Molecular Insights into the Behavior of Aqueous Amine Solutions for CO_2 capture in the Presence of Degraded Amine By-Products

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The most standard process used in industry today for CO_2 capture is the separation by absorption in aqueous amine solvents, usually monoethanolamine (MEA) due to its particular properties (e.g., high CO_2 cyclic capacity, high kinetic at low CO_2 partial pressure, low viscosity, high water solubility, low price, etc.). Nevertheless, it has some disadvantages such intensive energy required for desorption and solvent degradation. Furthermore, byproducts cause a noteworthy decrease in process efficiency with solvent losses, corrosion, fouling, foaming and an increase in viscosity. Most the studies available in the literature to quantify these effects has been performed experimentally [1]. To the best of our knowledge, there is no literature focused on the molecular modelling the thermophysical properties of such degraded amines and the relationship between the interaction of these molecules with MEA, CO_2 and water, and hence, the final performance of the solvent.

Hence, in this contribution, we present results concerning molecular dynamics simulations and soft-SAFT calculations concerning the effect of the presence of degradation amine products into the microscopic behavior of the CO_2 capture process with aqueous amines. Degraded amines include 1-(2-HydroxyEthyl)-2-ImidAzolidinone (HEIA), 2-oxazolidone (OZD) and N-(2-Hydroxyethyl) ethylene-diamine (HEEDA). Thermophysical properties as well as atomistic behavior have been analyzed for pure and multi-component systems. Results show that when cyclic degraded amines such as HEIA are present in the aqueous systems, it leads to the generation of molecular aggregates, which suppresses the carbamate reaction and therefore the absorption capacity of the solvent.

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References

[1]. GT Rochelle. Science, 325, 1652–1654 (2009).