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Vapor–Liquid Equilibrium in Binary and Ternary Azeotropic Solutions Acetonitrile-Ethanol-Water with the Addition of Amino Esters of Boric Acid

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Abstract: The effect of amino esters of boric acid (AEBA) on the conditions of vapor–liquid equilibrium in binary mixtures of acetonitrile–water, ethanol–acetonitrile and a three-component mixture of ethanol-acetonitrile-water was investigated. Residual curves and vapor–liquid phase equilibrium conditions (TPXY data) were experimentally measured at atmospheric pressure for a binary mixture of acetonitrile-AEBA and a triple mixture of acetonitrile-water-AEBA. Previously unknown energy binary parameters of groups B, CH_2N with group CH_3CN were determined for the UNIFAC model. The correction of the value of the binary parameter water—acetonitrile was carried out. On the basis of thermodynamic modeling, the degree of influence of AEBA on the relative volatility of acetonitrile in binary and ternary mixtures was analyzed. It is shown that the use of AEBA removes all azeotropic points in the studied mixtures. In this case, acetonitrile turns out to be a volatile component, and water is a non-volatile component in the entire concentration range.

Keywords: vapor–liquid equilibrium; azeotropic mixtures; UNIFAC model; extractive distillation

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1. Introduction

Acetonitrile and ethanol are important organic solvents that are used in many industries [1,2]. The areas of their use are quite wide and include components for chemical synthesis, solvents, entrainers, etc. For example, ethanol is an important source in the synthesis of esters, is used as a solvent for the production of paints and varnishes, for the manufacture of medicines, food, consumables in household chemicals and is one of the most common types of biofuels. [3]. Acetonitrile is necessary for the production of pharmaceuticals, purification of butadiene and fatty acids [4,5], as a medium for chemical reactions, where it can also serve as a catalyst [6].

In industrial technologies, acetonitrile and ethanol are often present in mixtures with water [7–9]. Since acetonitrile and ethanol are often used as mobile phases in liquid chromatography, a ternary mixture of ethanol-acetonitrile-water is formed at the final stage of the analytical process, requiring separation. This raises the problem of separating these mixtures into individual substances. The separation of acetonitrile and ethanol from their liquid solutions in water by using distillation is difficult due to the formation of both binary and ternary azeotropic mixtures by them [10–12]. Thus, the acetonitrile–water system forms an azeotrope boiling at 349.65 K and containing 83.7 wt.% acetonitrile [13]; the ethanol–acetonitrile system forms an azeotrope boiling at 345.65 K and containing 46.9 wt.% acetonitrile [13]; the ethanol–water system forms an azeotrope boiling at 351.35 K and containing 96 wt.% ethanol [13]; the ethanol-acetonitrile-water system forms a ternary azeotropic mixture boiling at 346.05 K and containing 55 wt.% ethanol, 44 wt.% acetonitrile [10]. From the point of view of ecology and economic benefits, the problem of separating such ternary systems is extremely important [14].