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Vapor-liquid equilibria of the binary system 2-methylfuran + 1-butanol, present in the production of 2,5-dimethylfuran from biomass

Luis A Follegatti-Romero, Iredé A L Dalmolin, Antonio J A Meirelles and Martín Aznar
University of Campinas, Brazil

Recently, the limitations of bioethanol as a direct substitute for petrol have inspired the development of chemical catalytic transformation for producing promising furan biofuels from carbohydrates or directly from other sources of biomass. 2,5-dimethylfuran (DMF) and 2-methylfuran (MF) furan biofuels can be directly used as motor fuels or blended with gasoline. The DMF production process begins with the acid dehydration of fructose in a two-phase reactor, producing 5-hydroxymethylfurfural (HMF), followed by separation, conversion and purification steps. In the separation step, HMF is evaporated from an aqueous solution containing also 1-butanol as solvent and HCl; in the conversion step, HMF is converted to DMF in a catalytic reactor, and in the purification step, DMF is evaporated from an aqueous solution containing 1-butanol and intermediate compounds, such as MF. In this way, the knowledge of the vapor-liquid equilibrium is essential for the design, operation and optimization of these DMF separation processes. In this work, vapor-liquid equilibria of the binary system 2-methylfuran + 1-butanol were measured at 101.325 kPa using a Fischer Labodest 602 ebulliometer. The experimental vapor-liquid equilibrium data were submitted to a thermodynamic consistency test using the equation of Gibbs-Duhem. The phase behaviour was predicted by the CPA EoS (Cubic-plus-Association equation of state), and a good predictive performance was achieved, using only the CPA pure compound parameters. In future works other systems present in the same process (DMF + butanol, water + DMF, water + MF) will be also studied.

lfollegatti@gmail.com