Molecular interaction establishment of amine-based absorption process for CO2 removal

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Abstract:
Amine absorption process is an approach for mitigation of carbon dioxide (CO2) from flue gas that was produced from the power plant. Modelling and simulation of amine absorption process for CO2 removal at macro-scale is well established. This study was aimed to investigate the amine-CO2 absorption process at the molecular level and their intermolecular interaction during the absorption process using molecular dynamics (MD) simulation. Several case studies were conducted to investigate the effect different types of alkanolamines for CO2 absorption process and comparison between single and blended amines for absorption process. Next, effect of different carbamate molecules for CO2 desorption process were also performed. MD simulation was installed in the HP240 workstation using the Material Studio (version 7.0) software. The MD simulation was carried out at NVE (constant number of moles, volume, energy) and NVT (constant number of moles, volume, temperature), which ensembles for 200 ps and 1 ns, respectively. Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies (COMPASS) and Ewald models were used for the force field and as summation method calculation within the simulation box. For case study 1, the simulation results show the MEA solvent showed the highest tendency to interact with CO2 compared to DEA (diethanolamine) and MDEA (methyl diethanolamine) because it can directly react with CO2 and easily form carbamate ions. A good performance of activator amine, PZ (piperazine) and steric hindered amine, AMP were observed in this study. Both showed high tendency to have intermolecular interaction with water and CO2.

Keywords: Molecular Dynamic Simulation; Radial Distribution Function; Alkanolamines; Absorption Process; Stripping Process; CO2 Capture

Acknowledgments

The authors acknowledge the support of the Ministry of Higher Education Malaysia for the financial support through the fundamental research grant scheme (FRGS) Project No. RDU130109 and Universiti Malaysia Pahang for providing the computational facilities and support.