

## **Impact of Organic Solvents on the Diffusivity of Carbon Dioxide in Alkanolamines**

John Dowdle<sup>S</sup>, Hangyao Wang<sup>C</sup>, Max Li, Ravi Dixit, Diego Ortiz-Vega and Diego Cristancho  
*2301 N. Brazosport Blvd, Dow Chemical Company, Freeport, TX, U.S.A.*  
*hwang@dow.com*

Optimal selection of solvents and process designs for the purification of industrial gas streams requires a fundamental understanding of the rate of mass transfer of acid gases from the gas phase into the liquid phase. Commonly, the gas industry uses aqueous alkanolamine solvents for the removal of acid gases and blended systems with organic solvents to selectively target additional contaminants such as organic sulfur compounds. The mass transfer of acid gases to aqueous alkanolamine solvents is a complex process that can be significantly impacted by the addition of an organic solvent. Understanding the effect of organic solvent addition on key thermophysical properties such as the liquid phase diffusivity is critical for accurate process design. However, direct experimental measurement of these properties is challenging or impossible due to the presence of chemical reactions, and complicated experimental setups. Analogies to similar compounds are typically required in order to make use of experimental data. Molecular simulation thus offers an attractive alternative to probe these systems. In this paper, we use molecular dynamics simulations to understand the effect of blending aqueous alkanolamines with organic solvents on the diffusion of carbon dioxide. Systematic studies are presented comparing the diffusivity of carbon dioxide in aqueous alkanolamines and blends with methanol and triethylene glycol. Conclusions relevant to gas treating applications are drawn from these studies.