A Simple and Generalized Model to Represent the Vapor-Liquid Equilibira and the Liquid-Densities of Alcohol-Alkane Binary Mixtures

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A simple model based on a two-parameter cubic equation of state translated in volume and the Huron-Vidal-NRTL mixing rules were developed to describe vapor-liquid equilibria and liquid densities of alcohol-alkane mixtures. To get a semi-predictive model, generalized expressions in terms of critical pressure and critical temperature of alkanes and alcohols were developed for the NRTL binary interaction parameters (A_{12}, A_{21}, a_{ij}). The model was proposed employing the homologous series concept as follows: in first place, for 4 series composed by an alcohol between ethanol and 1-pentanol with some n-alkanes between butane and n-undecane, linear generalized expressions in terms of the ratio RT_c/P_c of n-alkanes were developed for A_{12}, A_{21}, a_{ij} in each series. The parameters of the generalized expressions were determined minimizing the total absolute relative deviation in bubble pressure. In second place, the parameters of all the series were correlated as quadratic functions in the RT_c/P_c ratio of alcohols. In total, 22 mixtures were used to develop the model and the average absolute relative deviation in bubble pressure (AADP) estimated is 1.65%. Also, the average absolute deviation in the vapor phase molar fraction (DY) is 0.007. Additionally, to validate the model, predictive calculations were made for 31 binary mixtures that include branched alcohols and branched alkanes. In general, predictions are adequate and results are similar to those reported in literature by associating models like the CPA, the SAFT and the GCA equations of state. The AADP for the new model is 2.80%, while the DY value is 0.009. Finally, liquid densities predictions were performed for 22 alcohol-alkane mixtures and it was found that calculated values are in good agreement with experimental data. The average absolute relative deviation calculated in liquid density is 1.16%. In total 645 densities and 1030 bubble pressures were predicted satisfactorily with the proposed model.