

MOL2NET'23, Conference on Molecular, Biomedical, Computational, & Network Science and Engineering, 8th ed.



# Prediction of Amine Transformation Products in the Absorption of CO<sub>2</sub> in Ternary Solvent Systems Consisting of Triethanolamine (TEA) / 2-Amino-2-methyl-l-propanol (AMP), Piperazine (PZ), and Water

Adonis P. Adornado<sup>a</sup>, Allan N. Soriano<sup>b</sup>, Rugi Vicente Del Castillo Rubi<sup>c</sup>

 <sup>a</sup>General Education Department, Colegio de Muntinlupa, Mayor J. Posadas Avenue, Sucat, Muntinlupa City, Philippines
<sup>b</sup>Department of Chemical Engineering, Gokongwei College of Engineering, De La Salle University, 2401 Taft Avenue, Manila, Philippines
<sup>c</sup>Chemical Engineering Department, College of Engineering Department, San Marcelino Street, Ermita, Manila, Philippines



### Abstract.

The process of post-combustion amine based *CO*<sup>2</sup> *capture relies on large scale use of aqueous* amine solutions. In such operations, it is associated with minor release of amine through the cleaned exhaust gas, as degraded solvent, as accidental spills, and amine transformation products in both liquid waste streams and atmosphere along with the treated flue gas. In this regard, it is necessary to study the concentration profiles of the by-products formed in aid of treating liquid waste streams. The present work includes chemistry and reaction mechanism studies of the reaction between CO<sub>2</sub> and ternary solvent systems consisting of triethanolamine (TEA) / 2-Amino-2-methyl-lpropanol (AMP), piperazine (PZ), and water. The chemical reactions of  $CO_2$  with TEA, a tertiary amine is described by base-catalyzed hydration were carefully derived. The calculation was carried out using the Electrolyte Non-Random Two Liquid (NRTL) model in a rigorous rate-based non-equilibrium process simulation on Aspen Plus® 8.6. The results yield reasonable predictions on product concentration profiles and can be used as reference in future assessment of the by-products formed in  $CO_2$ capture using the considered amine solvent system.

#### **Introduction** (optional)

Materials and Methods (optional)

**Results and Discussion** (optional)

- . .
- •

## **Conclusions** (optional)

- .
- .
- •

### **References** (mandatory)

- .
- .
- .

3