

## **ABSTRACT**

### **Absorption of Carbon Dioxide and Hydrogen Sulfide into Blended Alkanolamines**

by

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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> and simultaneous absorption of CO<sub>2</sub> and H<sub>2</sub>S into single and blended alkanolamine solvents incorporating the most extensive set of important reversible reactions in the liquid phase. The bulk equilibrium concentrations as well as the interfacial concentration profiles of fourteen chemical species can be predicted at any point in a gas-liquid contactor using the model. The seven coupled nonlinear partial differential equations along with seven coupled nonlinear algebraic equations are solved numerically using method of lines with uniform nodal spacing. The model is validated by comparing its predictions with experimental results of steady-state absorption of CO<sub>2</sub> and simultaneous absorption of CO<sub>2</sub> and H<sub>2</sub>S into aqueous single amine solvents and amine blends in a wetted wall column. The model has been used for rigorous parametric sensitivity analyses to see the effects of different pertinent parameters such as CO<sub>2</sub> interfacial concentration (CO<sub>2</sub> partial pressure), Henry's law constants for CO<sub>2</sub> and H<sub>2</sub>S, diffusion coefficients of CO<sub>2</sub>, H<sub>2</sub>S and all chemical species, and rate coefficients on the rate of absorption of CO<sub>2</sub>, H<sub>2</sub>S and selectivity factor. Steady-state absorption measurements of this work have shown that the CO<sub>2</sub> absorption rate into aqueous N-methyldiethanolamine (MDEA) and aqueous 2-amino-2-methyl-1-propanol (AMP) increases significantly with the addition of small quantities of monoethanolamine (MEA) or diethanolamine (DEA) in these amines, with more pronounced effect for the MDEA based solvents. Thus establishing the usefulness of the blended amine solvents for sour gas treating. By varying the relative concentrations of the primary or secondary amine in the blended amine solvents, the blends' performance can be varied from H<sub>2</sub>S selective absorption at one end, to total removal of CO<sub>2</sub> and H<sub>2</sub>S from the

sour gas streams at the other. The comprehensive mathematical model developed in this work should be useful for the rational design of gas treating processes employing single or blended alkanolamine solvents.

Extensive physicochemical properties of  $\text{CO}_2$  and the aqueous alkanolamine solvents needed in the model have been measured in this work, extending the data in the literature for the specific single and blended amine solvents studied in this work. The diffusion coefficients and physical solubilities of  $\text{N}_2\text{O}$  in the aqueous alkanolamine solutions have been measured and the diffusivities and physical solubilities of  $\text{CO}_2$  in these solvents have been estimated by “ $\text{N}_2\text{O}$ -analogy”. The densities and viscosities of the aqueous alkanolamine solvents have been measured over a wide range of amine concentration and temperature. The Henry’s law constants and diffusion coefficients of  $\text{H}_2\text{S}$  needed in the model have been taken from the published literature. In addition, several correlations developed in this work, will allow prediction of blend properties from single amine properties for process design and research work in gas treating.