**Vapor-Liquid Phase Equilibrium for Binary Systems Containing**

**1,2,4-Trimethylbenzene and Aromatic Compounds**

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**Highlights**

* **The isothermal VLE data were measured for 1,2,4-trimethyl benzene + *m*-xylene and 1,2,4-trimethyl benzene + *p*-xylene systems at temperatures from 363.15 K to 473.15 K using a static apparatus.**
* **Experimental VLE data were correlated well with the NRTL-HOC model.**

**1. Introduction**

For conducting the process simulation for an oil refinery plant, we need vapor-liquid equilibrium (VLE) data of the mixtures containing alkyl aromatics and xylenes. Among several others, the VLE data of binary mixtures of 1,2,4-trimethylbenzene + *m*-xylene and + *p*-xylene are still unavailable from open literature. In this work, the total pressure method was used to measure the isothermal VLE data for the binary systems of 1,2,4-trimethylbenzene with *m*-xylene or *p*-xylene at 363.15 K, 393.15 K, 433.15 K, and 473.15 K with 8:2/6:4/4:6/2:8 in mole ratios of the consitituent compounds in the liquid phase. Using the NRTL-HOC model, we determined the optimal values of the binary interaction parameters for each investigated system via data correlation.

**2. Methods**

The Isothermal VLE data were measured for the binary systems of 1,2,4-trimethylbenzene + *m*-xylene and + *p*-xylene by using total pressure method with a static apparatus. The operation of this static apparatus is briefly described as follows. The air impurities were adequately evacuated from the cell with a vacuum pump (Model GLD-N136, a minimum pressure of 6.7×10-1 Pa, ULVAC). The high-purity chemicals were degassed to remove the non-condensable dissolved gases before use. Each of binary mixture was prepared from the degassed compounds with an electronic balance (Model FA-2204C, Chrom Tech Co., Ltd., Taiwan), which can be accurate to ± 0.1 mg and then mixed well by using magnetic stirrer under a certain composition. The prepared solution was then charged into the evacuated equilibrium cell by pressure difference between vaccum and atmospheric pressure [1]. The charging process was terminated before the liquid level in the degassing bottle lower than the bottom of the feeding tube to prevent non-condensable gas from entering the equilibrium cell. After the charging process, the temperature of the bath was adjusted to the desired value. Since this equipment has no circulating pump, it is necessary to shake the cell manually to accelerate the system to achieve a vapor-liquid equilibrium state. As the equilibrium state is attained, the pressure reading will reach a constant value, which was recorded as the equilibrium pressure (*P*) at the specific temperature (*T*). The equilibrium pressure was measured at different temperatures by an increment of about 30 K. Additonally, the composition of each loaded liquid sample was analyzed by gas chromatography. The uncertainties of the reported equilibrium temperature, pressure, and liquid phase composition are estimated to be 0.1 K, 0.01 bar, and 0.005 in mole fraction, respectively.

**3. Results and discussion**

The total pressures (*P*) at given *T* and liquid composition (*x*i) were measured for 1,2,4-trimethylbenzene + m-xylene and 1,2,4-trimethylbenzene + p-xylene at 363.15 K, 393.15 K, 433.15 K, and 473.15 K over the entire composition range. The experimental results show that equilibrium pressure increases as increasing temperature and no azeotrope was formed in both two systems. The VLE data were correlated using the (γ-φ) method. The NRTL model [2] and the two-term virial equation of state with Hayden-O’Connell method [3] for estimation of the second virial coefficient (HOC) were adopted to represent the non-idealilties of liquid and vapor phases, respectively. Figures 1 and 2 indicate that the NRTL-HOC model correlates satisfactorily the VLE data. The average absolute relative deviations (AARDs) between measured and calculated values are 0.003 % and 0.14 % for the systems containging *m*-xylene and *p*-xylene, respectively.

 **Figure 2.** Deviation distribution of the calculated values from the NRTL-HOC model with the measured values for 1,2,4-trimethylbenzene + *p*-xylene system.

 **Figure** **1.** Deviation distribution of the calculated values from the NRTL-HOC model with the measured values for 1,2,4-trimethylbenzene + *m*-xylene system.

**4. Conclusions**

In the present study, the VLE data of 1,2,4-trimethyl benzene + *m*-xylene and 1,2,4-trimethyl benzene + *p*-xylene were measured at temperatures from 363.15 K to 473.15 K. The experimental results exhibit no azeotropic behavior over whole temperature ranges studied here.The calculated results reveal that the NRTL-HOC model can accurately represent the VLE behaviour for these two investigated systems. These experimental data are fundamentally important to conduct the optimal process simulation and design for an oil refinery plant.

**References**

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