A Multiscale Approach for the Thermophysical Characterization of Phosphonium-based Ionic Liquids in CO2 Capture Applications

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The development of efficient separation systems for CO_2 capture is a key area of research to reach green-house gas control. To this end, different solvents are applied in absorption circuits. Among them, amines are the most extensively used solvents in industrial applications, but they pose important environmental and economic issues due to their evaporation and degradation during operation. In addition to these problems, there is nowadays a need to find alternative solvents that can operate at different CO_2 concentrations of the treated streams, ranging from 15 % in flue-gases to ppm in air.

Ionic Liquids (ILs) are actively being researched as CO_2 sorbents, given their low vapor pressure and the possibility of tuning their solvent power by combining different ions, considering the specific stream composition and conditions for the absorption. Particularly, some phosphonium cation/anion combinations have been studied in literature with promising performance, although their complete characterization is still required to select the most appropriate CO_2 absorber.

In this work, a multiscale approach was applied to study the CO_2 gas absorption in phosphonium-based ILs with a variety of anions. New molecular models were developed through the soft-SAFT [1] approach for these ILs based on: a) previous soft-SAFT coarse-grain models for this ILs family already available in the literature [2], b) the analysis of the charge distribution of molecules performed through Turbomole-COSMO software for new ILs; and c) the approximation of association parameters via DFT calculations. Then, soft-SAFT has been used to effectively reproduce/predict the thermodynamic and absorption properties [2] of these CO_2 absorbents in wide ranges of pressure and temperature. The molecular models consider specific CO_2-IL cross-association interactions to account for chemisorption phenomena when present. Additionally, the presence of hydration is also discussed. The analysis is carried out at different CO_2 compositions and completed with the estimations of Henry's law constants, solvation enthalpies and entropies to finally propose the most promising solvents.

Acknowledgements

This research is supported by the Spanish Ministry of Science and Innovation MCIN/AEI/10.13039/501100011033 and by the European Union Next Generation EU/PRTR under R + D + I project NEW-F-TECH (TED2021-130959B-I00). S. B. Rodriguez Reartes acknowledges the financial support of the "María Zambrano" grant awarded by Universitat Rovira i Virgili for the requalification of the Spanish university system for 2021-2023.

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