Modeling and Simulation of Catalysts in Amine-Based Solvents for Capturing CO_2

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The scientific groups at the Center for Applied Energy Research, University of Kentucky (UKy) have developed a series of catalysts that, when combined with amine-based solvents, perform CO_2 hydration under conditions similar to post-combustion capture. The catalysts were inspired by the function of carbonic anhydrase, but are water soluble, stable, and show an enhancement in mass transfer in concentrated aqueous primary amine solutions. These catalysts have the purpose of improving carbon capture by decreasing the capital costs. However, some of the catalysts tested experimentally were associated with unfavorable outcomes, such as foaming. UKy scientists would like to have a better understanding of the relationship between the structure of a given catalyst and its catalytic properties. Furthermore, it is highly relevant to be able to predict the modifications induced by a given catalyst on various properties of the amine solution such as viscosity, surface tension, and gas mass transport. Addressing these goals are difficult and sometimes impossible with the current state-of-the-art experiments, but relatively easier using computational chemistry which we use in the present work.

We first compare the force field parameters available in the literature for the classical simulation of amines. Based on the calculated properties against measured experimental values, we picked the best force force field parameters for amines. Force fields for catalysts were generated using quantum-mechanical calculations along with available AMBER force field parameters. Once force fields in hand, we use molecular dynamics (MD) simulations to calculate the physical properties (density, CO_2 diffusivity, surface tension, viscosity) of the amine-water solutions when the catalysts are present, as well as to describe the involvement of the catalysts with the CO_2 hydration reaction. Finally, the problem of foaming will be addressed which depends on the solution density, viscosity, surface tension, surface elasticity, and operating conditions, such as gas velocity, and the packing materials. Preliminary MD simulations suggest that foaming happens due to the surfactant behavior of catalysts, which were verified using experiments.

Modeling and calculated properties are very helpful in describing the underlying chemistry happening in the CO_2 capture process, and will be further helpful in improving the efficiency of catalysts as well as in predicting new catalysts for CO_2 capture.