

ICAMS Advanced Discussion

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**Prof. Dr. Mansour Kanani**  
Shiraz University, Shiraz, Iran**Insight into CO<sub>2</sub> Capture in Biphasic Solvents:  
Molecular Dynamics Simulations using Reactive Force Fields  
and Experimental Verification**Maryam Alipour<sup>a</sup>, Mansour Kanani<sup>b</sup>, Ali Hafizi<sup>a</sup><sup>a</sup> Department of Chemical Engineering, Shiraz University, Shiraz, Iran<sup>b</sup> Department of Materials Science and Engineering, Shiraz University, Shiraz, Iran

This study employs Molecular dynamics (MD) simulation to investigate effects and governing mechanisms of diethylenetriamine (DETA) and diethylethanolamine (DEEA) as the mutual amine solvent, along with N-methyl-2-pyrrolidone (NMP) and water as co-solvents, on the efficiency of CO<sub>2</sub> absorption within a biphasic solvent system. To parametrize the CO<sub>2</sub> loading in terms of atomic scale evolution, partial radial distribution function (PRDF) as well as atomic coordination number (CN) are carefully defined for carbon in CO<sub>2</sub> and N in the solution. Using these two parameters, efficiency of solution as well as kinetic of the reactions could be captured for variety of compositions. PRDF graphs mostly provide qualitative results on the beginning of capturing reactions and C-N bond length, while CN outputs can quantitatively monitor the CO<sub>2</sub> loading and C-N bonding creations. Comparing different solution ratios over time showed that increasing DETA can intensify the absorption rate significantly by adding more absorption sites in the solution. CN analysis for 1, 2 and 3M of DETA shows that 17, 24 and 29% of active DETA sites (i.e. their N atoms) can capture a CO<sub>2</sub> molecule in the same time period. An experimental methodology was followed to validate the MD results.