Modeling of Liquid-Liquid Equilibrium for BTX extraction using COSMO-SAC model

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The most commonly used plastics, clothing, film, rubber, etc. are made by benzenes, toluenes, and xylenes (BTX) among the ingredients of petroleum. BTX are not easy to separate from C4 to C10 aliphatic hydrocarbon mixtures that make up crude oil because aromatic hydrocarbons form azeotropes with similar boiling points to other aliphatic hydrocarbons. More recently, ionic liquids (ILs) owing to thermal and chemical stability, and negligible vapor pressure try to use as an extraction solvent, which can be extracted from aromatic compounds through simple processes such as flash distillation or stripping in crude oil. The NRTL, UNIQUAC, and UNIFAC models require the binary interaction parameters to be determined by regressing the experimental data, and have a limit to use them widely because of the huge amount of possible cation-anion combinations. On the other hands, COSMO-base models as a predictive model are free in this problem because they do not need the fitting parameters and recently was used widely. In this work, COSMO-SAC model applies to predict the extraction efficiency of different ILs for the mixtures of alkanes, cycloalkanes and aromatic compounds mixtures.