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Liquid-liquid Equilibrium Determination and Data Correlation for 2,2,4-trimethyl Pentane - tripropylene Glycol Binary System

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Abstract

Liquid-liquid equilibrium at temperatures between 293.16K and 353.1K for the mixture of 2,2,4- trimethylpentane + 2- [2- (2-Hydroxypropoxy) propoxy] -1-propanol was determined using the cloud point method. The measured data was used to estimate the binary interaction parameters of NRTL thermodynamic model, through non-linear regression using MATLAB® software. The binary interaction parameters resulting from regression were used further in a chemical simulation software (PRO/II 9.3) to determine the LLE for the studied mixture. The LLE calculation results obtained with the NRTL model were compared with the results of LLE calculations using the predictive thermodynamic model-UNIFAC. It was determined that the results of the calculation of the LLE using binary interaction parameters obtained through regression have a smaller deviation from the experimental data than the results of the calculation performed using the UNIFAC model. Moreover, the binary interaction parameters obtained from regression were utilized for the estimation of the solvency properties of tripropylene glycol considering the extraction of C8 aromatics from a mixture containing 2,2,4-trimethyl pentane, ethylbenzene and xylenes.

Author Keywords

LLE, Isooctane, Tripropylene glycol, Regression, NRTL

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