INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

Name of the Student	:	**Anirban Dey**
Roll Number	:	**146107017**
Programme of Study	:	**Ph.D.**

Thesis Title: **Experimental and Modeling Study on the Absorption of CO_2 in Aqueous Single and Blended Amines**

Name of Thesis Supervisor(s)	:	**Prof. Bishnupada Mandal & Dr. S.K.Dash (External)**
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SHORT ABSTRACT

The present work investigates two potential amine activators, 1-(2-aminoethyl) piperazine (AEP) and N-(3-aminopropyl)-1,3-propanediamine (APDA) for its applicability in efficient CO_2 capture from flue gas streams. The study reports new experimental CO_2 solubility data of absorption in various compositions of aqueous AEP and APDA system over the broad temperature and pressure range of (303.2–323.2) K and (3-300) kPa, respectively. Along with binary system, different blended system with non-carbamate forming amines such as N-methyldiethanolamine (MDEA), 2-amino-2-methyl-1-propanol (AMP) and 1-dimethylamino-2-propanol (1DMAP) have been also explored in the current work. The blended amine systems considered in this work are aqueous (AEP + MDEA), (AEP + AMP), (APDA + MDEA), (APDA + AMP) and (APDA + DMAP), respectively. The experimental solubility data is modeled using modified Kent-Eisenberg (KE) equilibrium model. The equilibrium constants related to amine deprotonation, and carbamate formation reactions are regressed as a function of important operating parameters such as, CO_2 partial pressure, amine concentration and temperature to fit the equilibrium CO_2 solubility data. The model predicted solubility results from KE model are in good agreement with the experimental data. The application of the modified KE model developed in this study can be further extended in estimating the pH and the overall speciation profile of all the molecular as well as ionic species prevailing in the solvent system. The CO_2 solubility data are also analyzed in view of estimating the heat duty requirement for the absorption process.The solubility data is also correlated using Feed forward Artificial Neural Network (ANN)

model. The ANN architecture used in this work consists of Levenberg-Marquardt back propagation algorithm as training function. The predicted value from the feed forward neural network model shows very good agreement with the experimental data. In addition to this, ATR-FTIR and qualitative ^{13}C NMR have been also conducted to interpret the various important reaction products as well as to assess the reaction scheme of CO_2-amine reaction. A comprehensive comparison of CO_2 loading with other conventional solvents has been presented to assess the performance of studied solvents in the present work.

For detail characterization of the solvent, important thermophysical properties are measured and correlated throughout the experimental range. Thermophysical properties such as density, viscosity and surface tension of aqueous binary and ternary system have been measured in the temperature range of (303.2 to 343.2) K. 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. The model results of these temperature dependent physical properties are also in good agreement with the experimental data. The surface tension data of the aqueous amine system has been correlated with temperature based correlation and multiple linear regression technique. The experimental viscosity data can be further utilized to analyze various thermodynamic properties such as Enthalpy (ΔH^o), Entropy (ΔS^o) and Gibbs energies (ΔG^o) of activation of viscous flow. The generated experimental solubility, thermophysical property data and the correlations developed in this work will allow for prediction of blend properties, thus significantly enhances the prediction capability of aqueous alkanolamines solutions for process design.