

# Modeling of CO<sub>2</sub> post-combustion capture process using biphasic solvents

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Since the preindustrial period, carbon dioxide anthropogenic emissions have increased sharply. In order to mitigate the climate change, industrial solutions such as improvement of energy efficiency, development of renewable energies, and applicability of carbon capture and reuse (CCU) or storage (CCS) technologies have been proposed. Cement industries represent 30% of the total annual CO<sub>2</sub> emitted from industrial sectors [1]. In this context, the European Cement Research Academy (ECRA) and the University of Mons (UMONS) established a research Chair with the purpose of studying the applicability of carbon capture in cement industry and its re-use. Previous studies presented in the different ECRA reports highlighted that two CO<sub>2</sub> capture processes can be applied in a cement plant: post-combustion and oxy-fuel combustion. Post-combustion CO<sub>2</sub> capture with absorption-regeneration using solvents is by far the most advanced technology. However, the use of conventional monoethanolamine (MEA)-based absorption process involves high energy consumption. An innovative alternative to improve the process performances is the use of biphasic solvents-based CO<sub>2</sub> absorption processes [2], [3].

Indeed, biphasic solvents exhibit a liquid-liquid phase separation, CO<sub>2</sub> rich and lean phases, for given temperature and/or CO<sub>2</sub> loading conditions. This phenomenon allows an important energy saving by regenerating only the heavy rich phase coming from the decanter unit. Thus, the energy required for the regeneration step in the stripper can be substantially reduced (see Fig.1).

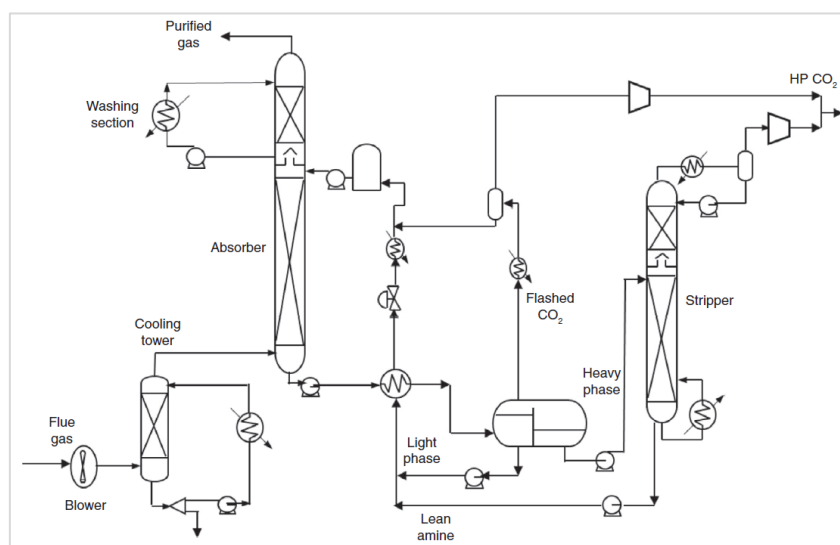
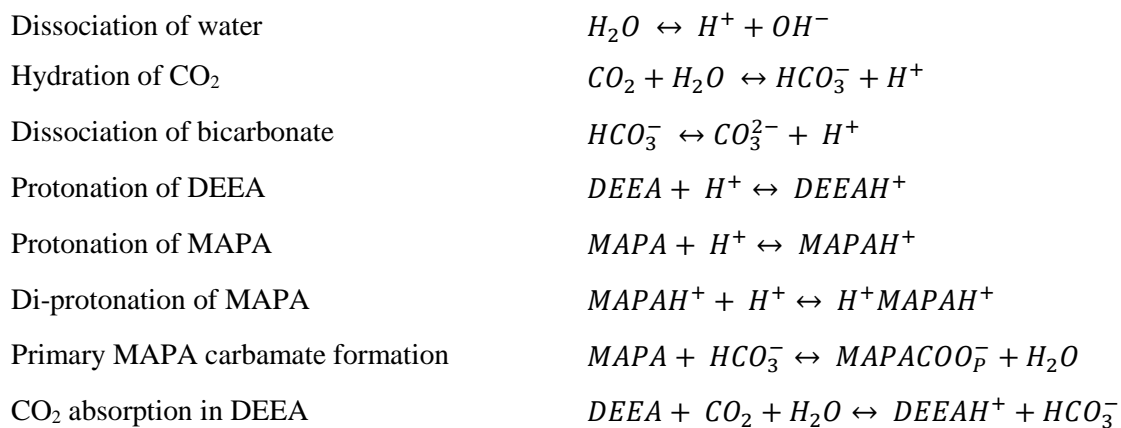


Fig.1. Simplified process flow diagram of the IFP Energies nouvelles DMX process

This work is focusing on the study of CO<sub>2</sub> post combustion capture technology using demixing solvents applied to cement plant flue gases containing high CO<sub>2</sub> amount (from 20 to 30%wt). Innovative

simulation model requiring both thermodynamic and kinetic parameters is under development. Moreover, economical evaluation of the energy consumption in such application will be carried out.

A comprehensive bibliographic review was carried out to highlight the most promising biphasic system. The solvents presenting required properties for CO<sub>2</sub> capture are necessarily composed of mixed amines. Usually, the mixture may contain amines with good absorption properties (primary/secondary or multifunctional amines) and amines as a regeneration promoter (tertiary amine). A mixture of a tertiary amine diethylaminoethanol (DEEA) and a diamine N-Methyl-1,3-Propanediamine (MAPA) has been chosen to be widely studied in this work. This aqueous mixture is interesting not only for its good absorption and regeneration properties, but also for allowing phase separation when loaded with CO<sub>2</sub>. CO<sub>2</sub> absorption into DEEA-MAPA mixtures will be firstly modeled in Aspen Plus using non-random two liquid (eNRTL) thermodynamic model at concentrations without demixing phenomenon. The modeling of this process can be validated by absorption-regeneration tests in a micro pilot unit available in our department [4]. It is of great interest and innovative to demonstrate the performances of this solvent, even without demixing. When CO<sub>2</sub> is dissolved in aqueous amine solutions, several reactions take place depending on the type of amine. The following speciation equilibria were considered for the thermodynamic modeling:



A separate vapor liquid-liquid equilibrium modeling using Extended UNIQUAC of DEEA-MAPA mixture at demixing concentrations will be realized to determine the composition of each phase leaving the decanter unit, the lean and the heavy ones. To carry out the process modeling in Aspen Plus software, maximum availability of data is needed for the system. Published experimental data will be regressed and might be completed with our own experimental measures of equilibrium and kinetic data. Finally, technico-economic investigations are scheduled to optimize biphasic CO<sub>2</sub> capture process specifically for the cement industry application.

## References

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