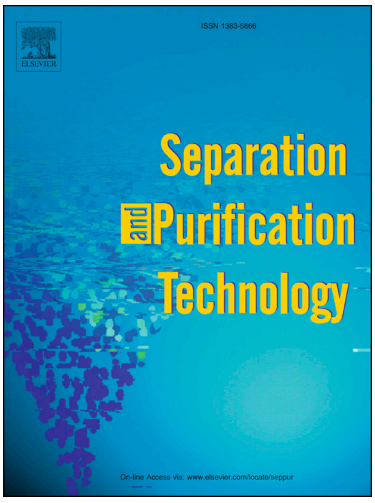

Extraction of nitrogen compounds from model fuel using 1-ethyl-3-methylimidazolium methanesulfonate

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Abstract[1]

Removal of nitrogen compounds is an essential process in the fuel processing industry. In this work, the extraction performance of 1-ethyl-3-methylimidazolium methanesulfonate ([Emim][$MeSO_3$]) ionic liquid in removing pyrrole, indoline, pyridine and quinoline from cyclohexane is investigated. The ternary liquid-liquid equilibria for four systems containing [Emim][$MeSO_3$] + pyrrole/indoline/pyridine/quinoline + cyclohexane were predicted using COSMO-RS and validated experimentally at 298.15 K under atmospheric pressure, with feed concentrations of nitrogen compounds ranging from 5 to 50 wt. %. Othmer-Tobias and Hand correlations confirmed the consistency of the experimental data. The tie-lines obtained experimentally and predicted with COSMO-RS were in good agreement. Additionally, the non-random two-liquid (NRTL) model was successfully employed to correlate the experimental tie-lines. The effects of basicity of nitrogen compounds toward extraction efficiency were also investigated. The selectivity and distribution ratio results demonstrated the suitability of [Emim][$MeSO_3$] as an extraction solvent for removing nitrogen compounds from fuel. Finally, the multicomponent extraction confirmed the performance of [Emim][$MeSO_3$] for extractive denitrogenation. In all ternary systems investigated in this work, the concentration of cyclohexane in the extract phase was very small and the presence of the IL in the raffinate phase was negligible indicating minimum cross contamination between the extract and raffinate phases.

Keywords: Denitrification; Ionic liquid; Liquid-liquid extraction; COSMO-RS; NRTL

[1] **Abbreviations:** COSMO-RS, Conductor-like Screening Model for Real Solvents; BP functional, Becke-Perdew functional; DFT, density functional theory; EDN, extractive denitrogenation; HDN, hydrodenitrogenation; IL, Ionic liquid; LLE, liquid-liquid extraction; NRTL, non-random two-liquid; RI, resolution of identity; RMSD, root mean square deviation.