Abstract

Liquid–liquid equilibrium (LLE) data for water + acetic acid + solvent (dichloromethane + methyl isobutyl ketone) ternary systems are measured experimentally at $T = 301.15$ K and $p = 1$ atm. Different proportions of pure solvents dichloromethane (DCM) and methyl isobutyl ketone (MIBK) are investigated. The cloud-point titration technique is employed in order to determine the equilibrium solubility data. The chemical species' concentrations, in both the light and heavy phases, were estimated using refractive index measurements. For activity coefficients prediction, the non-random two liquids (NRTL) model was used to correlate the measured tie-line data. Two evolutionary optimization methods (i.e., the genetic algorithm and the particle swarm optimization) are used in order to estimate the binary interaction parameters for the NRTL model. In addition to this, both the Othmer–Tobias and the Hand correlations are used to verify the thermodynamic consistency and reliability of the experimental tie-line measured data. Finally, the distribution coefficients and the separation factors are calculated in order to determine the suitability of the mixed solvents for the acetic acid extraction from water. The present results indicate that the mixed solvent (50% DCM + 50% MIBK) is the most suitable solvent for the separation the acetic acid from water.

Keywords: Acetic acid extraction; Liquid–liquid equilibrium; Distribution coefficient and separation factor; Genetic algorithm; Particle swarm optimization

1. Introduction

The determination of accurate phase equilibrium data for multicomponent mixtures has paramount importance to the study of various chemical processes. For example, good design of an extraction equipment requires experimental determination and/or theoretical prediction of liquid–liquid equilibrium (LLE) data. In recent years, several authors [1–6] have investigated LLE of ternary systems. Recently, mixed solvents have been investigated as potential candidates for extraction processes [6,7] including mixtures containing water and acetic acid [8,9].

A water-free acetic acid is called glacial acetic acid, which is a colorless liquid and has a distinctive sour taste and a pungent smell. Concentrated acetic acid is corrosive and can attack skin. On the other hand, when mixed with water it forms vinegar [10]. It is used as a precursor to poly(vinyl acetate) and cellulose acetate.

It is not possible to separate this acid from water by distillation due to a severe tangent pinch. Thus, solvent extraction is a promising alternative for the recovery of the acetic acid diluted in water. Selecting a good extraction solvent has a substantial effect on pure acetic acid retrieval. Several authors [2,11] have studied LLE data for ternary mixtures, which are composed of acetic acid and water. In the present work, we have tried solvents composed of dichloromethane (DCM) and methyl isobutyl ketone (MIBK) mixed in different proportions. These solvents are attractive since they possess low toxicity, are relatively cheap and have less solubility in water.