(Liquid + Liquid) Equilibrium for Ternary System of (Water + Phenol + Cyclohexane) at \( T = 298.2 \text{ K} \)

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ABSTRACT
Experimental solubility curves and tie-line data for the (water + phenol + 2-ethyl-1-hexanol) system was obtained at \( T = 298.2 \text{ K} \) and atmospheric pressure. The tie-line data was determined by techniques karl-fischer and refractometry. This ternary system exhibits type-2 behavior of LLE. Distribution coefficients and separation factors were measured to evaluate the extracting ability of the solvent. The consistency of the experimental tie-line data was determined through the Othmer–Tobias and Bachman equations. The data were correlated with the NRTL (\( \alpha = 0.25 \)) and UNIQUAC models and the parameters estimated present root mean square deviations below 0.50%.

Keywords: Cyclohexane, Extraction, Liquid + Liquid Equilibrium (LLE), NRTL, Phenol, UNIQUAC

INTRODUCTION
Liquid + liquid equilibrium (LLE) investigations for ternary aqueous mixtures of phenol with organic solvents are important in evaluation of industrial solvent extraction units. Accurate ternary equilibrium data are always needed for efficient separation of phenol from water.

One of the important sections of the petrochemical industry is phenol production, especially for the production of resins (Matar & Hatch, 2001). Phenol is formed by oxidation of cumene in liquid phase, leading to cumene hydroperoxide (CHP); in following order: the CHP suffers a catalytic decomposition, producing phenol and acetone with water and \( \alpha \)-methyl styrene as byproducts. So, a stream including phenol, water and small amounts of acetone and \( \alpha \)-methyl styrene is produced at the end of the process (Speight, 2002). The remotion of

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phenol from aqueous solutions is an environmental interest for a very toxic stream (Dohnal & Fenclová, 1995). To remove phenol from wastewater, liquid extraction can be more economically feasible than distillation, since these streams contain low concentrations of phenol and (phenol + water) forms an azeotrope at 9.2 wt% of phenol (Pinto et al., 2005). Additionally, Brazilian law restricts the mass fraction of total phenol from \((0.3 \times 10^{-6} \text{ to } 1.0 \times 10^{-6})\) wt% in fresh water, \(6.0 \times 10^{-6}\) wt% in salt water, and \(0.3 \times 10^{-6}\) wt% in brackish waters. Various solvents have been proposed for this process. According to the authors, the esters are most appropriate for the separation of phenol from water because of their present better selectivity ratio versus distribution coefficient results (González et al., 1986). The distribution coefficients of phenol for systems (water + phenol + 1-decanol) and (water + phenol + tridecanol) have been published at \(T = 293.15\) K (Scott et al., 1992). The LLE data for the systems (water + phenol + tert-butanol) at 298.15 K and (water + phenol + 1-butanol), (water + phenol + 2-butanol) are reported at \(T = (298.15\) and 313.15) K (Oliveira & Aznar, 2010). The systems (water + phenol + dimethyl carbonate), (water + phenol + diphenyl carbonate) have been studied at \(T = 358.15\) K (Hwang & Park, 2011).

**EXPERIMENTAL**

**Material**

The phenol and 2-ethyl-1-hexanol with stated mass fraction purities higher than 0.99 were purchased from Chem-lab and Merck, respectively. The organic chemicals were dried over molecular sieves. Distilled and deionised water was used throughout all experiments. All materials were used as received without any further purification. Some measured physical properties for the chemicals used in this study along with the literature values are listed in (Table 1).

**Apparatus and Procedure**

The solubility curve (binodal) was determined by the cloud point method in an equilibrium glass cell with a water jacket to maintain isothermal conditions. The temperature of the cell was controlled by a water jacket and maintained with an accuracy of within \(\pm 0.1\) K. At each system, the third component was progressively added using a microburet. The end-points were determined by observing the transition from an appearance to disappearance mixtures. All the measurements were repeated at least three times. The average of these readings was taken for the component compositions (Table 2).

A 250 cm\(^3\) glass cell connected to a thermostat was used to measure the tie-line data. The equilibrium data were determined by preparing the ternary mixtures of known compositions. The prepared mixtures were agitated vigorously for at least 4 h, and then left to settle for 5 h for complete phase separation. For these ternary systems, this time long enough to achieve equilibrium. When the equilibrium was attained, the system separated into two liquid phases that become clear and transparent with a well-defined interface. The sample of the organic-rich phase was carefully taken from the top sampling port of a syringe, and that of the water-rich phase was taken from a bottom sampling port of the cell.

<table>
<thead>
<tr>
<th>Presence</th>
<th>(\text{n})</th>
<th>(\rho) (Kg.m(^{-3}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>cyclo-hexane</td>
<td>1.4234</td>
<td>773.86</td>
</tr>
<tr>
<td>Water</td>
<td>1.3325</td>
<td>997.06</td>
</tr>
</tbody>
</table>

*Table 1. The refractive index \(\text{n}\) and density \(\rho\) of the pure components at \(T = 298.2\) K*
The Dispersion Effect of Carbon Nanotubes on the Viscoelastic Properties of Epoxy by Perez Model

Optimizing the Size of Drug-Loaded Nanoparticles Using Design of Experiments: Solid Lipid Nanoparticles
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