Aqueous ammonia is a rising sorbent for the CO₂ capture in the post combustion. Some technical barriers for commercialization to be mentioned are the control of ammonium speciation and ammonia slip. Due to the intrinsic nature of its high volatility, the suppression of its vaporization bears criticality. Some efforts to suppress its vaporization have been endeavoured such as cooling down of flue gases and/or the absorbent solution or pressurization of the system. However, these remedies can cause the increase of operation cost. In this study, we employed a computational chemistry approach, i.e. molecular simulation, for the additive search to minimize the ammonia loss. The suggested additives feature amphoteric nature or having both the acidic and basic functional groups within a molecule. We expect that the CO₂ loading capacities would be preserved (due to the basic functional group) and ammonia vaporization loss would be reduced (due to the acidic functional group). The effects of candidate additives were tested both in the non-carbonated ammonia solution and in the carbonated ammonia solution. Significant reduction in the vapor pressure of ammonia was observed in both types of solutions. Although some candidate additives showed good feature of vapor suppression of ammonia, we stress that the addition of candidate chemicals to the absorbent solutions in the process need caution. Other factors including the recovery of additives, CO₂ absorption capacity, reaction mechanisms, and environmental risk should be taken into consideration to develop a commercial facility, and this will be the subject of our future investigation.
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