Separation and Purification Technology 190 (2018) 211–227

Contents lists available at ScienceDirect

Separation and Purification Technology

journal homepage: www.elsevier.com/locate/seppur

COSMO-based/Aspen Plus process simulation of the aromatic extraction from pyrolysis gasoline using the {[4empy][NTf_2] + [emim][DCA]} ionic liquid mixture

Marcos Larriba[a,*], Juan de Riva[a], Pablo Navarro[b], Daniel Moreno[a], Noemí Delgado-Mellado[c], Julián García[c], Victor R. Ferro[a], Francisco Rodríguez[c], José Palomar[a]

[a] Sección de Ingeniería Química, Universidad Autónoma de Madrid, 28049 Madrid, Spain
[b] CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Aveiro, Portugal
[c] Departamento de Ingeniería Química, Universidad Complutense de Madrid, 28040 Madrid, Spain

ARTICLE INFO

Keywords:
Aromatic-aliphatic separation
Ionic liquids
Aspen Plus
COSMO-RS
Process simulation

ABSTRACT

The ionic liquids (ILs) have been widely studied as potential replacements of conventional solvents in the extraction of aromatic hydrocarbons from alkanes. However, most of the literature is focused in obtaining liquid-liquid equilibria experimental data without studying the complete extraction and IL regeneration process. In this paper, a computer-aided methodology combining COSMO-based molecular simulations and Aspen Plus process simulations has been used to study the extraction process of aromatic hydrocarbons from pyrolysis gasoline employing a binary mixture of 1-ethyl-4-methylpyridinium bis(trifluoromethylsulfonyl)imide ([4empy][NTf_2]) and the 1-ethyl-3-methylimidazolium dicyanamide ([emim][DCA]) ILs as solvent. An extensive comparison (more than 600 points) between experimental data and the predictions obtained by the COSMO-based thermodynamic model of liquid–liquid and vapor–liquid equilibria and ILs physical properties was made for validation purposes. Process simulations were performed in three system configurations: with one, two, or three flash distillations in the IL recovery section. The potential advantage of using binary IL-IL mixture as extracting solvent was studied in the whole range of composition. The configuration with three flash distillations and the binary IL-IL mixture with a 75% of [4empy][NTf_2] were selected as the optimal conditions to increase aromatic recovery and purity, improving the separation performance respect to the neat ILs.

* Corresponding author.
E-mail address: marcos.larriba@uam.es (M. Larriba).

http://dx.doi.org/10.1016/j.seppur.2017.08.062
Received 15 June 2017; Received in revised form 21 August 2017; Accepted 24 August 2017
Available online 01 September 2017