INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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SHORT ABSTRACT

Over the last few decades, the increasing concentration of carbon dioxide (CO_2) in the atmosphere has contributed adversely to the environment and has been a subject of worldwide attention. The capture of CO_2, which is one of the main greenhouse gas (GHG), currently represents an essential step in the performance of electric power stations, petroleum refineries, chemical fertilizer plants, coal gasifiers, cement factories, and the steel industries. In the recent days, gas scrubbing using activated aqueous alkanolamine solutions is the most reliable retrofit option for post combustion CO_2 capture. The present study investigates a novel activator, bis(3-aminopropyl)amine (APA), which can be an effective mode of eliminating CO_2 from flue gas. The kinetics of CO_2 absorption into chosen aqueous solution of APA was carried out at 303, 308, 313 and 323 K over a concentration range of 0.1-0.5 kmol m^{-3} and at different CO_2 partial pressure. A wetted-wall column absorber was used for the kinetics measurement. The reaction mechanism of CO_2 with primary and secondary amines (zwitterionic mechanism) is described and accordingly the experimentally obtained kinetic data are interpreted. A qualitative nuclear magnetic resonance [NMR (1D and 2D)] spectroscopy method has been applied to develop the reaction scheme for novel aqueous APA with CO_2. The kinetic rate parameters were investigated according to the pseudo-first-order condition for CO_2 absorption at each experimental condition. The values of second-order rate constant, $k_{2\text{-APA}}$ and reaction rate with CO_2 reported in this study were higher than many existing amine activators like ethylenediamine (EDA), N-(2-aminoethyl ethanolamine (AEEA), piperazine (PZ), 2-(1-piperazinl)-ethylamine (PZEA), etc. Two blended solvents such as aqueous blend of APA with N-Methyldiethanolamine (MDEA) and 2-Amino-2-methyl-1-propanol (AMP) were considered for potential use in CO_2 capture. It was observed that the enhancement factor increases significantly in comparison to single amine (aqueous MDEA) solutions when the APA concentrations increased in the blends with MDEA. Based on the pseudo-first-order condition for the CO_2 absorption, kinetic data for amine blend measurement

are reported. Furthermore, the absorption of CO_2 into (APA + MDEA +H_2O) solutions using the same absorber was investigated over the range of temperature and CO_2 partial pressure. The molar concentration of APA was varied while maintaining the total concentration of the amine blends at 3.0 $kmol.m^{-3}$. Based on the zwitterion mechanism, overall reaction scheme for (APA+AMP+H_2O)-CO_2 system was established. According to the pseudo-first-order condition, the reaction rate parameters were estimated for (APA+AMP+H_2O)-CO_2 system from the kinetics measurement. A substantial enhancement of rate in comparison to the single AMP solution was observed due to the addition of a small amount of APA in the blend. A parametric sensitivity analysis has been performed to examine the effect of important physicochemical and kinetic parameters on the specific rate of absorption of CO_2 into (APA+H_2O) and (APA+AMP+H_2O) solutions. For the analyses, the involved parameters are Henry's law constant for CO_2, diffusivity of CO_2 into the amine solutions and the second order reaction rate constants for the absorption of CO_2.

Physicochemical properties such as density and viscosity of aqueous novel APA and an aqueous novel blend of APA with MDEA and AMP solutions as well as solubility and diffusivity of N_2O into these binary and ternary solutions were measured over a wide range of temperature and relative amine composition. The "N_2O-analogy" has been used to determine Henry's constant and diffusivity for CO_2 into the chosen solvents. The experimental binary and ternary density data as well as binary viscosity data were correlated by Redlich–Kister equation whereas ternary viscosity data were correlated by Grunberg and Nissan model. On the other hand, solubility and diffusivity were correlated with different models like the semiemperical model, the modified Stokes Einstein model, arrhenius type equation and polynomial model. All the correlations based on the different model performed are capable for adequately predicting experimental physicochemical data. It is expected that the kinetics and the physicochemical properties this generated will be useful for process design.