Soft-SAFT Transferable Molecular Models for the Description of Gas Solubilities in Eutectic Ammonium Salt Solvents

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The use of different amine-based organic solvents is very extensive in post-combustion CO2 capture. Despite their great properties to capture CO2 with high efficiency, the energetic penalty in the regeneration stage and their corrosive character have pushed research towards the evaluation of alternative solvents. Recently, Deep Eutectic Solvents (DESs) have claimed the industrial attention for the possibility to tune their physicochemical properties for a wide range of applications [1]. While sharing many of the characteristics of ionic liquids, such as a near-zero vapor pressure, these eutectic mixtures of a salt with a hydrogen bonding donor are generally biodegradable and can be easily synthesized at low cost. Different computational studies have demonstrated that the existence of multiple hydrogen-bonding interactions between the halide salt and a neutral complexing agent forming the eutectic are the key factor to understand their physicochemical behavior, including a decrease of the melting point of the mixture [2]. To reduce the number of experiments needed to study the relevant properties of these compounds, molecular modeling tools and, in particular, molecular-based equations of state that contain a specific term to deal with hydrogen-bonding effects, are an excellent option to screen these new solvents. In this work, different tetralkylammonium-based DESs are modelled within the soft-SAFT EoS framework using a consistent and transferable molecular model approach that considers the molecular parameters of each individual compound forming the eutectic [3]. A careful search of optimal and transferable parameters is carried out. Particular attention is later paid to the solubility of relevant gases such as CO_2 and SO_2 in DESs, evaluating the solvent capabilities for gas separations.

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References:

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