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Separation of benzene from methylcycloalkanes by extractive distillation with cyano-based ionic liquids: Experimental and CPA EoS modelling

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ABSTRACT

The aromatic/aliphatic separation using ionic liquids (ILs) has been proposed as an enhanced technology when compared to conventional liquid-liquid extraction and extractive distillation processes. Some ILs show extractive properties (distribution ratios and selectivities) greater than those of conventional solvents, like sulfolane and N-methylpyrrolidone, positioning these solvents to address challenging separations. Methylcycloalkanes and benzene are close-boiling mixtures in the petrochemical industry, presented at the hydrogenated pyrolysis naphtha where benzene is at a high concentration (ca. 70 wt%). Aiming to tackle this separation, cyano-based ILs were tested as mass agents in the benzene separation from methylcycloalkanes. A complete phase equilibria characterization with the most promising ILs, $[C_2C_1im][DCA]$ and $[C_2C_1im][SCN]$, were done, using a recently developed experimental-modelling strategy. Isothermal vapour-liquid equilibria for binary, ternary and quaternary systems was measured by Headspace Gas-Chromatography (HS-GC) and modelled using the Cubic Plus Association (CPA) Equation of State (EoS). The presence of the ILs improved the methylcycloalkane/benzene relative volatilities by one order of magnitude, whereas homogeneous and heterogeneous regions were determined by HS-GC, leading to a consistent model.

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