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CO2 capture, transport, storage & valorisation **Oral**

Modeling of the CO_2-AMP-H_2O system for simulation of the carbon dioxide removal absorption + regeneration process

Stefania Moioli[1], Ricardo R. Wanderley[2], Laura A. Pellegrini[1], Hanna K. Knuutila[2]

[1]GASP, Group of Advanced Separation Processes and GAS Processing, Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta", Politecnico di Milano, Piazza Leonardo da Vinci 32, I-20133 Milano, Italy

[2]Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), NO-7491 Trondheim, Norway

Corresponding author e-mail: stefania.moioli@polimi.it

The increase in the concentration of carbon dioxide in the atmosphere is causing an increase in the Earth's temperature so, in order to decrease global warming, a reduction of anthropogenic carbon dioxide emissions is needed. Power production units, in particular those fed with coal, are among the most relevant sources of CO_2 emitted to the atmosphere, making the treatment of flue gases from this type of plants of major importance. For this purpose, several technologies may be considered and absorption by chemical solvents is generally preferred.

AMP (2-amino-2-methyl-1-propanol) is a sterically hindered amine which had been studied in mixtures with promoters such as piperazine and which is now subject of research for its use in mixtures also with nonaqueous solvents, as N-methyl-2-pyrrolidone (NMP), to form precipitating solvents.

As single solvent in aqueous solution, it is characterized by a good absorption capacity and it is more resistant to degradation than the traditionally employed monoethanolamine (MEA) solvent. Moreover, it is easy to regenerate, because of extensive formation of the bicarbonate instead of the carbamate due to the steric hinderance of the amine.

This work focuses on the thermodynamic modeling of the solubility of CO_2 in the AMP+H_2O solvent, for which literature works are scarce. Considering the formation of ions in the liquid phase, a γ/ϕ model, with γ calculated according to the Electrolyte-NRTL method and ϕ obtained by employing the Redlich-Kwong EoS, has been selected and the values of the parameters for the calculation of the activity coefficient have been determined by regression to best represent the experimental data for AMP+H_2O and AMP+H_2O+CO_2 systems.

The model has been implemented in the commercial software ASPEN Plus® for the simulation of carbon dioxide removal from a flue gas exiting a coal-fired power plant.