Evaluation of the Performance of Single or Mixed Amine Solvents for CO_2 Capture from Exhaust Gases

Introduction

Reducing carbon dioxide (CO_2) emissions is essential to address global warming and achieve the 2050 net-zero goal (IPCC, 2018). While active research is underway to replace fossil fuels with renewable energy sources such as hydrogen, the continuous increase in global energy demand is making the temporary use of fossil fuels inevitable. Consequently, Carbon Capture, Utilization, and Storage (CCUS) has emerged as a critical transition technology. Among various methods, Post-Combustion Carbon Capture (PCC) via Chemical Absorption is widely recognized as the most commercially mature technology. (Rochelle, 2009). Monoethanolamine (MEA) is used as a primary solvent in the industry due to its rapid absorption rate and low chemical costs. However, MEA-based processes face challenges such as high thermal regeneration costs (reboiler load) and serious equipment corrosion issues. The costs required for solvent regeneration and amine regeneration account for more than 70% of OPEX (Shirdel et al., 2022). To overcome these limitations, active research is being conducted on alternative amine solvents. Piperazine (PZ), a cyclic amine, exhibits excellent thermal stability and low corrosiveness. (Borhani and Wang, 2019). Conversely, tertiary amines such as methyldiethanolamine (MDEA) have the disadvantage of slow reaction rates despite significantly lower regeneration energy. Sterically hindered amines, such as 2-amino-2-methyl-1-propanol (AMP), have reaction pathways altered by structural hindrances that promote bicarbonate formation more than carbamates, which essentially facilitates solvent removal (Kim et al., 2024). Due to the site requirements, costs, and various process challenges involved in experimenting with multiple amines in wet amine plants, simulation methods were devised. Aspen HYSYS, a process simulation software, provides reliable data as it includes a built-in Amine package. Literature on combined cycle gas turbine power plant (CCGT) flue gas is limited. The CO_2 composition of CCGT flue gas is approximately 3–5% (Arshad and Alhajaj, 2023). In this study, we simulate the process of capturing CO_2 from the exhaust gases of coal-fired power plants and CCGTs using Aspen HYSYS and examine the potential of amines to replace MEA.

Theory

Primary and secondary amines react with CO_2 to form carbamates. Tertiary amines react with water and carbon dioxide to form bicarbonates. Primary and secondary amines react directly with CO_2, so they have a fast absorption rate and high regeneration energy. Tertiary amines have a slow absorption rate but low regeneration energy. There is a trade-off between absorption rate and regeneration energy. Recently, due to the synergistic effect of mixed amines, a mixed amine has been reported that has an absorption rate slightly lower than MEA and regeneration energy similar to MDEA.

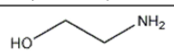
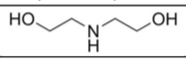
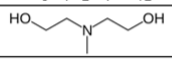
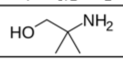
Alkanol amine	1°amine	2° amine	3° amine	Steric Hindrance amine
Molecular Formula	MEA $(C_2H_4OH)NH_2$	DEA $(C_2H_4OH)_2NH$	MDEA $CH_3N(C_2H_4OH)_2$	AMP $H_2NC(CH_3)_2CH_2OH$
Molecular structure				
Reaction	Carbamate($R\text{-}NHCOO^-$)	Carbamate(R_2NCOO^-)	Bicarbonate(HCO_3^-)	Bicarbonate(HCO_3^-)

Figure 1 *Chemical characteristics and reaction behaviors of primary, secondary, tertiary, and sterically hindered amines*

The simulation program used in this study is Aspen HYSYS v15. The process flow diagram of the PCC process is shown in Figure 1.

Method

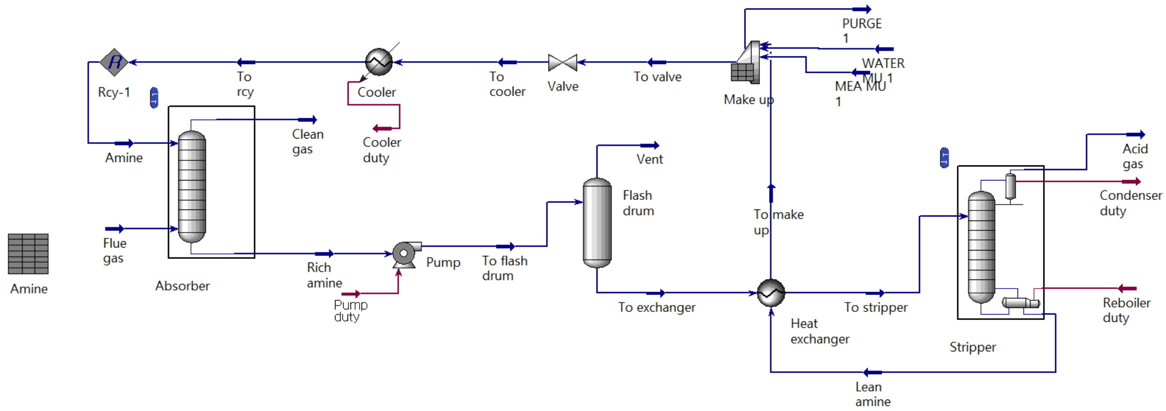


Figure 2 *Aspen HYSYS simulation flowsheet for evaluating single amine performance under varying CO_2 flue gas concentrations.*

Process simulations were performed using acidic gas chemical solvents as fluid packages. This process consists of an absorption tower, a desorption tower, heat exchangers, pumps, etc. The amine absorbent and combustion gases undergo countercurrent contact inside the absorption tower, and the CO_2-rich amine moves to the top of the desorption tower after heat exchange with the regenerated lean amine. The CO_2-absorbed amine is regenerated by high-temperature steam rising from the bottom of the desorption tower. The desorbed CO_2 is compressed and captured at the top of the desorption tower. The captured CO_2 can then be utilized in various industrial sectors through compression. The regenerated lean amine passes through a heat exchanger and moves to the recycle block. In Aspen HYSYS, a recirculation block is required to calculate the recirculation flow. It then passes through the recirculation block and flows back into the absorption tower. Amine and water evaporated or lost in the absorption and regeneration towers are refilled by the make-up device. The process for each amine is designed to achieve a CO_2 capture rate of 90% and a minimum CO_2 purity of 95%. In the calculation process for the absorption and desorption towers, accuracy was improved by applying rigorous velocity-based calculations using advanced modeling rather than efficiency. The following criteria were adopted to evaluate absorption and regeneration performance: 1) Cyclic capacity (Rich Loading - Lean Loading), 2) Reboiler duty, and 3) L/G ratio.

Conclusions

CO_2 capture processes targeting coal-fired power plant flue gas and SOFC flue gas were simulated using single and mixed amines. The performance of single and mixed amines was evaluated. As the proportion of the tertiary amine MDEA increased, rich loading decreased, but reboiler duty decreased. In the case of PZ, acting as an additive, the absorption rate of tertiary amines could be significantly increased. The applicability of mixed amines was confirmed. As a follow-up study, research will be conducted to improve performance through process modification.

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