OFFICIAL ABSTRACT and CERTIFICATION

An Investigation of the Ideal Reaction Conditions for Optimal Carbon Dioxide Absorption using Amino Acid Salt Solutions

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Carbon dioxide (CO_2) is one of the most prominent greenhouse gases in the atmosphere and has been implicated in global temperatures. Post-combustion carbon capture (PCC) has been recognized to reduce CO_2 emissions from fossil fuel combustion sources. Chemical absorption is a popular type of PCC that utilizes reversible reactions to absorb CO_2. Common solvents are amine-based, but due to several disadvantages, amino acid salt solutions (AAS) are currently being examined. Amino acid molecules react with CO_2 to form carbamates and bicarbonate. Reaction ensemble Monte Carlo simulations (RxMC) were used to investigate amino acid solutions of glycine, lysine, proline, alanine, and glutamate under varying conditions of concentration, CO_2 loading, and temperature. The RxMC method samples these reactions in order to determine the equilibrium distribution of vaious solutions, which were then analyzed. Generally, higher concentration and CO_2 loading trials indicated more absorption. The temperature trials had less conclusive results, but the AAS displayed relatively high performance at high temperatures. Optimal simulations were run in order to verify these results. A glutamate slution at a 0.9 wt % concentration had the greatest CO_2 absorption. Ultimately, this study provided greater information regarding optimal conditions for maximum CO_2 absorption, allowing for an ultimate identification of the ideal solution to be implemented in power plants.

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