

Isobaric vapor–liquid equilibrium for binary systems of toluene + *o*-xylene, benzene + *o*-xylene, nonane + benzene and nonane + heptane at 101.3 kPa



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ABSTRACT

Isobaric vapor–liquid equilibrium (VLE) data for the binary systems of toluene + *o*-xylene, benzene + *o*-xylene, nonane + benzene and nonane + heptane were measured at 101.3 kPa by using a modified Othmer still. The thermodynamic consistency of these new VLE data was checked by using the point to point test of Van Ness. No azeotrope was found in these binary systems investigated. While nonane + benzene were found to have large positive deviation, toluene + *o*-xylene, benzene + *o*-xylene, and nonane + heptane exhibited large negative deviation from ideal behavior. The binary interaction parameters of the Wilson, the NRTL, the UNIQUAC models and the SRK equation of state for these four binary systems were determined through the VLE data reduction. These new VLE data were compared with the predicted values from the UNIFAC and the COSMO-RS (conductor-like screening model for realistic solvents) models as well. Generally, reasonable agreement was found between the predicted results and the experimental values, except for nonane + benzene system.

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1. Introduction

Hydrocarbons are the main components in crude oils. The separation of paraffins and aromatics, such as benzene (B), toluene (T) and xylenes (X), from petroleum fractions, is commonly encountered in refinery processes. Since distillation is the most popular separation method in the chemical and petroleum industries, vapor–liquid equilibrium (VLE) data of the related mixtures are basically important for development of the separation processes. Although a plenty of VLE data of the mixtures containing paraffins (from C₆ to C₉) and aromatics (BTX) are available from literature [1–14], the VLE data for some specific systems are still insufficient. As a part of our continued studies on the isobaric VLE data measurements for the mixtures containing C₆–C₉ and BTX [3,9], we measured the isobaric VLE data for four binary systems, including toluene + *o*-xylene, benzene + *o*-xylene, nonane + benzene, and nonane + heptane, at 101.3 kPa in this work. According to the results of literature survey, no isobaric VLE data of these four binary systems at 101.3 kPa has been reported in literature. Chen et al. [8] reported the density and the isothermal VLE data (*P*–*T*–*x* at 333.15 K and 353.15 K) for nonane + benzene and toluene + *o*-xylene, but they did not measure the vapor compositions (*y*) and thus

thermodynamic consistency test cannot be made for those VLE data. In the present study, *P*–*T*–*x*–*y* data were measured and subsequently checked with the thermodynamic consistency test by using the point to point test method of Van Ness [15] modified by Fredunslund et al. [16].

In VLE data reduction, vapor phase was considered as non-ideal. The two-term virial equation and the Hayden and O'Connell (HOC) model [17] were used to estimate the fugacity coefficient and the second virial coefficient for each component in the vapor phase, respectively, and the non-ideality of each liquid component were represented by the Wilson [18], the non-random two-liquid (NRTL) [19], and the universal quasi-chemical (UNIQUAC) [20] activity coefficient models. These new VLE data were also correlated with the Soave–Redlich–Kwong (SRK) equation of state [21]. In addition, the predicted results from both the UNIFAC [16] and the COSMO-RS [22] models were also compared with these new experimental VLE data.

2. Experimental

2.1. Materials

All the chemicals used in this study are listed in Table 1, including the suppliers and the purity levels. The purity level of each substance has been confirmed by gas chromatography (GC) analysis. In addition, the density (ρ) and the normal boiling point

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Table 1Materials description, densities (ρ) at 298.2 K and the normal boiling points (T_b) of the pure components.^a

Compound	Source	Mass fraction purity	$\rho/(\text{g cm}^{-3})$		T_b/K	
			This work	Literature	This work	Literature
Nonane	Aldrich, USA	0.9998	0.71407	0.71402 [23]	423.8	423.8 [24]
Benzene	R.D. Germany	0.9997	0.87366	0.87360 [25]	353.3	353.20 [26]
Heptane	Acros, USA	0.9998	0.67952	0.67950 [7]	371.4	371.55 [7]
Toluene	Aldrich, USA	0.9996	0.86218	0.86219 [25]	383.4	383.75 [25]
<i>o</i> -Xylene	Alfa Aesaer, USA	0.9995	0.87566	0.87557 [7]	417.5	417.55 [7]

^a $u(\rho)=0.00005 \text{ g cm}^{-3}$; $u(T)=0.1 \text{ K}$.

(T_b) of each compound were measured with a vibrating-tube densimeter (DMA 4500, Anton Paar, Austria) to an uncertainty of $\pm 0.00005 \text{ g cm}^{-3}$ and a modified Othmer VLE apparatus facilitated with a thermocouple calibrated to an uncertainty of $\pm 0.1 \text{ K}$, respectively. The results are also compared with the literature values [7,23–26] in Table 1, which shows that the agreement is excellent. No further purification has been made for the chemicals before use.

2.2. Apparatus and procedure

The VLE measurements were conducted by using an Othmer-recirculation still [27] with some modification as reported by

Johnson et al. [28]. The schematic diagram and the operating technique are similar to those reported in literature [29,30]. In each experimental run, about 100 cm^3 of freshly prepared mixture was injected in the still and then heat was provided gradually by means of external heater. The pressure was maintained at $101.3 \pm 0.2 \text{ kPa}$ during the course of measurement by a pressure adjustment system, which has been described in our previous articles [3,9]. This pressure controlling system is composed of a graduated burette, directly connected with an elevation-adjustable water reservoir. By adjusting the required water level difference between the burette and the water reservoir, the pressure difference between local atmospheric pressure and 101.3 kPa was compensated during each

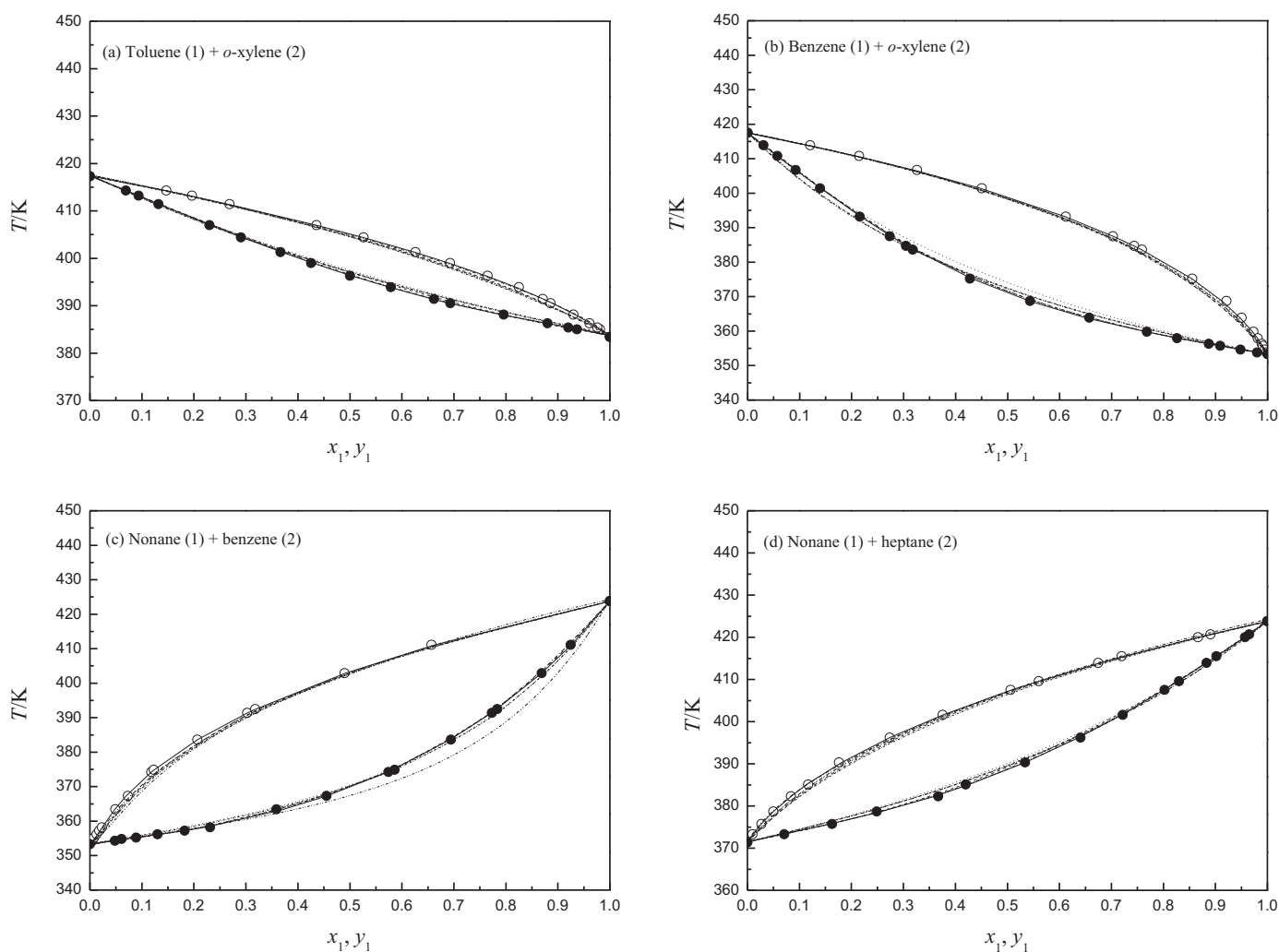


Fig. 1. (a–d) (T , x_1 or y_1) plot for the investigated binary systems at 101.3 kPa: (●), experimental liquid phase and (○); experimental vapor phase compositions; (---), calculated liquid and vapor phase compositions from the Wilson model; (—), calculated liquid and vapor phase compositions from the NRTL model; (-.-), calculated liquid and vapor phase compositions from the SRK equation of state; (....), predicted liquid and vapor phase compositions from the UNIFAC model; (-.-.-), predicted liquid and vapor phase compositions from the COSMO-RS model.

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