

Deep eutectic solvents : designing extracting agents for liquid-liquid extraction

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**DEEP EUTECTIC SOLVENTS:
DESIGNING EXTRACTING AGENTS FOR LIQUID-LIQUID EXTRACTION**

Congress: ECCE10

Topic: Fluid separations processes and technologies

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Abstract:

The separation of azeotropic mixtures, specifically the separation of aromatic and aliphatic compounds, is of crucial importance in the petrochemical business. Industrially, the sulfolane process is used for this separation. The sulfolane process implies liquid-liquid extraction using sulfolane as extracting agent followed by distillation for the sulfolane recovery. The main disadvantages of the sulfolane process are the usage of a volatile, flammable and toxic extracting agent together with the enormous energy requirements needed for the solvent recovery step.

In order to develop a more sustainable process, several green and novel solvents have been studied as alternative to the sulfolane. Ionic liquids (ILs) have been widely investigated for the separation of aliphatic-aromatic mixtures via liquid-liquid extraction [1]. However, the high price of ILs, associated mainly to the complicated synthesis and purification, is their main drawback for large scale application. Contrarily, deep eutectic solvents (DESs), which are ILs analogues in terms of properties, can be prepared cheaply, with low price starting materials and without purification requirements, overcoming the main disadvantage of ILs [2]. DESs are a mixture of one hydrogen bond donor (HBD) and one hydrogen bond acceptor (HBA), generally solids, that when mixed in the proper ratio, show a large decrease in the melting point compared to the initial compounds. In the last years, the scientific community has started to explore the applicability of this new generation of green solvents as extracting agents in liquid-liquid extraction, mainly for the separation of aliphatic-aromatic mixtures [3,4].

In this work, several new DESs have been tested as extracting agents for the separation of aliphatic-aromatic mixtures. The liquid-liquid equilibrium (LLE) of the ternary mixtures {hexane + benzene + DES} have been measured at two different temperatures (298.15 K and 398.15 K) and atmospheric pressure. The solute distribution coefficient and the selectivity have been calculated and compared to literature. The effect of the temperature and composition (e.g. chain length) has been studied. Moreover, the solvents have satisfactorily been recovered. The obtained experimental results show that DESs are promising extracting agents for the separation of aromatic components from aliphatic-aromatic mixtures. An economic evaluation of the sulfolane process compared to the process using ILs and DESs will be also presented.

Reference 1: A. Pereiro, J. Araújo, J. Esperança, I. Marrucho, I. Rebelo, *the journal of chemical thermodynamics*, 2012.

Reference 2 : M. Francisco, A. van den Bruinhorst, M. C. Kroon, *Angewandte Chemie International Edition*, 2013.

Reference 3 : M. A. Kareem, F. S. Mjalli, M. A. Hashim, I. M. AlNashef, *Fluid Phase Equilibria*, 2011.

Reference 4 : A. S. Gonzalez, M. Francisco, G. Jimeno, S. L. G. de Dios, M. C. Kroon, *Fluid Phase Equilibria*, 2013.

Highlight 1: Deep eutectic (DESs) solvents have been used as extracting agents

Highlight 2: The LLE data of the systems {aliphatic + ethanol +DES} have been measured

Highlight 3: The distribution coefficient and selectivity have been calculated and compared