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Design calculations of an extractor for aromatic and aliphatic hydrocarbons separation using ionic liquids

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The study concentrates on the separation of aromatic hydrocarbons from aliphatic hydrocarbon mixtures using ionic liquids as a new alternative of extraction solvents. Influence of the phase equilibrium description accuracy on the separation equipment design using different thermodynamic models was investigated. As a model system, a heptane–toluene binary mixture was chosen, employing 1-ethyl-3-methylimidazolium ethyl sulfate (EMIES) ionic liquid as an extractive solvent. Liquid–liquid equilibrium (LLE) data of the ternary system were calculated using NRTL equations with different quality model parameters. Model 1 corresponds to the NRTL equation with the original binary parameters evaluated independently from the respective binary equilibrium data. Model 2 is represented by an NRTL equation extended by the ternary correction term (with the original binary parameters and ternary correction term parameters evaluated from the ternary tie-lines). Model 3, i.e. the NRTL equation with binary model parameters determined via ternary LLE data regression using ASPEN Plus, was taken from Meindersma et al. (2006). Continuous-flow liquid-phase extraction was simulated considering a cascade of mixer–settler type extractors according to the Hunter–Nash scheme (Hunter & Nash, 1934). Based on the simulation results, for a preset separation efficiency criterium, different accuracies of the equilibrium description caused serious discrepancies in the separation equipment design, e.g. in the number of theoretical stages, solvent to feed ratio, and product purity.
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Introduction

Fossil materials (coal, crude oil, natural gas) are a common source of hydrocarbons. In past, aromatics, namely benzene, were obtained as by-products of coal coking. Nowadays, most of the aromatic hydrocarbons (over 90 % of the total consumption) are produced from crude oil, only a small portion is produced from coal (Wauquier, 2000). Practically all liquid fractions obtained by fractional distillation of naphtha contain aromatics; however, due to their low content, their separation is not profitable. In order to increase the aromatics' content, primary fractions obtained by crude oil distillation are submitted to aromatization and the obtained aromatics are separated from the product. Aromatic hydrocarbons are typically obtained from the product of catalytic reforming of primary gasoline or from pyrolysis of gasoline after selective hydrogenation of dienes (Blažek & Rábl, 2006).

Feed of ethylene producing units in most refineries contains about 10 mass % to 25 mass % of aromatics depending on its source. This stream serves as a source of aromatic hydrocarbons. In praxis, there are several procedures for selective separation of aromatics from hydrocarbon mixtures: liquid extraction for aromatic contents from 20 mass % to 65 mass %, extractive distillation for 65 mass % to 90 mass %, and azeotropic distillation for aromatic content higher

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