

Vapor-liquid equilibrium study on the γ -valerolactone-water binary system

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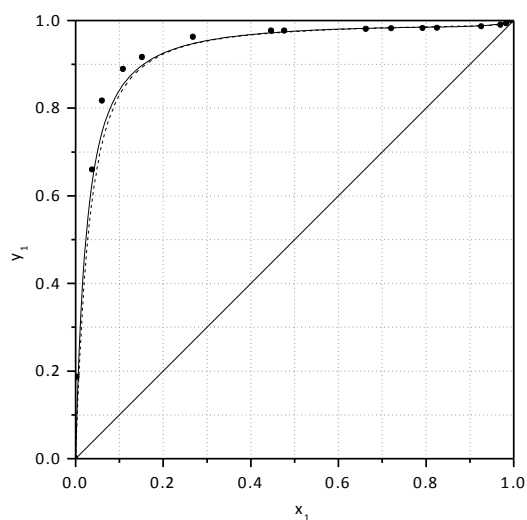
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Keywords: distillation, γ -valerolactone, vapor-liquid equilibrium

The intensive research activities on biomass conversion has resulted in the identification of key platform molecules such as 5-hydroxymethyl furfural (5-HMF), levulinic acid (LA), γ -valerolactone (GVL), which could either replace the currently used fossil-based chemicals or serve as the renewable feedstock for their production. The catalytic hydrogenation of LA using molecular hydrogen or formic acid as a hydrogen source resulted in equimolar formation of GVL and water. The latter has to be separated for the production of pure GVL. In order to design an efficient separation process for GVL-water final reaction mixture, the vapor-liquid equilibrium (VLE) data are required.

Although, numerous papers have been published concerning the production and utilization of GVL, the VLE data for this binary mixtures has not been reported yet.

In the present study, the vapor pressure, Antoine-constants, and isobaric vapor-liquid equilibrium properties of the water (1) – GVL (2) system at different pressures were investigated by the use of a modified Gillespie-still.



Experimental vapor-liquid equilibrium data (•) of the system water (1) – GVL (2) at $p = 101.325 \text{ kPa}$ with Wilson (---) and NRTL (—) simulations

It was demonstrated that the water can be removed from GVL without formation of azeotropic mixture. According to the Herington test, the experimental data was considered as thermodynamically consistent. Both experimental and simulated VLE data will be presented including the modelling by the use of Wilson and NRTL activity coefficient methods.

We are grateful for the support of Budapest University of Technology and Economics under project number KMR_12-1-2012-0066.