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Effect of Temperature on Diffusivity of Monoethanolamine (MEA) on Absorption Process for CO_2 Capture

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Abstract- Diffusion coefficient study gains an interest to know the mass transfer properties of molecules especially in study of the absorption process. The main objective of this study is to investigate the effect of temperature on diffusivity of MEA absorption process for CO_2 capture. Three different values of process temperature were chosen for simulation in this study, 298 K, 313 K and 318 K. The MD simulation was carried out at NVE (200ps) and NPT (1ns) ensemble in Material Studio 7.0 software. Mean Square Displacement (MSD) analysis was done to compute the self-diffusion coefficient of molecules in tertiary system ($MEA+H_2O+CO_2$). The results show that the rate of the diffusion coefficient is increased as temperature increased. Diffusion coefficient at 318 K is the highest compared to others temperature. MD simulation is used to study details about absorption process and capture CO_2 acid gases. The simulation diffusivity result obtained from this work shows higher compared with theoretical results.

Index Terms- Molecular Dynamic, Simulation, Amine Absorption Process, Monoethanolamine, Carbon Dioxide, Mean Square Displacement.

I. INTRODUCTION

Recently, the increment of CO_2 composition in air will be contributing the increment of the global temperature. IPCC (Intergovernmental Panel on Climate Change) is an international agency, whose plays a role in preparing a report about the global climate change [1]. IPCC is one of agencies in this world which extensively conduct the research to overcome the global climate change problem. At present, there are many CO_2 capturing chemical materials are known such as amine-solvent, organic molecular cages, ionic liquids, metal-organic framework, zeolite and carbon-materials [2]. In this study, amine-solvent is used to determine the diffusivity of CO_2 in amine-based absorption process. Absorption process is a process in the scope of post-combustion capture process. This technology has been established over the year since 1930"s [3]. MEA, monoethanolamine (C_2H_7NO) is a primary amine. Which has been used as solvent in CO_2 capture due to higher performance in the absorption process [4].

Molecular Dynamic (MD) simulation was run on molecules species to calculate the diffusion coefficient. This computational method has become an effective tool to explore more deeply about absorption process and also CO_2 capture. MD simulation used to study the molecular properties such as the diffusion coefficient [5]. This computation technique can also study others thermodynamic condition at atomic level that cannot be study by doing experimental. Moreover, this technique has many advantages compare to chemical experimental study such as environmental friendly and money saving [6]. In CO_2 capture cost process, more than half is distributed to the absorbent regeneration part [7]. Study on the thermodynamic properties is essential before operating the absorption process in pilot plant. In addition, cost for experimental research to study the diffusion coefficient is high particularly at operating condition of higher pressure and temperature [8]. Besides that, the equipment used for study diffusion coefficient of solute in liquid solvent in low concentration is expensive. MD simulation also is an option to study the diffusion coefficient of solute in supercritical fluid because it"s difficult to run by experimental [9]. Therefore, the computation measurement study offers better approach to do the research on diffusivity.

Factors that affected the diffusion are concentration gradient, pressure gradient and temperature gradient [10]. Diffusion coefficient, density and viscosity are used to calculate the mass transport