MODELING AND SIMULATION OF POST-COMBUSTION CO₂ CAPTURE PROCESS FOR 6.4 MWE BAGASSE FUELED POWER PLANT

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Abstract

The emission of carbon dioxide, a greenhouse gas, contributes to the phenomenon of climate change; the largest source of carbon dioxide emissions are fossil fuel power plants. Post-combustion carbon capture (PCC) technology, which is based on solvents, is currently the most advanced technology for reducing carbon dioxide emissions from power plants. The Post-combustion Process, which uses conventional solvents, has a number of disadvantages, including high energy consumption for regeneration, solvent losses, corrosion of equipment, thermal instability, and environmental impact. Ionic liquids (ILs) and IL-based solvents have produced a novel method of CO₂ capture that is highly efficient, economical, and environmentally friendly. A rate-based steady-state model of the PCC process using the ionic liquid 1-hexyl-3-methylimidazolium glycine ([Hmim] [Gly]) was investigated using Aspen Plus®. In Aspen Plus® Electrolyte NRTL method and RK equation of state are used to compute liquid and vapor properties. From the process analysis carried out, it was found that the height and diameter of the absorber packing, the liquid-to-gas ratio and the solvent and flue gas temperatures have a positive effect on the CO₂ capture efficiency. The result showed a maximum CO₂ capture efficiency of 92% at a packed height of 12m and diameter of 0.9m. The best capture efficiency of 98.82% was achieved at an L/G ratio of 4.0. The process simulation study examined five key parameters for ([Hmim] [Gly]) solvent which may reduce the energy and cost required for CO₂ capture. The results show that aqueous ([Hmim] [Gly]) is a promising absorbent for CO₂ capture. Offering a pathway towards more sustainable and efficient carbon capture technologies. This study contributes to the advancement of carbon capture technologies and underscores their significance in mitigating climate change impacts.

Keywords: post-combustion CO₂ capture, chemical absorption, 1-hexyl-3-methylimidazolium glycine, Ionic liquid

1.0 Introduction

Forecasts indicate that fossil energy sources will remain the backbone of power generation worldwide in the coming decades (Reichl et al., 2014). As of now, fossil fuels are still used to generate most of the world’s electricity. In 2019, fossil fuels were responsible for 65.3% of global electricity production (IEA, 2021). Fossil fuel power plants are the major source of greenhouse gas (Wang et al., 2011).

CO₂ is the main greenhouse gas (GHG) and its emissions have been directly linked to global warming (Yew et al., 2022). A study undertaken in Europe reported that global warming would lead to a significant increase in cold weather moisture levels of up to 15% by the mid-2030s and 25% by the middle of this century. The average CO₂ concentration rose to approximately 414 ppm CO₂ as of October 2021, which is an increment of approximately 47.86 % as compared to the
pre-industrial era of 280 ppm (Chai et al., 2022). Based on NASA’s Goddard Institute for Space Studies, it has been found that the land-ocean temperature index has increased from −0.16°C in the year 1880 to 1.02°C in 2020. Carbon capture and storage (CCS) represents an option for the mitigation of CO₂ caused by fossil fuel use. CCS consists of the separation of CO₂ from industrial sources, transportation of CO₂ to a storage location, and long-term isolation of CO₂ from the atmosphere. Three technological pathways can be used for CO₂ capture from coal-derived power generation: oxy-combustion, pre-combustion, and postcombustion capture (Wang et al., 2011).

Post-combustion carbon capture is the suitable choice in the near-to middle-term, since it can be retrofitted to the existing power plants compared to the other two approaches. In the post-combustion capture, the separation of CO₂ from flue gas derived from combustion fossil fuels is carried out using amine solvents then the absorbed CO₂ is liberated from the solvent and is compressed for transportation and storage (Akadiri et al., 2019; Arroyave et al., 2020). Post-combustion CO₂ capture can be divided into three categories: biological, physical, and chemical methods. As to the biological method, CO₂ is fixed by photosynthesis of plants, algae, and photosynthetic bacteria without energy consumption. The drawback of this method is low absorption capacity and its efficiency (Wu et al., 2014). The physical method contains physical absorption, cryogenic condensation, and membrane separation technology (Wu et al., 2014). Compared with the biological method, the physical method has higher CO₂ absorption efficiency, but the cost of absorbent is higher because of some special requirement (Wu et al., 2014). As to chemical method, CO₂ is removed from power plant flue gas by reacting with chemical absorbents. The chemical method includes chemical adsorption, absorption, and chemical looping combustion. By comparison, the chemical absorption method has a lot of obvious advantages, high efficiency, mature technology, and low cost. CO₂ scrubbing or absorption is the most predominantly proposed post-combustion capture (PCC) process, since it is the most developed process of all CCS options that has been used for decades for applications, such as in the chemical industry.

Ionic liquids (ILs) were well-known a few years ago as a possible substitute for conventional solvents in the industrial chemical processes because of their special qualities (Kaur et al., 2022; Greer et al., 2020). The great degree of property tunability exhibited by ILs, which could be achieved by varying the structural characteristics of anions, cations, and/or their substituents, was another noteworthy aspect that set them apart (Silva et al., 2021). Owing to their low vapor pressure, excellent thermal stability, and diverse composition, ionic liquids have emerged as efficient absorbents for the chemical conversion of CO₂ (Kanjilal et al., 2023).

Guo et al. (2013) conducted an experimental study using a double stirred cell absorber with a smooth gas-liquid interface and compared the CO₂ absorption rates for different solvents of [Hmim] [Gly], MEA, DEA and AMP solution absorbers. The result showed that [Hmim] [Gly] had the highest absorption rate. This study deals with the process modelling of post-combustion CO₂ capture in a 6.4 MWe biomass power plant (sugarcane bagasse). The process analysis of CO₂ capture from flue gas streams using [Hmim] [Gly] liquid was performed for both absorber and stripper performance.
2.0 Methodology
2.1 Model Development
The absorber and stripper model were developed using RADFRAC model in Aspen Plus®. RADFRAC supports a rate-based approach for mass transfer modeling. The rate-based method assumes equilibrium only at the vapor-liquid interface and considers reaction kinetics and film reaction in the calculation of the rate of mass transfer between the phases. The rate-based model includes detailed mass transfer calculations based on the two-film theory.
The following assumptions were made during the model development (Akinola et al., 2019).
• Steady-state model
• Negligible heat loss to the surroundings
• N₂ and hydrocarbon not readily soluble in IL
• Chemical reactions are completed in liquid film only.

2.2 Physical Properties
The electrolyte NRTL method and RK equation of state are used to compute liquid and vapor properties respectively H₂, CO₂, N₂, O₂ and CO are treated as Henry-components to which Henry’s law is applied and the Henry’s constants are retrieved from Aspen Plus databanks for these components with water in the reaction’s calculations, the activity coefficient basis for the Henry’s components was chosen to be Aqueous. Therefore, in calculating the unsymmetrical activity coefficients (GAMUS) of the solutes, the infinite dilution activity coefficients were calculated based on infinite-dilution condition in pure water.

2.3 Critical Properties.
The critical parameters of the ionic liquids were computed utilizing the modified Lydersen Joback-Reid group contribution method as elaborated in Table 1.

Table 1: shows the critical parameters of the ionic liquid.

<table>
<thead>
<tr>
<th>M</th>
<th>Tb</th>
<th>Tc</th>
<th>Pc</th>
<th>Vc</th>
<th>Zc</th>
<th>Ω</th>
</tr>
</thead>
<tbody>
<tr>
<td>g.mol⁻¹</td>
<td>K</td>
<td>K</td>
<td>Mpa</td>
<td>cm³.kmol⁻¹</td>
<td></td>
<td></td>
</tr>
<tr>
<td>242.34</td>
<td>710.3</td>
<td>906</td>
<td>2.08693e+06</td>
<td>0.7603</td>
<td>0.211</td>
<td>1.108</td>
</tr>
</tbody>
</table>

2.4 Kinetic Models
The kinetics of CO₂ absorption into the aqueous ionic liquid was the fast pseudo-first order reaction regime. The reaction kinetics can be well described using the zwitterion mechanism proposed originally by (Caplow, 1968) and later reintroduced by (Danckwerts, 1979) according to the zwitterion mechanism the equilibrium reactions in the liquid phase were suggested as follows:
\[ \text{NH}_2^- + \text{CH}_2 - \text{COO}^- \text{R}^+ + \text{CO}_2 \longrightarrow \text{OOC}^- \text{NH}_2^+ + \text{CH}_2 - \text{COO}^- \text{R}^+ \]  ... R1
\[ \text{NH}_2^+ + \text{CH}_2 - \text{COO}^+ \text{R}^- + \text{B}_1 \longrightarrow \text{OOCHN}^- \text{CH}_2 - \text{COO}^- \text{R}^+ + \text{B}_1 \text{H}^+ \]  ... R2
\[ \text{OOCHN}^- \text{CH}_2 - \text{COO}^- \text{R}^+ + \text{H}_2 \text{O} \longrightarrow \text{NH}_2^- \text{CH}_2 - \text{COO}^- \text{R}^+ + \text{HCO}_3^- \]  ... R3
\[ \text{NH}_3^+ + \text{CH}_2 - \text{COOR}^- \longrightarrow \text{NH}_2^- \text{CH}_2 - \text{COO}^- \text{R}^+ + \text{H}^+ \]  ... R4
\[ \text{H}_2 \text{O} \longrightarrow \text{H}^+ + \text{OH}^- \]  ... R5
\[ \text{HCO}_3^- \longrightarrow \text{H}^+ + \text{CO}_3^{2-} \]  ... R6
\[ \text{CO}_2 + \text{H}_2 \text{O} \longrightarrow \text{H}^+ + \text{HCO}_3^{2-} \]  ... R7
CO$_2$ reacted with the [Hmim] [Gly] through the formation of zwitterion, subsequently deprotonated by a base present in solution, where B might be [Hmim] [Gly], H$_2$O, and OH$^-$. 

5 Transport properties models

The transport properties are essential as they are part of the correlations used to calculate the mass transfer, heat transfer and liquid holdup in the RadFrac model. The transport properties are calculated using models within the ElecNRTL property method as shown Table 2.

<table>
<thead>
<tr>
<th>Properties</th>
<th>Viscosity</th>
<th>Molar volume</th>
<th>surface tension</th>
<th>thermal conductivity</th>
<th>binary diffusivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>Jones-Dole electrolyte correction model</td>
<td>Clarke model, Onsager-Samaras model</td>
<td>Riedel electrolyte correction model</td>
<td>Nernst-Hartley model</td>
<td></td>
</tr>
</tbody>
</table>

2.6 Simulation flowsheet

The pilot plant unit has been simulated using the flowsheet shown in Figure 1, utilizing Aspen Plus. The sizing and specifications used in the process simulation are detailed in Table 3.

Figure 1. Rate-Based ([Him] [Gly]) simulation flow sheet.
Table 3: Sizing and specification for the Absorber, heater, Pump, and the Stripper

<table>
<thead>
<tr>
<th>Unit Operation</th>
<th>Specification</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Absorber</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Column height</td>
<td>6</td>
<td>m</td>
</tr>
<tr>
<td>Top stage Pressure</td>
<td>1</td>
<td>atm</td>
</tr>
<tr>
<td>Packing Type</td>
<td>Sulzer BX</td>
<td></td>
</tr>
<tr>
<td>Packing dimension</td>
<td>STANDARD</td>
<td></td>
</tr>
<tr>
<td>Packing Material</td>
<td>STANDARD</td>
<td></td>
</tr>
<tr>
<td>Number of stages</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td><strong>Heater</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temperature approach</td>
<td>120</td>
<td>°C</td>
</tr>
<tr>
<td>Hot side pressure drops</td>
<td>1</td>
<td>atm</td>
</tr>
<tr>
<td><strong>Pump</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pressure Increase</td>
<td>2</td>
<td>atm</td>
</tr>
<tr>
<td><strong>Stripper</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Condenser</td>
<td>Partial vapour</td>
<td></td>
</tr>
<tr>
<td>Top stage pressure</td>
<td>3</td>
<td>atm</td>
</tr>
<tr>
<td>Column height</td>
<td>6</td>
<td>m</td>
</tr>
<tr>
<td>Packing Type</td>
<td>Sulzer BX</td>
<td></td>
</tr>
<tr>
<td>Packing dimension</td>
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</tr>
<tr>
<td>Packing material</td>
<td>STANDARD</td>
<td></td>
</tr>
</tbody>
</table>

3.0 Results and Discussions
3.1 Process simulation results
The CO$_2$ capture efficiency and other key factors of the absorption process are discussed. The CO$_2$ removal efficiency of the PCC facility in this paper is defined as follows:

\[
\text{CO}_2\% = \frac{Q_{L_{\text{in}}} - Q_{L_{\text{out}}}}{Q_{L_{\text{in}}}} \quad \ldots 1
\]
Where $Q_{in}$ mole flows in the flue gas entering the absorber and $Q_{out}$ moles flow of CO$_2$ exiting the absorber in the depleted or treated gas.

### 3.2 Effect of the absorber packed height on the CO$_2$ capture efficiency
The absorber packed height varied between 8 m and 12 m with diameter from 0.5 m to 0.9 m. Capture efficiency increases with increase in packing height and diameter. The Reason is the solution contact area is increasing with the increase of packing height and diameter. Therefore, residence time for reacting system is increased as the capture efficiency increased. Figure 1 showed the 3-D plot of capture efficiency as a function of absorber-packed height and diameter, the results showed a maximum CO$_2$ capture efficiency of 92% at the packed height of 12 m and Diameter of 0.9 m. The same observation was also demonstrated by Basha et al., (2013).

![Figure 2](image.png)

**Figure 2.** Effect of the absorber packed height and diameter on the CO$_2$ capture efficiency

### 3.1.2 Effect of the liquid-to-gas (L/G) ratio on the CO$_2$ capture efficiency
Solvent recirculation rate is an important parameter in decision making regarding the operating cost of a PCC process plant. A high L/G ratio means a large amount of solvent regenerated in the reboiler, resulting in high reboiler duty. Also, if the L/G ratio is too low, we expect a lower CO$_2$ recovery rate in the absorber. Therefore, it is necessary to know the impact of the L/G ratio on the system performance of the PCC process. The L/G ratio varied from 1.52 to 4.00 as shown in Figure 3. The CO$_2$ capture efficiency
increases with the increase in the L/G ratio. This is due to the increase in CO\textsubscript{2} absorption rate in the absorber as high superficial velocity enhances mass transfer. At higher L/G ratio, more CO\textsubscript{2} is absorbed by the ([Hmim][Gly]) solution, resulting in higher enhancement factor due to increased ([Hmim][Gly]) concentration and sufficient contact time for absorption even with increase in liquid flow. Higher L/G ratio improves CO\textsubscript{2} capture efficiency but also increases the overall energy consumption for solvent regeneration. This observation was possibly due to the higher availability of amine molecules at the higher ratio, which react with CO\textsubscript{2} molecules, consequently leading to higher absorption efficiency, which is consistent with the result of (Rajiman et al., 2020).

![Figure 3. Effect of the liquid-to-gas (L/G) ratio on the CO\textsubscript{2} capture efficiency](image)

### 3.1.3 Effect of the [Hmim][Gly] Concentration on CO\textsubscript{2} capture efficiency

Increasing Solvent concentration leads to higher capture level and greater tendency for equipment corrosion. A good understanding of this relationship is needed to determine the needed concentration that gives the best capture level with the least consequence for corrosion. [Hmim][Gly] concentration was varied from 22.4 to 33.6wt%. The results in figure 4 showed that Capture efficiency increases with increase in [Hmim][Gly] concentration. The behavior reflects, increase in hydroxide ions per unit volume resulting in a higher degree of CO\textsubscript{2} absorption in the lean solvent. Since there is a direct correlation between the liquid mass transfer coefficient and the pace of the chemical reaction, the CO\textsubscript{2} capture efficiency increases as the concentration of [Hmim][Gly] increases. This is because the rate of the chemical reaction between [Hmim][Gly] and CO\textsubscript{2} increases. Conversely, as the chemical reaction rate rises, the gas in the microchannel moves more slowly because the gas volume is getting smaller. In this
instance, the length of the gas residence time is greater, and as the concentration of the amines and the volume percentage of amine modes increase, so does the absorption between amines and CO$_2$, the aforementioned explanation is in agreement with the findings of (Guo et al., 2013).

3.1.4 Effect of the Lean-[Hmim][Gly] Temperature on CO$_2$ capture efficiency

The simulations are carried out in solvent temperature range from 298 – 318 K. The results showed in Figure 5, lean-[Hmim][Gly] temperature on CO$_2$ capture efficiency at different lean-[Hmim][Gly] concentrations of (20 wt% [Hmim][Gly] and 60 wt% [Hmim][Gly]) increases significantly. The reason is that, as the solvent temperature increases, rate of reaction and diffusivity increase, and efficiency of the CO$_2$ capture is increased. At a higher lean amine temperature, the absorber as a whole will be operated at a higher temperature. This higher operating temperature will increase the evaporation rate of [Hmim] [Gly] from the top of the absorber. This identical observation was also illustrated by (de Riva et al., 2017; Vadillo et al., 2022).

![Figure 4. Effect of the [Hmim][Gly] Concentration on CO$_2$ capture efficiency](image-url)
3.1.5 Effect of flue gas temperature on CO\textsubscript{2} Capture efficiency

Effect of flue gas temperature on CO\textsubscript{2} capture efficiency. The moisture content of a flue gas is dependent on temperature, pressure and the type of fuel used. Studying flue gas temperature is necessary since additional cost will be incurred in cooling flue gas prior to entering conventional absorber. Figure 6 showed that the CO\textsubscript{2} capture efficiency was maintained or slightly decreases as the temperature increases. The flue gas temperature at the concentration of 20 wt\% and 60 wt\% of [Hmim][Gly] gives the same trend, this shows that even if the solvent is having higher [Hmim][Gly] concentration, this is due to fact that CO\textsubscript{2} solubility decreases as the temperature increases. The same observation was also discovered by (Vadillo et al., 2022).
3.1.6 Effect of [Hmim] [Gly] concentration on the Reboiler heat duty
Concentration of [Hmim] [Gly] solution influences the reboiler heat duty for solvent regeneration. In Figure 7 The reboiler heat duty of [Hmim] [Gly] solutions at five different concentrations (20, 28, 30, 35, 40 wt%) was studied. findings demonstrate that an increase in [Hmim][Gly] concentration from 20, 28, 30, 35 and 40 wt% results in a reduction in the reboiler heat duty. The relationship between rising [Hmim][Gly] concentration and reboiler heat duty is inverse (Sakwattanapong et al., 2005). The reason is that the reboiler duty reduction is attributed to the decrease of sensible and latent heat during regeneration, the latent heat decreases due to the reduction of the amount of water vaporized, which is achieved by using IL to reduce vapor pressure of the solvent or increase the reboiler temperature (Zacchello et al., 2018).
Figure 7. Effect of [Hmim] [Gly] concentration on the Reboiler heat duty

4.0 Conclusion
In this study, the process performance of the [Hmim][Gly] IL solvent, which could replace the conventional MEA solvent, is evaluated. Process analyses were conducted to investigate the influence of absorber packing height and absorber diameter, liquid-to-gas ratio, lean solvent concentration, flue gas and lean solvent temperature, on reboiler heat duty and capture efficiency. The height and diameter of the absorber, the liquid-to-gas ratio (L/G) and the lean solvent concentration increase with increasing capture efficiency. The temperature of the lean amine increases the CO₂ capture efficiency over the entire temperature range because the reaction rate and diffusivity increase with the capture efficiency. The increase in flue gas temperature shows a decrease in capture efficiency slightly. This is because CO₂ solubility decreases with increasing temperature. The thermal duty of the reboiler is strongly dependent on the [Hmim][Gly] concentration. The reason for this lies primarily in the heat of reaction with CO₂ and the heat of evaporation of water. The result showed a maximum CO₂ capture efficiency of 92 % with a tower packing height of 12 m and a diameter of 0.9 m. Finally, the height and diameter of the absorber, the L/G ratio, the lean [Hmim][Gly] temperature, the flue gas temperature, and the heating capacity of the reboiler have a significant influence on the absorption efficiency and therefore play an important role in improving the capture efficiency. Therefore, aqueous ([Hmim][Gly]) is a promising absorbent for CO₂ capture.

Reference
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