Combining Theoretical Tools to Characterize the Thermophysical Profile of Deep Eutectic Solvents for CO2 and F-Gas Capture Applications

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In recent years, there has been a growing interest in the thermophysical characterisation of Deep Eutectic Solvents (DES) [1, 2]. These unique eutectic mixtures consist of the combination of a Hydrogen Bonding Acceptor (HBA) and a Hydrogen Bonding Donor (HBD), whose interaction results in a significant reduction in the melting point, well below that of the individual components and far from that of an ideal system, thereby expanding the liquid state range while maintaining low volatility. Moreover, DESs exhibit tunability comparable to Ionic Liquids, as the HBA:HBD combination can be easily modified, altering the hydrogen-bonding dominance and influencing thermophysical properties. Despite ongoing research, the underlying mechanisms are still being explored to better understand their thermophysical behavior. Multiscale simulation proves to be a valuable tool in gaining additional insights to guide experimental efforts effectively.

This contribution outlines a practical methodology for thermophysical characterization of DESs in the context of greenhouse gas capture applications. The soft-SAFT equation of state, in conjunction with modeling tools like Turbomole-COSMO and machine learning, has been employed. By analyzing molecular simulation data or charge analysis distribution, a rational selection of a molecular model and the predominant number of hydrogen bonds is suggested. A comprehensive approach treating each entity within the DES as an independent compound is adopted to describe density, as well as the impact of water and co-solvents. The study of additional of properties, such as viscosity, is completed using artificial neural networks. Subsequently, the solubility of CO_2 and fluorinated refrigerants in various DESs is presented, emphasizing the influence of different variables (pressure, temperature) and structural characteristics of the DES (type of HBA, HBD, number of fluorine atoms, etc.) on the results [3-5]. This facilitates a rapid screening process to identify optimal conditions for specific gas capture or separation applications.

Acknowledgments

This research is supported by the Spanish Ministry of Science and Innovation and by European Union EU/PRTR under R+D+I projects STOP-F-Gas (PID2019-108014RB-C21) and NEW-F-TECH (TED2021-130959B-I00). S. B. Rodriguez Reartes acknowledges the financial support of the "María Zambrano" grant for the requalification of the Spanish university system for 2021-2023.

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