Measurements of Carbon Dioxide Solubility in Cyrene and Simulation of the Absorption Process

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Physical absorption is one of the most applied and efficient methods for CO_2 removal and it is primarily employed for CO_2 separation from industrial gases, such as natural gas and syngas.

N-Methyl-2-Pyrrolidone (NMP) is one of the main employed solvents for CO_2 removal from gas streams via physical absorption, but it has been classified as a "Substance of Very High Concern" under European Regulation No. 1907/2006. Consequently, alternative solvents are under consideration. One of these candidates is Cyrene (dihydrolevoglucosenone) that is a biodegradable, non-mutagenic and non-toxic solvent derived from biomass, which has emerged as a promising bio-based alternative to NMP. Due to its properties similar to those of NMP, some studies in the literature suggest Cyrene as a potential bio-based substitute. Despite its promise, to the authors' knowledge, the studies of CO_2 solubility in Cyrene already performed are a few, with experimental data available only at 313.15 K [1], consisting of eight measurements, and at 333.15 K [2], with only a single reported measurement.

This work aims at investigating the use of Cyrene as solvent for CO2 absorption from both an experimental and modelling point of view.

The measurements of the solubility of CO2 in Cyrene have been performed at the Process Thermodynamics laboratory (PT lab) of Politecnico di Milano at 313.15 K, 333.15 K and 363.15 K following the model employed in the literature [1] for data processing.

In detail, the series at 313.15 K reported in [1] has been used for the validation of the solubility unit installed at the PT lab. Upon confirming that these measurements closely matched the reference values, the experiments have been extended to two additional temperatures, 333.15 K and 363.15 K, chosen because they lie within the typical range for physical absorption processes for CO2 removal. These newly solubility data have, then, been used to simulate the physical absorption process in Aspen Plus®.

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[1] M. Kerleaux, et al., 2022. *GL2022*. [2] A. Hajlaoui, et al., 2023. *ICR2023*.

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