Evaluation of thermodynamic modeling in the description of phase equilibrium for systems composed by components present in fusel oil

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The production of bioethanol generates byproducts, such as fusel oil, which consists of a mixture of higher alcohols. In countries where there is a large production of bioethanol, like Brazil, alternatives to the use of these byproducts are of great importance, to make the ethanol production less polluting and more profitable. Isoamyl alcohol and others alcohols may be separated from fusel oil by fractionation processes, since these compounds find several applications in the chemical industry. For the accurate design and optimization of these processes, reliable knowledge of the phase equilibrium behavior is required. In this work, the description of phase equilibrium, Vapor-Liquid Equilibrium (VLE) or Liquid-Liquid Equilibrium (LLE) of the components found in fusel oil was investigated using the parameters found in the data bank of Aspen Plus. The components present in fusel oil were chosen on the basis of samples from Brazilian refineries and literature sources. Nine components were selected to represent the fusel oil: water, ethanol, isoamyl alcohol, 2-methyl-1-butanol, isobutanol, 1-pentanol, butanol, propanol and methanol. Thirty six binary systems were evaluated for Vapor–Liquid Equilibrium and twelve ternary systems for Liquid-Liquid Equilibrium. For VLE, the NRTL model was used to calculate the activity coefficient and the Hayden and O'Connell model, for the fugacity coefficient. When the average absolute deviation in vapor phase between experimental and calculated data was larger than 0.03, the NRTL parameters were readjusted using the corresponding experimental data. For the LLE, NRTL and UNIQUAC models were tested. It was observed that the UNIQUAC model described better the system behavior with an average percent absolute deviation in phase compositions equal to 3.41 %, with the readjustment of some parameters, the deviation was reduced to 2.51 %. This new parameter data bank will enable more accurate computational simulation for recovering of some compounds present in fusel oil.

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