LIQUID-LIQUID EQUILIBRIA AND TRANSPORT STUDIES OF TERNARY SYSTEMS COMPOSED OF IONIC LIQUID, 1-HEXANETHIOL AND *N*-DODECANE

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Abstract: Sulphur emissions from fossil fuels and refinery industries have a great impact in health and environment. In order to minimize the negative effects, environmental regulations have been more strict, aiming near-zero sulphur levels (< 10ppmw S) [1]. This deep desulfurization, performed with the conventional process (hydrodesulfurization), is very difficult, since it becomes inefficient and expensive when more stable sulphur compounds are presented at the petroleum streams.[1] In view of that, it is necessary an upgrading of the existing technologies and the development of new ones. An alternative that receive great expectation, at the academic and industrial community, is the use of ionic liquids (ILs) applied as solvent in extraction processes. The research developed so far is mainly based on aromatic sulphur compounds. Nonetheless, aliphatic sulphur compounds extraction behaviour also requires an understanding, in order to design and improve the processes efficiency. Thus this work addresses the use of imidazolium based-ionic liquids on a selective extraction of 1-hexanethiol from *n*-dodecane. Its feasibility was evaluated by the characterization of the liquid-liquid equilibrium (LLE) and the mercaptan transport between the phases, experimentally determined. However, due to the huge number of possible ionic liquids, a comprehensive selection via experimental observation is impossible, being important to model the LLE of mixtures containing ILs. Therefore, the experimental data was compared with the predicted results by the COSMO-RS model to evaluate its performance on describing and predicting these types of systems, aiming its appliance on identifying the ionic liquids with greater potential.

References: [1] P. S. Kulkarni and C. A. M. Afonso, Deep desulfurization of diesel fuel using ionic liquids: current status and future challenges. *Green Chemistry* 12 (2010) 1139-1149.