

Measurement and Correlation of Ternary Liquid-Liquid Equilibria of Acetonitrile and Water with n-Dodecane, 1-Dodecene, Nonanol and Heptanoic Acid at 323.15 K and 1 atm

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Liquid-liquid extraction is important as it provides prospects for substantial energy saving when compared with distillation, when a minor but high density constituent of the feed mixture is to be recovered [1]. Reliable phase equilibrium data are required for the design and evaluation of industrial units for separation processes, especially ternary liquid-liquid equilibrium data [2].

A binary mixture of acetonitrile and water is primarily used as an extraction solvent for unsaturated hydrocarbons and as a general purpose solvent for many compounds based on its selective miscibility. Liquid-liquid equilibria data on a number of ternary mixtures containing acetonitrile have been published in the literature [3]. However, there is little or no data published on systems showing the effect of acetonitrile and water as a binary solvent on heavy components. This research investigates the effect of the acetonitrile-water binary solvent on heavy components. An alkane, alkene, alcohol and a carboxylic acid were chosen for this study. Hence, ternary liquid-liquid equilibrium measurements of acetonitrile and water with n-dodecane, 1-dodecene, nonanol and heptanoic acid were undertaken at 323.15 K and 1 atm.

The liquid-liquid equilibrium relations were measured using the direct analytical method in a double-walled glass cell. The cell is a modification of the one used by Raal and Brouckaert [4]. The modifications, undertaken by Ndlovu [5], improved sampling and provided an excellent seal for the cell. The samples were analyzed by gas chromatography. The obtained liquid-liquid binodal phase equilibrium data were correlated using a modified Hlavaty equation [6], a beta function and a log gamma equation using the methods previously described by Letcher et. al. [7]. The experimental tie lines were correlated using the liquid activity coefficient NRTL model of Renon and Prausnitz [8]. The parameters of the correlations were found by optimization of a non-linear least squares objective function.

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