

Ionic-Liquid Based Separation of Azeotropic Mixtures - DTU Orbit (08/11/2017)

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methodology for the screening of ionic liquids (ILs) as entrainers for ILs-based separation processes in binary aqueous azeotropic systems (e.g., water + ethanol and water + isopropanol) is presented. Ionic liquids as entrainers were first screened based on a combination of criteria such as stability, toxicity, and environmental impacts of the ILs. A Hildebrand solubility parameter group contribution model for ILs is highlighted to screen the miscibility of the ILs with the target solute component which was considered as a key target property to further screen the candidates from the previous step. The best candidates for aqueous systems were selected for final evaluation as follows: 1-ethyl-3-methylimidazolium ethylsulfate [C2MIM][EtSO₄], 1-ethyl-3-methylimidazolium acetate [C2MIM][Ac], 1-ethyl-3-methylimidazolium dicyanamide [C2MIM][N(CN)₂], and 1,3-dimethylimidazolium dimethyl phosphate [C1MIM][DMP]. For the final evaluation, the best candidates for aqueous systems were used as entrainers, and then the vapor-liquid equilibrium (VLE) of the ternary systems containing ILs was predicted by the Non Random Two Liquids (NRTL) model to confirm the breaking of the azeotrope. Based on minimum concentration of the ILs required to break the given azeotrope, the best ILs as entrainers for water + ethanol and water + isopropanol azeotropic mixtures were [C1MIM][DMP] and [C2MIM][N(CN)₂], respectively.

General information

State: Published

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Pages: 517-522

Publication date: 2014

Host publication information

Title of host publication: Proceedings of the 17th Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction

Volume: 39

ISBN (Print): 978-88-95608-30-3

Series: Chemical Engineering Transactions

ISSN: 2283-9216

Main Research Area: Technical/natural sciences

Conference: 17th Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction, Prague, Czech Republic, 23/08/2014 - 23/08/2014

DOIs:

10.3303/CET1439087

Publication: Research - peer-review › Article in proceedings – Annual report year: 2015