



Frontiers in Catalysis Science and Engineering
Seminar Series

CO₂ Capture in Amine Solutions: Modeling and Simulations of Key Chemical Reactions

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Abstract: Amine solutions are still at the heart of the most mature technology for post-combustion CO₂ capture. Monoethanolamine (MEA) is the prototype. However, serious concerns exist about the related costs, e.g., for the release process in MEA solutions, and several problems must be solved before their application can be extended to large scale. The need for both solvent and process optimization has promoted fundamental research, mainly using experimental methods. During the past decade, several models and simulations have been performed, with the aim of deepening our understanding of the key elemental reactions of CO₂ involved in its capture in solution. Our own study of the CO₂ uptake and release was based on DFT-based molecular dynamics aided by metadynamics. We applied it to selected aqueous amines: monoethanolamine, 2-amino-2-methyl-1,3-propanediol (AMPD), 2-amino-2-methyl-1-propanol (AMP) and benzylamine (BZA). The scenario emerging from our simulations has provided new insights into the reaction mechanisms and also into the origin of the different behavior of different amines. In particular, the role of water—previously strongly underestimated in computational studies—was established as essential in facilitating the development of all the relevant reactions.