Liquid-Liquid Equilibrium of the Ternary System Water/Formic Acid/1-Pentanol at $T=308.2$ K

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ABSTRACT

Liquid–liquid equilibrium data for the (water + Formic acid + 1-pentanol) ternary system were determined at $T=(308.2)$ K in ambient pressure. This ternary system exhibits type-1 behavior of LLE. Distribution coefficients and separation factors were measured to evaluate the extracting capacity of the solvent. The consistency of the experimental tie-line data was determined through the Othmer–Tobias and Bachman equations. The raw experimental data were correlated using the NRTL and UNIQUAC models. The average root-mean-square deviation between the experimental and calculated mass fractions was 0.488% and 0.465%.

Keyword: 1-Pentanol, Formic Acid, Liquid–Liquid Equilibrium (LLE), NRTL, Separation Factor, Tie-Line Data, UNIQUAC

INTRODUCTION

Phase equilibrium data of ternary systems composed of (water + carboxylic acid + organic solvents) are important in both theoretical and industrial applications. As the separation of carboxylic acids from aqueous solutions resulting from fermentation processes or synthetic methods is industrially and scientifically important, the precise LLE data are needed and required in design of many chemical processes, separation operations, and fermentation industry. Many researchers have investigated various kinds of the multi-component systems in order to understand and provide further information about the phase behaviour and the thermodynamic properties of such systems (Ghanadzadeh Gilani, & Golpour, 2011). Formic acid is one of the most widely used carboxylic acids, which has many industrial applications. Formic acid is a colorless liquid having a highly pungent, penetrating odor (Steyer & Sundmacher, 2005) at room temperature. It is miscible with water and most polar organic solvents, and is somewhat soluble in hydrocarbons. In hydrocarbons and in the vapor phase, it consists of

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hydrogen-bonded dimers rather than individual molecules. (a b c d e f g Werner Reutemann & Heinz Kieczka, 2002-Roman.a b, Balabin, 2009) Formic acid can be produced by chemical synthetic or fermentation methods. So, the extraction of this acid from aqueous mixtures using the liquid + liquid extraction technique is still an important problem. As the separation by solvent extraction depends on mutual solubility of the (water + Formic acid) mixture, the variation of solubility of organic solvent in the mixture is an important feature in the LLE investigations. Significant investigation has been carried out in recent years on the LLE measurements and the extraction of Formic acid from aqueous solutions (Baslıo˘glu & Cehreli, 2011; Hwang, Park, & Choi, 2008). This work presents a useful LLE data for the extraction of Formic acid from aqueous solution. Complete phase diagrams are obtained by solubility and tie-line data for each temperature. Separation factors (S) are also determined from the tie-line data to establish the possibility of the use of this solvent for the separation of (water + Formic acid) binary mixture.

EXPERIMENTAL

Material

The supplier, purity, and some properties for the organic chemicals used in this study are listed in Table 1. The organic chemicals were dried over molecular sieves (Merck 4Å). Distilled and deionized water was used throughout all experiments. All materials were used as received without any further purification.

Binodal Curve Measurement

The binodal curves for the ternary mixtures were determined by the cloud point method in an equilibrium glass cell (GhanadzadehGilani & Ghanadzadeh Gilani, 2010). The prepared binary mixtures of known compositions were introduced into the glass cell. The temperature of the cell was controlled by a water jacket and maintained with an accuracy of within ±0.01 K. The third component was progressively added using a micro-burette. The end point was determined by observing the transition from a homogeneous to a heterogeneous mixture. All the measurements were repeated at least three times. The average of these readings was taken for the component compositions Table 2.

Tie Lines

Two-phase three-component solutions were prepared by weighing the components. The prepared mixtures were introduced into the extraction cell and were stirred for 4 h, and then left to settle for 4 h for phase separation. After being allowed to reach equilibrium, samples were carefully taken from each phase and analyzed. The analysis for the two phases was done by direct titration of weighted sample against 0.1N sodium hydroxide with phenolphthalein as the indicator.

Table 1. Supplier, purity and the measured and literature physical properties of the materials at T = 293.2K (D.R. Lide (Ed.),2010 (1), D.R. Lide (Ed.), 2009 (2))

<table>
<thead>
<tr>
<th>component</th>
<th>Molar mass (g / mol)</th>
<th>Supplier</th>
<th>Mass fraction purity</th>
<th>nD</th>
<th>$\rho$/(Kgm-3)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Exp.</td>
<td>Lit.</td>
</tr>
<tr>
<td>Formic acid</td>
<td>46.026</td>
<td>Merck</td>
<td>&gt; 0.99</td>
<td>1.3712</td>
<td>1.3714(1)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Exp.</td>
<td>Lit.</td>
</tr>
<tr>
<td></td>
<td>1-Pentanol</td>
<td>88.148</td>
<td>Merck</td>
<td>1.41</td>
<td>1.4101(1)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Exp.</td>
<td>Lit.</td>
</tr>
<tr>
<td></td>
<td>Water</td>
<td>18.015</td>
<td></td>
<td>1.331</td>
<td>1.3330(2)</td>
</tr>
<tr>
<td></td>
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