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Molecular Dynamic Simulation of CO2 Absorption into Mixed Aqueous Solutions MDEA/PZ

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Abstract : Amine absorption process is an approach for mitigation of CO2 from flue gas that produces from power plant. This process is the most common system used in chemical and oil industries for gas purification to remove acid gases. On the challenges of this process is high energy requirement for solvent regeneration to release CO2. In the past few years, mixed alkanolamines have received increasing attention. In most cases, the mixtures contain N-methyldiethanolamine (MDEA) as the base amine with the addition of one or two more reactive amines such as PZ. The reason for the application of such blend amine is to take advantage of high reaction rate of CO2 with the activator combined with the advantages of the low heat of regeneration of MDEA. Several experimental and simulation studies have been undertaken to understand this process using blend MDEA/PZ solvent. Despite those studies, the mechanism of CO2 absorption into the aqueous MDEA is not well understood and available knowledge within the open literature is limited. The aim of this study is to investigate the intermolecular interaction of the blend MDEA/PZ using Molecular Dynamics (MD) simulation. MD simulation was run under condition 313K and 1 atm using NVE ensemble at 200ps and NVT ensemble at 1ns. The results were interpreted in term of Radial Distribution Function (RDF) analysis through two system of interest i.e binary and tertiary. The binary system will explain the interaction between amine and water molecule while tertiary system used to determine the interaction between the amine and CO2 molecule. For the binary system, it was observed that the –OH group of MDEA is more attracted to water molecule compared to –NH group of MDEA. The –OH group of MDEA can form the hydrogen bond with water that will assist the solubility of MDEA in water. The intermolecular interaction probability of –OH and –NH group of MDEA with CO2 in blended MDEA/PZ is higher than using single MDEA. This findings show that PZ molecule act as an activator to promote the intermolecular interaction between MDEA and CO2.Thus, blend of MDEA with PZ is expecting to increase the absorption rate of CO2 and reduce the heat regeneration requirement.

Keywords : amine absorption process, blend MDEA/PZ, CO2 capture, molecular dynamic simulation, radial distribution function

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