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Density and vapor–liquid equilibria at 101.3 kPa of binary mixtures containing ethyl acetate and a branched naphthenic compound: experimental data and modeling

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Density and VLE of pure compounds and mixtures are fundamental thermodynamic properties for the design of many industrial processes and for the development and improvement of thermodynamic models. Despite the vast amount of such experimental data currently available, a lack of data can be noticed for certain kinds of mixtures.

For example, the binary system ethyl acetate + cyclohexane was widely studied in the past. But very few VLE data are available for binary systems containing ethyl acetate and a branched naphthene. Indeed, to our knowledge, only a limited number of data are available for the system methylcyclohexane + ethyl acetate whereas the binary mixture methylcyclopentane + ethyl acetate has never been studied.

To fill this gap, the present work reports experimental densities and isobaric VLE data (at $P = 101.3$ kPa) for the following binary systems: methylcyclopentane + ethyl acetate and methylcyclohexane + ethyl acetate.

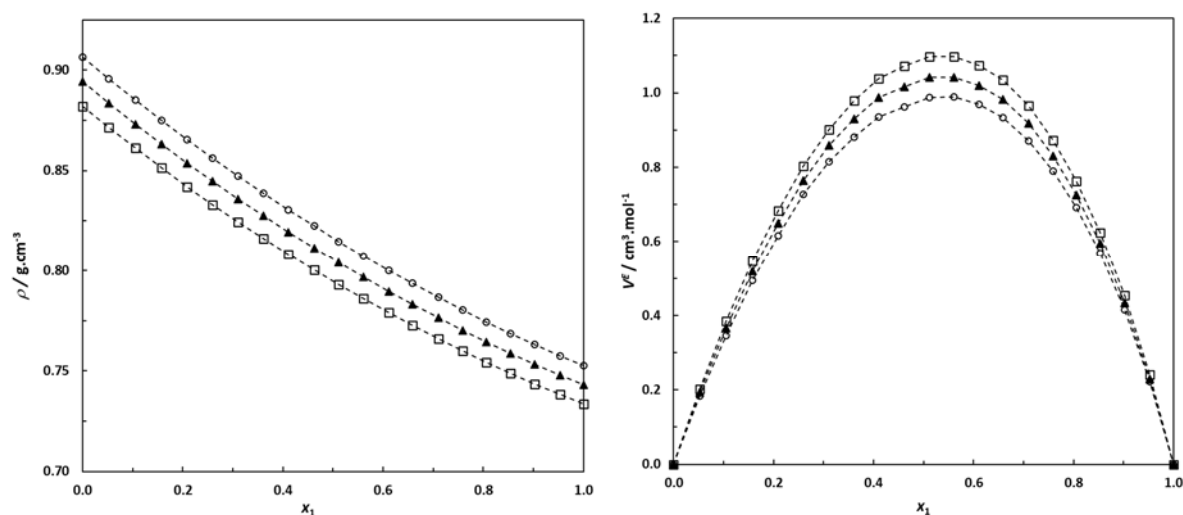


Figure 1. Densities (ρ) and excess molar volumes (V^E) for the binary system methylcyclopentane (1) + ethyl acetate (2) at 0.1 MPa measured in this work.

○: 288.15 K, ▲: 298.15 K, □: 308.15 K.

Density (ρ) measurements under atmospheric pressure were carried out in an oscillating tube density meter (DMA 4500 M, Anton Paar) from (288.15 to 308.15) K. The experimental densities obtained were used to calculate the excess molar volumes (V^E) of the mixtures at each temperature.

Densities and excess molar volumes are shown in Figure 1 for the binary mixture methylcyclopentane (1) + ethyl acetate (2), as an example of the results obtained in this study. Excess molar volumes derived from density measurements were correlated with composition using a Redlich-Kister type expression.

Isobaric VLE measurements were conducted in a Gillespie-type recirculation still in which pressure was maintained at 101.3 kPa under inert nitrogen atmosphere. After equilibrium had been reached, the compositions of the liquid and condensed vapor phases were determined indirectly by density measurements.

Wisniak L-W and Fredenslund consistency tests were used to check the accuracy of the measurements. VLE data acquired in this study were found to be thermodynamically consistent and were successfully correlated using activity coefficient models such as Wilson and NRTL.

The main conclusion of this investigation is that both binary systems present significant deviations from ideal behavior. Moreover, both binary mixtures investigated exhibit minimum boiling azeotropes at 101.3 kPa. VLE data measured in this work were used to determine azeotropic coordinates ($x_{1\text{ az}}$; T_{az} at 101.3 kPa) for each mixture.