Vapor-Liquid Equilibrium for mixtures containing higher alcohols at 560 and 760 mmHg

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The design and optimization of separation processes involving direct contact of vapor and liquid phases, such as ethanol distillation, require information on Vapor-Liquid Equilibrium (VLE). The higher alcohols are byproducts of the ethanol distillation process related also to the flavor of alcoholic beverages and that, when purified, can act as a solvent. This study aimed to obtain isobaric Vapor-Liquid Equilibrium (VLE) data for binary and ternary systems involving higher alcohols. Vapor Liquid Equilibrium were measured for the binary system composed by 2-propanol/2-methyl-1-butanol at 560 and 760 mmHg and for the ternary systems composed by 2-propanol/1-butanol/3-methyl-1-butanol and 2-propanol/2-methyl-1-propanol/2-methyl-1butanol, both at 760 mmHg. The experimental measurements were performed in a Fischer ebulliometer (VLE 602) and the phase compositions were determined by gas chromatography. Thermodynamic consistency of the VLE binary data P-T-x-y was evaluate by area test and van Ness-Fredenslund test and the results proved the good quality of the VLE data determined in this work. The binary interaction parameters of the NRTL, Wilson and UNIQUAC models were fitted to the experimental binary VLE data in the commercial software Aspen Plus 12.1. The results showed a good description of the VLE data. In the binary system at 760 mmHg, it was observed average percent relative deviations in vapor phase composition equal to 1.31 % for the Wilson model, 1.56 % for the NRTL model and 1.90 % for the UNIQUAC model. To the same binary at 560 mmHg, the deviations were 2.02 %, 1.63 % and 1.22 % for the Wilson, NRTL and UNIQUAC models, respectively. These parameters were used to describe the VLE data for the ternary systems and the results showed a good agreement between experimental and calculated data. These parameters will ensure the assurance of the results of computational simulation in ethanol production.

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