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Liquid-liquid Equilibrium Determination and Thermodynamics Modeling for Extraction of Isopropanol from Its Aqueous Solution

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Abstract

To separate isopropanol from its aqueous solution, isobutyl acetate, butyl acetate and butyl propionate were adopted as the extractive solvents, and the liquid-liquid equilibrium (LLE) data for the ternary systems (isobutyl acetate / butyl acetate / butyl propionate) + isopropanol + water were determined at 298.15 K and 308.15 K under atmospheric pressure. The experimental LLE data were correlated by the NRTL and UNIQUAC models, and the values of the root mean square deviations (*RMSD*) were less than 1%. And the binary interaction parameters of the NRTL and UNIQUAC models were optimized. Meantime, the distribution coefficient and selectivity were calculated to evaluate the extraction capacity of the solvents. As a result, butyl propionate is a desirable extractive solvent compared with the other two solvents.

Keywords: liquid-liquid equilibrium; isopropanol; extraction; extractive solvents

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