Effect of Temperature and Organic Solvent Structure on Ternary Liquid-Liquid Equilibria of (Water + Short-Chain Normal Alcohol + Organic Solvent) Systems

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Anhydrous short-chain normal alcohols have numerous applications, from fuel additives or replacements to the pharmaceutical and cosmetic industries. The alcohols are often produced in aqueous streams, such as in the Fischer-Tropsch process, or in biofermentation processes. Thus, alcohol dehydration is an important consideration for these processes. The complex phase behavior seen in (water + short-chain alcohol) systems, including the formation of azeotropes, necessitates the use of advanced separation techniques, such as heterogenous azeotropic distillation (HAD) and liquid-liquid extraction. In these two processes, an additional component is chosen such that a two-liquid-phase mixture is formed in a way that allows recovery of the component of interest to the desired liquid phase. For alcohol dehydration, recovery of the alcohol to the organic phase is preferred. Liquid-liquid equilibria (LLE) data provide crucial insight into the alcohol recovery to both phases for solvent selection, as well as the necessary data for the design and optimization of decantation processes.

This work aims to evaluate and qualitatively define the effect of the organic solvent structure and temperature on the liquid-liquid behavior in ternary (water + ethanol/n-propanol/n-butanol + organic solvent) systems between 25°C and 45°C. The organic solvents of interest include an aliphatic branched hydrocarbon (isooctane), a cyclic hydrocarbon (cyclohexane), and two oxygenates (diisopropyl ether (DIPE) and isoamyl alcohol). Data were measured for these systems where no literature data were available. These experimental data, along with the literature data, were used to fulfill the aim of this work. The alcohol distribution between the organic and aqueous phases, the alcohol and water selectivity, as well as the size of the miscibility region, were investigated for the various solvent and alcohol combinations. Further, the influence of temperature on these parameters was considered.