## ABSTRACT

## Absorption of Carbon Dioxide into Piperazine Activated Alkanolamines

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In this work, a coupled mass transfer-reaction kinetics-equilibrium model has been developed for absorption of CO<sub>2</sub> into aqueous piperazine (PZ), PZ activated aqueous N-methyldiethanolamine (MDEA) and PZ activated aqueous 2-amino-2methyl-1-propanol (AMP) solvents incorporating the important reversible reactions in the liquid phase. The bulk equilibrium concentrations as well as the interfacial concentration profiles of all chemical species can be predicted at any point in a gasliquid contactor using the model. The set of partial differential equations along with nonlinear algebraic equations are solved numerically. The model is validated with experimental results of steady state absorption measurements of  $CO_2$  into aqueous PZ, aqueous (MDEA + PZ), and aqueous (AMP + PZ) in a wetted wall contactor. The rates of absorption of CO<sub>2</sub> into these solvents have been measured at various temperatures, CO<sub>2</sub> partial pressures, and various relative compositions of MDEA/PZ and AMP/PZ in the blends. New kinetic parameters for the reactions of  $CO_2$  with aqueous PZ, aqueous (MDEA + PZ) and aqueous (AMP + PZ) have been obtained using the developed mathematical model and the measured rates of absorption. The model has also been used for parametric sensitivity analyses to determine the effects of various important parameters, such as CO<sub>2</sub> interfacial concentration, Henry's law constants for CO<sub>2</sub>, diffusion coefficients of CO<sub>2</sub> and all liquid phase chemical species, and the reaction rate coefficients on the rates of absorption of  $CO_2$  and the enhancement factors. Steady state absorption measurements of this work have shown that the CO<sub>2</sub> absorption rates into aqueous MDEA and aqueous AMP increase significantly with the addition of small amounts of PZ in these alkanolamines, while more pronounced effect has been observed for aqueous (AMP + PZ) solvent at high  $CO_2$  partial pressures. This indicates the importance of the PZ activated aqueous AMP solvent for sour gas treating besides

the PZ activated aqueous MDEA solvent. The comprehensive mathematical model developed in this work can be used for the process design of gas treating units using aqueous (MDEA + PZ) and (AMP + PZ). By using appropriate model parameters and considering relevant chemical reactions, the model can also be used for other single and activated alkanolamine solvents.

Extensive physicochemical properties of  $CO_2$ , aqueous PZ, aqueous (PZ + MDEA), and aqueous (AMP + PZ) solvents have been measured in this work, extending the literature database for the physicochemical properties of these amine solvents. In addition, several correlations developed in this work, will allow calculation of the physicochemical property data of these solvents for process design and research work in gas treating.