I&EC research
Industrial & Engineering Chemistry Research

Article

Cite This: *Ind. Eng. Chem. Res.* 2019, 58, 19681−19692

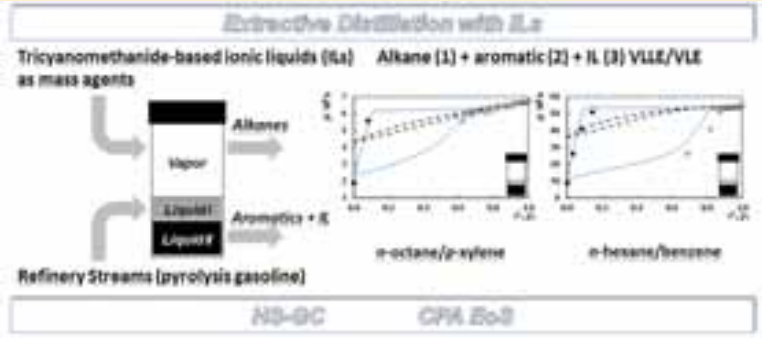
pubs.acs.org/IECR

Toward Modeling the Aromatic/Aliphatic Separation by Extractive Distillation with Tricyanomethanide-Based Ionic Liquids Using CPA EoS

Miguel Ayuso,[†] Pablo Navarro,[*,‡,§] André M. Palma,[‡] Marcos Larriba,[†,‡] Noemí Delgado-Mellado,[†] Julián García,[†] Francisco Rodríguez,[†] João A.P. Coutinho,[‡] and Pedro J. Carvalho[‡]

[†]Department of Chemical Engineering, Complutense University of Madrid, Madrid, Spain
[‡]CICECO − Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Aveiro, Portugal
[§]Department of Chemical Engineering, Autónoma University of Madrid, Madrid, Spain

Supporting Information



ABSTRACT: Extractive distillation using tricyanomethanide-based ionic liquids (ILs) has been shown to be a promising and feasible process for effectively separate aromatics from pyrolysis gasolines. The high performance of these mass agents has been reported by evaluating simple synthetic *n*-heptane/toluene binary mixtures, on a wide temperature and solvent to feed (*S*/*F*) ratio ranges. However, industrial streams are much more complex with the presence of other aromatic and aliphatic compounds, like benzene, xylenes, and shorter and longer linear alkanes, creating further difficulties to the separation and thus must be studied. This work covers the phase equilibrium characterization of {*n*-hexane + benzene + IL} and {*n*-octane + *p*-xylene + IL} ternary systems with two tricyanomethanide-based ILs, namely 1-ethyl-3-methylimidazolium tricyanomethanide ([C_2C_1im][TCM]) and 1-butyl-4-methylpyridinium tricyanomethanide ([4-C_4C_1py][TCM]), addressing also the phase characterization of the corresponding {hydrocarbon + IL} binary systems. The phase equilibria were determined by headspace gas chromatography (HS-GC) in a wide range of hydrocarbon compositions, temperatures and *S*/*F* ratios and modeled using the Cubic Plus Association (CPA) Equation of State (EoS). This is the first work proposing a consistent EoS model for a multicomponent separation case involving ILs, demonstrating its suitability for a wide range of conditions in binary and ternary systems.

Received: August 12, 2019
Revised: September 12, 2019
Accepted: September 25, 2019
Published: September 25, 2019

DOI: 10.1021/acs.iecr.9b04440
Ind. Eng. Chem. Res. 2019, 58, 19681−19692