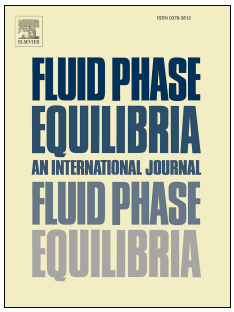

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Zhigang Zhang, Ru Yang, Wenxiu Li, Tao Zhang, Debiao Zhang, Qinqin Zhang

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Separation of acetonitrile and methanol azeotropic mixture using imidazolium-based ionic liquids as entrainers

Zhigang Zhang, Ru Yang, Wenxiu Li **, Tao Zhang, Debiao Zhang, and Qinqin Zhang *.

Liaoning Provincial Key Laboratory of Chemical Separation Technology, Shenyang University of Chemical Technology, Shenyang 110142, China.

Abstract:

In this work, three imidazolium-based ionic liquids (ILs) with different anions, namely 1-butyl-3-methylimidazolium chloride ([BMIM][Cl]), 1-butyl-3-methylimidazolium bromide ([BMIM][Br]) and 1-butyl-3-methylimidazolium acetate ([BMIM][OAc]), were tested as entrainers to separate acetonitrile and methanol mixtures. Isobaric vapor-liquid equilibrium (VLE) data of the acetonitrile (1) + methanol (2) + IL ternary systems were measured at 101.3 kPa. Addition of ILs produced a salting-out effect on acetonitrile, thus leading to the increase of the relative volatility of acetonitrile to methanol. As IL content increased to a certain value, the azeotropic point of acetonitrile and methanol could be totally eliminated. In addition, the separation performance of ILs was closely related to anion structure, with [BMIM][OAc] producing the most significant salting-out effect orderly followed by [BMIM][Cl] and [BMIM][Br]. Finally, the measured ternary VLE data were correlated with the nonrandom two-liquid (NRTL) model, and σ-Profiles were used to explain the separation performance differences of the three ILs.

Keywords:

Vapor-liquid equilibrium; ionic liquids; acetonitrile; methanol; NRTL model; σ-profiles.

1. Introduction

Acetonitrile and methanol are important solvents, and have been extensively used in chemical and pharmaceutical processes.[1,2] For example, they are used in reverse phase high performance liquid chromatography[3], and also used as raw material in organic synthesis to produce acetamidine hydrochloride which is widely served as a synthetic pharmaceutical intermediate of 4,6-Dihydroxy-2-methylpyrimidine. [4,5] Moreover, mass spectrum and chromatography techniques also produce some mixtures of them.[6-8] Those procedures inevitably produce a large quantity of mixtures of methanol and acetonitrile. Unfortunately, the binary system of methanol and acetonitrile forms an azeotrope at atmospheric pressure, and this azeotrope cannot be separated by conventional distillation process.[1]

Extractive distillation, which combines the virtues of extraction and distillation, is an effective special distillation and is widely adopted in industry to separate azeotropic or close-boiling mixtures. [9-11] the key to extractive distillation is the selection of competent entrainers. Yang Yu et al. [12] reported isobaric VLE data for the system of acetonitrile and methanol using traditional organic solvents (N,N-dimethylformamide and aniline) as entrainers. However, the traditional organic solvents used in extractive distillation have some disadvantages such as environment pollution caused by volatile emission and difficulty in recycling.[13] Therefore, new entrainers which are eco-friendly and easy to be recycled are urgently desired.

ILs, which are totally composed of ions, are regarded as green and designable solvents. They have many unique physic-chemical properties such as high thermal and chemical stability, excellent dissolving capacity