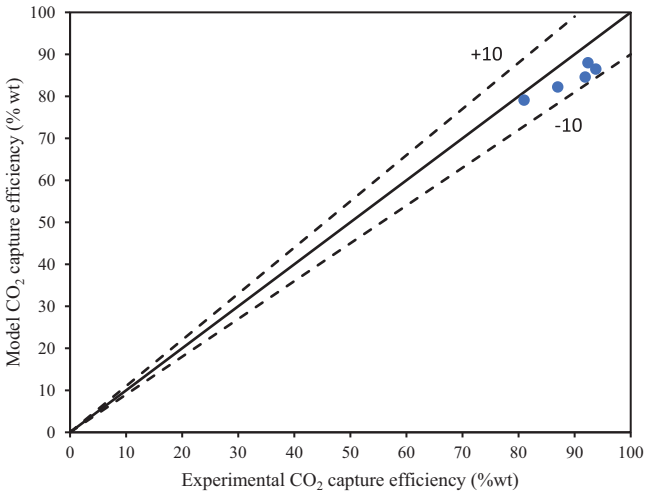


Figure 3. Parity plot on CO_2 capture efficiency.

is good.

$$\text{Capture efficiency} = \left(\frac{\text{kg } CO_2 \text{ in flue gas} - \text{kg}CO_2 \text{ in outlet gas}}{\text{kg } CO_2 \text{ in flue gas}}\right) \times 100 \quad (19)$$

$$\%\ \text{Error} = \left(\frac{\text{Experimental data} - \text{Validated data}}{\text{Experimental data}}\right) \times 100 \quad (20)$$

Results and discussion

The model was able to predict the experimental result with percentage error of less than 10%. Therefore, the

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Table 4. Input specification for model validation.[25]

Parameter	Value
packing type	stainless wire mesh
surface area per unit volume of the packing ($m^2 \cdot m^{-3}$)	1,533
inner radius of the packing, r_{in} (m)	0.025
outer radius of the packing, r_{out} (m)	0.075
axial height of the packing, H (m)	0.053
packing volume, VP (m^3)	8.33×10^{-3}
voidage of packing	0.904
inlet CO_2 concentration, yin, CO_2 (%, v/v)	30
inlet N_2 concentration, yin, N_2 (%, v/v)	70
temperature, T (K)	302.95–318.15
high gravity factor, β	40.0–160.0
MDEA concentration, CMDEA ($mol \cdot L^{-1}$)	0.84–2.94
PZ concentration, CPZ ($mol \cdot L^{-1}$)	0.12–0.58
gas volumetric flow rate, G ($m^3 \cdot h^{-1}$)	2
liquid volumetric flow rate, L ($L \cdot h^{-1}$)	12.6–47.6

Table 5. Flue gas composition and parameters

Parameters	Value
Power generation (MWe)	6.4
Volumetric flowrate (m^3/sec)	10
Temperature (°C)	216
Gas Composition (% mole)	
CO_2	16.3
O_2	6.4
N_2	63
H_2O	14.3
Stripper distillate rate (kg/s)	3.6
Stripper reflux ratio (mass)	1.2

model is then scaled-up to treat flue gas composition (Table 5) from typical 6.4 MWe power plant.

Model scale-up

The strategy used for the scale-up of the 6.4 MWe power plant involves knowing the feed conditions (flow rate, composition, temperature, and pressure) of the flue gas and then calculate the require solvent flow rate that can capture 90% of CO_2 from the flue gas, while ensuring that no flooding occurs. The basic dimensions of the RPB that is scale-up include the inner radius, the outer radius, and the axial width.

The ratio of liquid to gas (L/G) is a very important factor in determining the solvent recirculation rate. When the volumetric flow rate of a gas is increased, the volume of lean solvent must be increased to maximize CO_2 capture and minimize energy consumption in the reboiler. An approach proposed by Agbonghae *et al.*[22] was used to determine the required lean solvent flow rate (Eqn 21).

$$F_{\text{Lean}} = \frac{F_{FG} x_{CO_2} \varphi_{CO_2}}{100 z \left(\alpha_{\text{Rich}} - \alpha_{\text{Lean}}\right)} \times \left[\frac{M_{\text{Amine}}}{44.009}\left(1 + \frac{1 - \omega_{\text{Amine}}}{\omega_{\text{Amine}}}\right) + z\alpha_{\text{Lean}}\right] \quad (21)$$

The inner radius of the RPB must be chosen according to the feed conditions to avoid flooding. Although there are other approaches to determining the diameter or radius of the RPB, in this paper, an approach from Agarwal *et al.*,[23] was adopted, with which the radius of the RPB was determined directly according to Eqn (22). The width of an RPB directly depends on the superficial gas velocity near the flooding point, so there is a need to calculate the superficial gas velocity to obtain the RPB width. A suitable correlation to determine the superficial gas velocity is given by Wallis[24] as described in Eqn (23). The width of a rotating packed bed can therefore be determined using Eqn (24). Agarwal *et al.*[23] suggested that the outer radius of the RPB can be determined by the correlation described in Eqn (25).

$$r_i = \left(\frac{G}{\pi v_{jet}\left(1 - f_d\right)}\right)^{1/2}\left(\frac{\rho_G p}{\rho_L}\right)^{1/4} \quad (22)$$

$$U_G = \left[\frac{\beta N_g^a a_p^b \mu^c (\rho_L - \rho_G)^{0.25}}{\left\{\rho_G^{0.5} + \lambda\left(\frac{L}{\alpha G}\right)^{0.5}\rho_L^{0.5}\right\}}\right]^2 \quad (23)$$

For a low viscous liquid ($\beta = 130$, $a = 0.43$, $b = -0.93$, $\lambda = 1.51$, and $\alpha = 1$).

$$H = \frac{G}{2\pi r_i U_G} \quad (24)$$

$$G\, d_y = K_G^a \left(y^* - y\right) 2\pi r H d_r \quad (25)$$

The power plant has a boiler efficiency of 64.2% using bagasse as a fuel and generates 6.4 MW. In the initial phase, the power plant is operated with black oil, and as soon as the plant is stable, the oil is gradually replaced by sugarcane bagasse, so that the power plant can be

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Table 6. Scale-up results

Parameters	Absorber	Stripper
Capture efficiency (wt%)	90	
Lean solvent flow (kg/s)	84	
Rich solvent flow (kg/s)		87.19
Inner diameter (m)	1.15	1.01
Outer diameter (m)	3.0	2.3
Axial height (m)	0.53	0.35

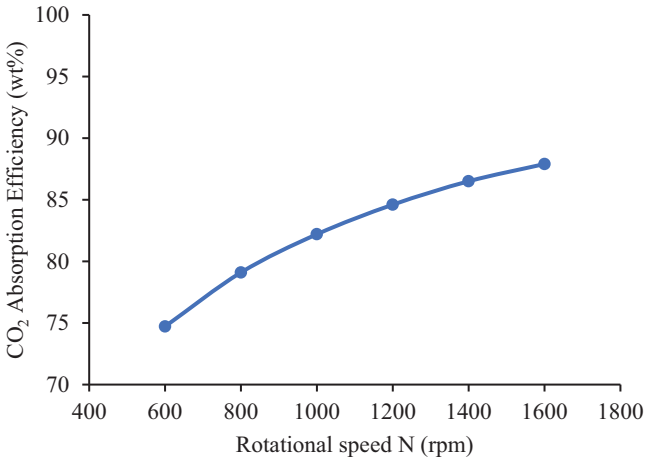


Figure 4. Rotational speed against CO_2 absorption efficiency. Reaction conditions: CPZ = 5wt% CMDEA = 30 wt%, P = 101.325 kN/m^2, T = 313 K.

operated with both non-renewable and renewable fuels. The scale-up of the model to the power plant capacity was carried out based on the validated model. After careful scale-up calculations and determining the dimensions of the RPB geometry, it is then simulated in Aspen plus® and visual Fortran according to the input conditions listed in Table 5. Table 6 shows the scale-up results calculated based on capture efficiency of 90%. The scale-up calculated for the RPB geometry and the results found from the Aspen plus® model agrees with the assumed 90% CO_2 capture efficiency.

Effect of rotational speed on absorption efficiency

Figure 4 shows the change in CO_2 absorption efficiency as a function of rotational speed in the range from 600 to 1,600 rpm with a step size of 200 rpm and a concentration of PZ and MDEA of 5 and 30 wt.%, respectively, at a gas and liquid temperature of 313.15 K. Increasing the speed from 600 to 1,600 rpm resulted in an increase in CO_2 removal efficiency from 74% to

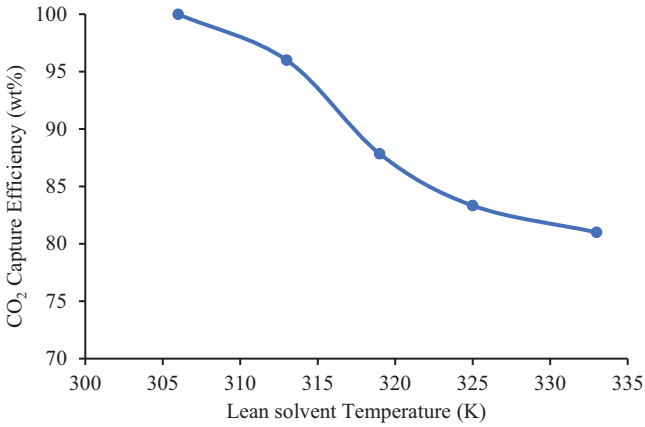


Figure 5. Effect of lean solvent temperature on CO_2 absorption efficiency. Reaction conditions: CPZ = 5wt% CMDEA = 30 wt%, P = 101.325 kN/m^2.

88%. Increasing the rotational speed causes shear and centrifugal forces to be generated by the rotation of the packing materials and the solvent in the RPB. This leads to better dispersion of the liquid and smaller droplet size, which in turn leads to a larger gas-liquid effective interfacial area and a reduction in mass transfer resistance due to the formation of a thin film that favors the absorption of carbon dioxide. The renewal rate of the liquid surface also increases when the rotation speed is increased, which in turn improves the mass transfer between gas and liquid. This study is consistent with Joel *et al.*,[10] who use MEA as the solvent for CO_2 absorption. This study is necessary because at higher rotor speed we expect higher energy would be needed for the rotation, therefore it is necessary to understand the relationship the rotor speed has with capture efficiency in order to minimize energy wastage.

Effect of lean solvent temperature on CO_2 capture efficiency

Lean solvent from the stripper needs to be cooled before it can be used in the absorber for CO_2 capture. Therefore, it is necessary to know the cooling temperature limit for the process to avoid the need for additional cooling units, which inevitably increase the capital and operating costs for CO_2 capture, hence the need for this study.

Figure 5 shows that the capture efficiency is highest at a lower temperature (305 K), but a lean solvent temperature of higher than 313 K requires additional cooling, resulting in an increase in capital and operating costs. When the temperature increases from

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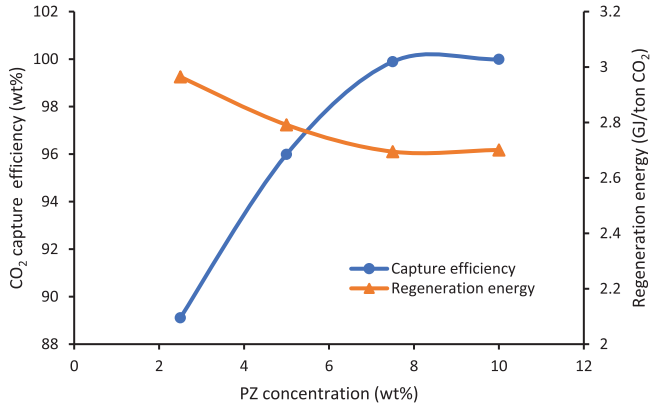


Figure 6. Effect of PZ concentration on CO_2 absorption efficiency. Reaction conditions: CPZ = 2.5 – 10 wt% CMDEA = 25 wt%, P = 101.325 kN/m^2, T = 313 K.

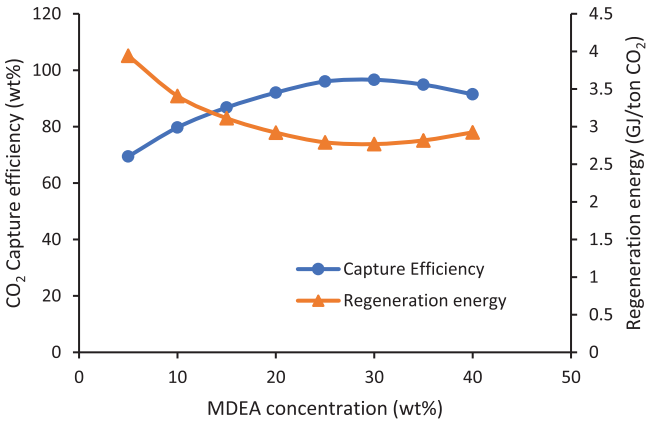


Figure 7. Effect of MDEA concentration on CO_2 absorption efficiency. Reaction conditions: CPZ = 5wt% CMDEA = 5 – 40wt%, P = 101.325 kN/m^2, T = 313 K.

306 to 333 K, capture efficiency drops from 99.99 to 81.00%. The decrease in capture efficiency is due to the temperature bulge that occurs in the column since the reaction between the CO_2 and solvent is exothermic, therefore higher temperature leads to a decrease in CO_2 capture efficiency. According to the findings of Zhan *et al.*,[25] an increase in temperature leads to a reduction in gas solubility and thus a decrease in the driving force for mass transfer on the gas side.

Effect of PZ concentration on CO_2 capture efficiency

According to the data presented in Fig. 6, it can be observed that increasing the concentration of PZ from 2.5 to 10 wt.% while maintaining a constant concentration of MDEA leads to an enhancement in capture efficiency, with values rising from 89.11% to 99.99%. The observed effect can be ascribed to the structural properties of PZ, which is a cyclic symmetric diamine possessing two amino groups. Each mole of PZ exhibits the theoretical capability to remove two moles of CO_2 and promotes the efficient generation of carbamates. According to Saidi and Inaloo,[26] the inclusion of two nitrogen groups in the molecule contributes to an increased capacity for CO_2 loading during the absorption process.

Nevertheless, it is important to emphasize that Fig. 6 shows no significant increase in capture efficiency beyond a PZ concentration of 7.5 wt%. This is because capture efficiency is close to 100%, which means that a further increase in PZ concentration will only result in a small increase in capture efficiency. Although the augmentation of PZ concentration presents benefits in terms of improved removal efficiency, it is accompanied by the disadvantage of high solvent volatility and higher solvent expenses. Therefore, it is imperative to determine the maximum solvent mixing ratio that can produce optimal separation efficiency while simultaneously minimizing solvent volatility and cost.

Furthermore, it can be seen in Fig. 6 that the specific energy required for regeneration tends to decrease with increasing PZ concentration. This phenomenon can be attributed to the continuous increase in the amount of CO_2 captured as the PZ concentration is increased. Svensson *et al.*[27] reported that MDEA has a lower heat of absorption compared to PZ. Consequently, when the PZ concentration is at 10 wt%, the energy requirement for regeneration increases.

Effect of MDEA concentration on CO_2 capture efficiency and regeneration energy

Figure 7 shows the effect of MDEA on CO_2 capture efficiency gradually increases with an increase in MDEA concentration from 5 to 30 wt.% and started decreasing as the result of low reactivity with CO_2 beyond 30 wt.%. This shows that higher MDEA concentration at a particular solvent ratio reduces the absorption efficiency. Similar studies were done by Zhan *et al.*[25] who reported that CO_2 first increased and then decreased with the increase of MDEA concentration because MDEA concentration has a significant effect on CO_2 absorption efficiency. The reason for the decrease in CO_2 capture efficiency as MDEA concentration increases is because MDEA is

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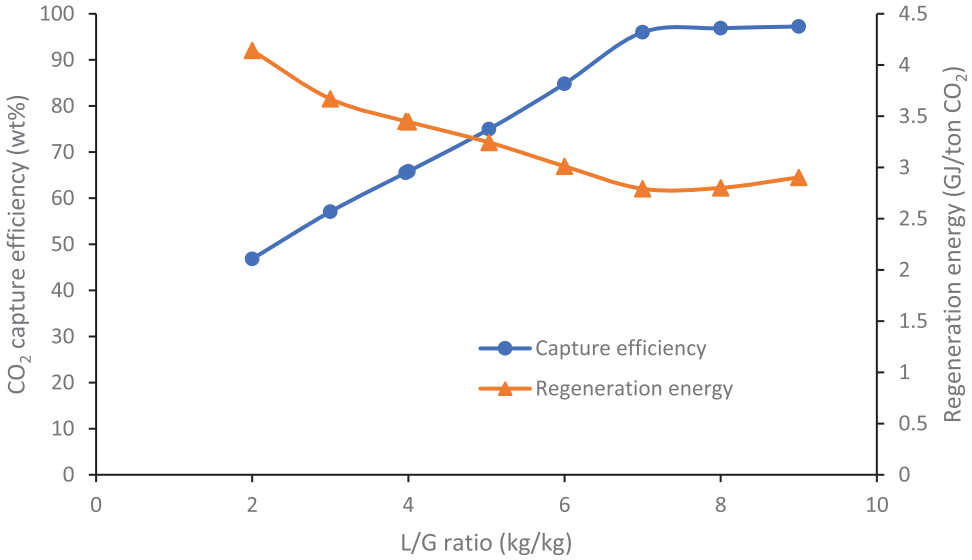


Figure 8. Effect of liquid-to-gas ratio on reboiler duty reaction conditions: CPZ = 5wt% CMDEA = 25 wt%, P = 101.325 kN/m^2, T = 313 K.

less reactive than PZ and then the reactivity of the solvent is now dominated by a less reactive solvent.

The data presented in Figure 7 show a negative correlation between the concentration of MDEA and the regeneration energy. The observed behavior can be attributed to the increased concentration of the solvent, which consequently enhances the capture of CO_2. This in turn leads to a decrease in the energy required for regeneration, as the heat of absorption is found to be quite low, as described in Svensson *et al.*[27] The trend changes when the MDEA concentration exceeds 30 wt%. This can be attributed to the high energy demand in the reboiler as the solvent becomes more viscous and the separation efficiency does not show significant improvement.

Effect of L/G ratio on capture efficiency and regeneration energy

The analysis of the liquid-to-gas (L/G) ratio becomes imperative when aiming to enhance capture rates in the absorber while minimizing the energy required for regeneration in the stripper. Figure 8 shows significant increase in CO_2 capture efficiency when the L/G ratio rises from 3 to 7 kg/kg. Nevertheless, it becomes apparent that above an L/G ratio of 7 kg/kg, there is no significant improvement in the efficiency of CO_2 absorption. This shows that the amount of solvent is already adequate to capture the bulk of carbon dioxide found in the exhaust gas. Hence, it is improbable that a higher L/G ratio will generate additional advantages in terms of CO_2 absorption within the absorber. Conversely, it could potentially lead to an adverse increase in energy requirement in the reboiler. This discovery is consistent with the study conducted by Joel *et al.*[28] using PZ solvent, which also demonstrated a positive relationship between L/G ratios and enhanced CO_2 removal efficiency. The observed trend correlation can be ascribed to the increased accessibility of solvent to capture CO_2.

The rate at which the solvent is recycled is an important parameter that influences the decision regarding the operating costs of a capture plant. A high liquid-to-gas ratio means that a significant amount of the solvent is regenerated in the reboiler, resulting in increased energy requirements for solvent regeneration. In addition, a reduction in the L/G ratio is expected to result in a lower CO_2 recovery rate in the absorber. Therefore, it is important to understand the impact of the L/G ratio on the operating efficiency of the capture system. Figure 8 shows that an increase in L/G ratio results in a corresponding decrease in regeneration energy (GJ/ton CO_2) for L/G ratios between 2 and 7 kg/kg, as the benefit of increased CO_2 capture is greater than the corresponding increase in reboiler duty, resulting in a decrease in specific regeneration energy. However, at L/G ratios higher than 7 kg/kg, the regeneration energy was found to increase, which is due to a decrease in CO_2 capture efficiency and an increase in the reboiler duty. The contribution of regeneration energy is mainly due to

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the heat of water evaporation and the sensible heat of the solution. According to Chakma,[29] the heat of vaporization of aqueous amine solutions depends on the water concentration, and since the water concentration does not change with increasing L/G ratio, the sensible heat of solution is the main factor for the increase in the regeneration energy with increasing L/G ratio, as confirmed by Nwaoha *et al.*[30]

Conclusion

The RPB absorber and stripper model was developed using Aspen Plus® and Intel® visual FORTRAN, and the model was validated based on capture efficiency with a percent error of less than 10%. The validated model was then scaled-up to treat the flue gas composition of a 6.4 MWe power plant. The effect of temperature on CO_2 capture efficiency was investigated and it was found that the capture efficiency decreased at higher temperatures which is attributed to phenomena known as temperature budge. Rotational speed, solvent recirculation rate (L/G ratio), and PZ concentration significantly increase CO_2 absorption efficiency, while higher MDEA concentration above 30 wt.% in the mixed solvent shows no improvement in absorption efficiency. An L/G ratio higher than 7 kg/kg does not result in a significant increase in CO_2 absorption efficiency but leads to higher reboiler energy requirements and thus higher capital and operating costs. Finally, the study shows that PZ can be used successfully as a promoter to enhance the capture performance.

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