## Characterization of aqueous ammonia modified with additives for removal of carbon dioxide

## 최봉길, 박호석, 유정균, 홍원희\*, 김종남<sup>1</sup> 한국과학기술원; <sup>1</sup>한국에너지기술연구원 (whhong@kaist.ac.kr\*)

Aqueous ammonia absorbent (10 wt%) was modified with four kinds of additives (1 wt%) including amine and hydroxyl groups, i.e. 2-amino-2-methyl-1-propanol (AMP), 2-amino-2-methyl-1,3-propandiol (AMPD), 2-amino-2-ethyl-1,3-propandiol (AEPD), and tri (hydroxymethyl) aminomethane (THAM), for CO2 capture. The loss of ammonia by vaporization was reduced by additives, while the removal efficiency of CO2 was slightly improved. These results were attributed to the interactions between ammonia and additives or absorbents and CO2 via hydrogen bonding, as verified by FT-IR spectra and computational calculation. Molecular structures as well as binding energies were obtained from the geometries of (ammonia + additives) and (ammonia + additives + CO2) at the optimized state. These experimental and theoretical findings demonstrate that additives including amine and hydroxyl group are suitable for modifying aqueous ammonia absorbent for CO2 removal.