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Liquid–liquid Equilibrium in Systems Used for the Production of 5–Hydroxymethylfurfural from Biomass Using Alcohols as Solvents

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ABSTRACT

The present work reports liquid–liquid equilibrium data for systems containing water + 5–hydroxymethylfurfural + {1–butanol, 2–butanol or 2–pentanol} at $T = 298.2$ K and atmospheric pressure (~ 0.1 MPa), determined by refractometry and density measurements. The results were evaluated by calculation of the overall mass balance, resulting in overall relative deviations lower than 1.05 %. Experimental data were correlated with the NRTL model to calculate the activity coefficient. The average root mean square deviation was equal to 0.65 % for all systems. Cloud points, tie lines, partition coefficients and selectivities indicated that 2–pentanol is better than the other studied solvents for 5–hydroxymethylfurfural recovery from water.

Keywords: Liquid–liquid equilibrium, extraction, 5–hydroxymethylfurfural, NRTL model

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