INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Programme of Study	:	**Ph.D.**

Thesis Title: Experimental and Modeling Study on the Absorption of CO_2 in Novel Activated Amine Solvents

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SHORT ABSTRACT

The increasing concentration of carbon dioxide (CO_2) in the atmosphere has had a negative impact on the environment over the previous few decades and has been a focus of global attention. CO_2 capture, one of the most important greenhouse gases (GHG), is now a critical stage in the functioning of electric power plants, petroleum refineries, chemical fertiliser plants, coal gasifiers, cement plants, and steel mills. Gas scrubbing with activated aqueous alkanolamine solutions has recently emerged as the most reliable post-combustion CO_2 collection retrofit option.

The current study looks into a new activator called tris (2-aminoethyl) amine (TAEA), which could be an excellent way to remove CO_2 from flue gas. The thesis presents novel experimental CO_2 solubility data of absorption in various aqueous (TAEA+MDEA+H_2O) and (TAEA+AMP+H_2O) systems compositions over wide temperatures and pressure ranges of (293.15-323.15) K and (2-500) kPa, respectively. The modified Kent-Eisenberg (KE) equilibrium model is used to model the experimental solubility data. To fit the equilibrium CO_2 solubility data, the equilibrium constants related to amine deprotonation and carbamate production reactions are regressed as a function of essential operating parameters such as CO_2 partial pressure, amine concentration, and temperature. The results of the KE model's projected solubility are in good accord with the experimental data. The modified KE model established in this study may also be used to estimate the concentrations of various ionic species in the solvent phase at equilibrium conditions. With the variation of α_{CO2}, the distribution of different reaction products arising from the CO_2 –amine reaction has been estimated. The pH of CO_2-loaded amine solvents can also be predicted using the KE model. From the standpoint of CO_2 capture process design, understanding the pH of the loaded solvent is essential.

Feed forward Artificial Neural Network (ANN) model is used to correlate the solub
The Levenberg-Marquardt back propagation technique is utilised as the training function in this ANN architecture. Hyperbolic tangent sigmoid and linear functions are used as transfer functions for the hidden and output layers. The experimental data and the anticipated value from the feed-forward neural network model agree pretty well. FTIR and qualitative ^{13}C NMR were also used to evaluate the many major reaction products and appraise the CO_2- amine reaction scheme. To assess the performance of the researched solvents in this study, a detailed comparison of CO_2 loading with other standard solvents was presented.

Over a temperature range of (293.15-333.15) K, important thermophysical parameters of the solvents, such as density and viscosity, are measured and reported. Diffusivity is also calculated using the measured viscosity values through the modified Stokes-Einstein relation. Along with physical solubility (Henry's law constant) of (TAEA+H_2O), (TAEA+MDEA+H_2O) and (TAEA+AMP+H_2O) are also investigated at different temperatures (293.15-323.15) K and other compositions. These features are essential in determining flow behavior, intermolecular interactions, the design of the absorber or regenerator column, solvent pumping costs, mass transfer, and CO_2 kinetic rates in solvents. The earliest principal models, Redlich-Kister and Grunberg-Nissan, were used to model density and viscosity. For the correlation, Henry's law constant an Arrhenius type equation is used. As a function of temperature and composition, all attributes were connected. The results showed a reduced variance between the experimental and predicted data, indicating that the models were accurate.