



Isobaric vapor–liquid equilibrium data of the binary systems of octane with p, o, m-xylene at 20 kPa

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ABSTRACT

Isobaric vapor–liquid equilibrium (VLE) data were determined at 20 kPa for the three binary mixtures composed of octane + p, o, m-xylene by using a recirculation type still. All the data passed the thermodynamics test and no azeotropic behavior was observed. The experimental results were used as a basis to check the validity of two predictive models, the UNIFAC (DORTMUND) and COSMO-RS. These new VLE data were also correlated with the Wilson, NRTL, and UNIQUAC activity coefficient models.

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1. Introduction

The vapor–liquid equilibrium (VLE) data provide the foundation in the design of distillation columns under reduced pressure. In refinery and petrochemical industries, vacuum distillation is commonly adopted to separate the systems of aromatic hydrocarbons (such as xylenes, trimethylbenzene) and aliphatic hydrocarbons (such as hexane, heptane, octane, nonane, and decane). In the present study, our interest focuses on the determination of vapor–liquid equilibrium data under reduced pressure for the systems of aromatic and aliphatic hydrocarbons. Among several other studies on the mentioned systems above, Lee and his coworkers have determined the isobaric VLE data for the systems of octane with o-, m-xylene [1] and nonane with m-, p-xylene [2] at 101.3 kPa. For the other properties of the similar systems, Changsheng Yang et al. [3] have measured the densities for octane with p-xylene from 298.15 to 353.15 K at atmospheric pressure. Moravkova et al. [4] have measured the densities for octane with m-xylene at temperatures between (298.15 and 328.15) K.

In this paper, we used a modified Rose–Williams type recirculation still to measure the isobaric VLE of the systems of p, o, and m-xylene at 20 kPa. The obtained VLE data were verified with the Herington [5] thermodynamic consistency test. In the VLE calculation, the fugacity coefficients of each constituent compound in the vapor phase were estimated from the two-term virial equation,

together with the Hayden–O’Connell (HOC) model [6] for calculating the second virial coefficients. The new VLE data were also correlated with three correlative models, the Wilson [7], NRTL [8], and UNIQUAC [9]. These new VLE data were also used to examine the predictive ability of two activity coefficient models, the UNIFAC (DORTMUND) [10] and the conductor-like screening model for realistic solvents (COSMO-RS) [11–13].

2. Experimental

2.1. Materials

The purity levels and sources of the chemicals used in this study are reported in Table 1. All substances were further purified by distilling twice at a low pressure (about 2.5 kPa), and the final purity were checked with gas chromatography (SP6890A, Shandong Lunan Ruihong Chemical Instruments Co., Ltd., China) analysis, also shown in Table 1.

In order to check the purity of the substances, their densities at $T=298.15$ K were determined by using a digital vibrating-tube densimeter (DMA 4500, Anton Paar, Austria) and refractive index values at $T=298.15$ K by using a full automatic refractometer (Hanon A610, Hanon Instrument, China). The densities and refractive index values were listed in Table 2, along with the literature values [13–15], showing the good agreement in general.

2.2. Apparatus and experimental procedure

In the present study, a modified Rose–Williams still (Beiyang Analytical Instrument Co. Ltd.) was employed to measure the

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Table 1
Materials description.

Chemical name	Source	Initial mass fraction purity	Purification method	Final mass fraction purity	Analysis method
Octane	Sinopharm Chemical Reagent Co., Ltd., China	0.9912	Distillation	0.9992	GC ^a
p-xylene	Tianjin Solvent Factory, China	0.9908	Distillation	0.9991	GC ^a
o-xylene	Tianjin Solvent Factory, China	0.9911	Distillation	0.9989	GC ^a
m-xylene	Tianjin Solvent Factory, China	0.9906	Distillation	0.9968	GC ^a

^a Gas chromatography.**Table 2**
Densities ρ and refractive index values n_D at $T=298.15$ K and $P=101.33$ kPa of the pure components, and their comparison with the literature.

Component	$\rho/(g\text{ cm}^{-3})$			n_D		
	Experimental	Literature	Reference	Experimental	Literature	Reference
Octane	0.69861	0.69862	[14]	1.3951	1.39505	[14]
p-xylene	0.85671	0.85658	[15]	1.4957	1.4958	[15]
o-xylene	0.85954	0.85966	[16]	1.4945	1.49466	[16]
m-xylene	0.85995	0.86009	[14]	1.4946	1.49464	[14]

^a Standard uncertainties: $u(\rho)=0.00005\text{ g cm}^{-3}$; $u(n_D)=0.0001$ and both with 0.95 level of confidence.**Table 3**
Experimental VLE data for binary system of octane (1)+p-xylene (2) at 20 ± 0.03 kPa.^a

T/K	x_1	y_1	γ_1	γ_2
359.75	0.000	0.000	–	1.000
358.72	0.042	0.078	1.31	1.000
357.21	0.116	0.191	1.226	1.004
355.96	0.191	0.287	1.170	1.013
354.99	0.259	0.364	1.133	1.023
354.22	0.322	0.428	1.102	1.035
353.35	0.402	0.505	1.075	1.049
352.75	0.462	0.559	1.058	1.063
352.10	0.537	0.623	1.039	1.082
351.58	0.603	0.679	1.028	1.096
351.03	0.678	0.740	1.017	1.118
350.53	0.751	0.799	1.010	1.140
350.15	0.812	0.848	1.005	1.159
349.77	0.879	0.902	1.002	1.178
349.37	0.953	0.962	1.000	1.194
349.13	1.000	1.000	1.000	–

^a $u(T)=0.02$ K; $u(x_1)=0.001$; $u(y_1)=0.001$.

isobaric VLE data, which a vacuum pump (SHZ-D (III), Yuhua Instrument, China) and a needle valve assembly hooked to the system to adjust the pressure, and a U-shaped mercury manometer (Nanjing Hengyuan Automatic Gauge Co. Ltd.) whose fluctuation was held within 0.03 kPa to measure the pressure. The diagrammatic sketch for this apparatus has been drawn and its detailed operating procedure has been given in our previous work [17].

Table 4
Experimental VLE data for binary system of octane (1)+o-xylene (2) at 20 ± 0.03 kPa.^a

T/K	x_1	y_1	γ_1	γ_2
365.16	0.000	0.000	–	1.000
363.73	0.063	0.110	1.037	1.000
361.94	0.148	0.242	1.032	1.000
360.17	0.239	0.363	1.019	1.004
358.71	0.320	0.462	1.020	1.003
357.34	0.401	0.548	1.013	1.007
356.00	0.485	0.630	1.010	1.009
354.69	0.572	0.707	1.007	1.011
353.38	0.664	0.779	1.002	1.022
352.43	0.734	0.832	1.003	1.018
351.57	0.800	0.877	1.001	1.026
350.54	0.882	0.930	1.000	1.030
349.54	0.965	0.980	1.000	1.033
349.13	1.000	1.000	1.000	–

^a $u(T)=0.02$ K; $u(x_1)=0.001$; $u(y_1)=0.001$.

In each experiment, about 100 cm³ liquid mixtures were injected into the still through a syringe and then starting vacuum pump. The needle valve was regulated to maintain the isobaric stable at 20 kPa in the equilibrium cell during the experimental course before heating up gently. The temperature was measured by a precise mercury thermometer (Tianjin Glass Instrument Factory) whose uncertainty is within ± 0.02 K. The vapor phases were continuously cooled and flowed back to the cell, providing intimate contact of the liquid phases. The equilibrium was deemed to establish when the temperature maintained constant at least half an hour. And then the vapor and liquid samples were withdrawn simultaneously to be analyzed under the equilibrium temperature.

2.3. Analysis

All the samples of the equilibrium phases are analyzed using a gas chromatograph (GC) with a flame ionization detector (FID) (SP6890A, Shandong Lunan Ruihong Chemical Instruments Co., Ltd., China). The GC column is a B-34 capillary column (28 m \times 0.25 mm \times 0.3 μ m). The carrier gas is nitrogen with a purity of 99.999% and a flowrate of 30 cm³ min⁻¹. For each binary mixture, we adopted several known composition standard mixtures, prepared gravimetrically over the whole composition range, to calibrate the response values of the gas chromatography. For each sample, the final composition was determined from the average

Table 5
Experimental VLE data for binary system of octane (1)+m-xylene (2) at 20 ± 0.03 kPa.^a

T/K	x_1	y_1	γ_1	γ_2
360.59	0.000	0.000	–	1.000
359.83	0.042	0.068	1.099	1.000
358.41	0.128	0.193	1.076	1.002
357.31	0.202	0.289	1.061	1.005
356.27	0.279	0.379	1.046	1.010
355.23	0.362	0.469	1.035	1.014
354.43	0.431	0.538	1.027	1.020
353.62	0.505	0.608	1.020	1.026
352.87	0.578	0.673	1.014	1.033
352.13	0.654	0.737	1.008	1.042
351.39	0.733	0.801	1.004	1.052
350.63	0.819	0.868	1.002	1.060
350.09	0.882	0.915	1.001	1.069
349.55	0.948	0.963	1.000	1.078
349.13	1.000	1.000	1.000	–

^a $u(T)=0.02$ K; $u(x_1)=0.001$; $u(y_1)=0.001$.

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