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Vapor−Liquid Equilibria in Alcohol + Cyclohexane + Water Systems

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Vapor−liquid equilibria in ternary systems were measured for ethanol + cyclohexane + water (mixture 1) at (35, 50, and 65) °C and isobutanol + cyclohexane + water (mixture 2) at (40 and 60) °C using an equilibrium still. The binary NRTL parameters for cyclohexane + water were obtained by optimization of fits to these experimentally measured data. These binary parameters were used to predict vapor−liquid equilibria for the systems 2-propanol + cyclohexane + water (mixture 3) and furanidine + cyclohexane + water (mixture 4). Excellent agreement was obtained. The mean deviation for the correlated data is 0.0207 for mixture 1 and is 0.0229 for mixture 2. The mean deviation for the predicted data is 0.0149 for mixture 3 and is 0.0110 for mixture 4.

Introduction

Compared to benzene, cyclohexane is a better water-entrainer when it is applied to remove water from higher alcohols.[1] Currently, published vapor−liquid equilibrium (VLE) data for alcohol + cyclohexane + water systems are limited. Data have been reported only for the 2-propanol + cyclohexane + water system.[2] To design a process to remove water from higher alcohols using cyclohexane as an azeotrope former, it is necessary to measure the VLE data for ternary systems containing alcohol, cyclohexane, and water. Multicomponent VLE data can be calculated by the use of the related binary model parameters. The binary parameters can be obtained from binary VLE data. Unfortunately, the binary VLE data of cyclohexane + water are difficult to obtain by a direct determination. This is because the cyclohexane + water system is an extremely nonideal solution.

The equilibrium still[3,4] used in this work has been successfully applied to VLE measurements for many systems.[4−8] In this work the ternary VLE data are presented for the systems ethanol + cyclohexane + water at (35, 50, and 65) °C and isobutanol + cyclohexane + water at (40 and 60) °C.

Experimental Section

Chemicals. Cyclohexane, isobutanol, and ethanol are analytical pure grade with a purity not less than 99.5% (by mass). They have no chromatographically detectable impurities. Before their use, they were dried with a zeolite and repurified by distillation. The water was distilled before use.

Apparatus and Procedures. An equilibrium still[3,4] was used for this study. A sketch flow sheet of the VLE measurement and a schematic diagram of the still are shown in Figures 1 and 2.

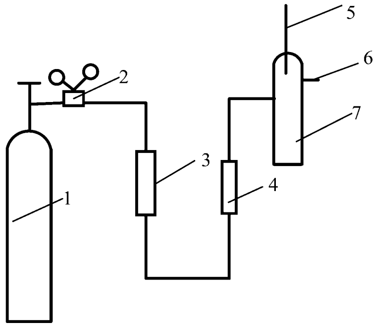

Figure 1. Sketch flow sheet: 1, H_2 cylinder; 2, reducing valve; 3, drying tube; 4, flow meter; 5, thermometer; 6, vapor phase sampling; 7, equilibrium still.

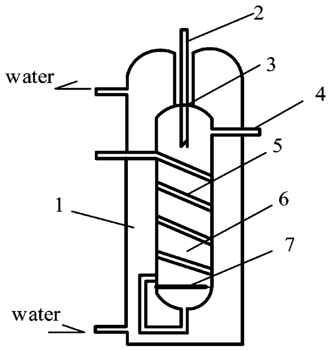

Figure 2. Schematic diagram of the equilibrium still: 1, water sleeve; 2, thermometer; 3, liquid phase sampling site; 4, vapor phase sampling site; 5, carrier gas preheating tube; 6, still body; 7, sieve plate.

The liquid phase was charged onto the sieve plate of the still (Figure 2, #7) via the liquid-phase sampling site (taking away the thermometer #2 to disclose the sampling site #3). The temperature of the still was kept unchanged by circulation water within ±0.1 °C. As the conditions were stabilized, the carrier gas, H_2, as shown in Figure 1, passed through a reducing valve, a drying tube, and a flow meter, and then it was introduced into the equilibrium still. In the still, as shown in Figure 2, the carrier gas H_2 was at first heated in a preheating tube (#5) winding along the still body (#6). The H_2 was dispersed into the liquid phase loaded on the porous sieve plate (#7) and finally flowed out from the vapor-phase sampling site (#4) together with the vapor in equilibrium with the liquid phase.

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On the equilibrium still, the vapor-phase samples were gathered from the vapor-phase sampling site (Figure 2, #4) by an injector (1 mL or 2 mL) directly. The liquid-phase samples were gathered at first via a liquid sampling site (#3) by a long capillary tube, and then the samples were transferred to an injector (1 μL or 10 μL) for assay. A type SP-501 gas chromatograph (provided with a thermal conductivity detector and a GDX-101 column 2 m long and 0.4 cm in diameter) was used in analyzing water and alcohols.

A type SP-6800 gas chromatograph (provided with a flame-ionization detector and a DEGS column 2 m long and 0.4 cm in diameter) was used in analyzing cyclohexane and alcohols.

Reliability of the Measurements. The following factors were considered to be the critical factors that affect the accuracy of the determined data (x, mole fraction of the liquid phase; y, mole fraction of the vapor phase on a hydrogen-free basis): analytical error, temperature fluctuation, entrainment of liquid in gas, the completeness of the mass transfer, and the possible condensation of the vapor phase.

The analytical error (including the error caused in sample gathering) for the liquid phase (mole fraction x) in this work was less than 0.002. This is normal for a gas chromatographic analysis. The error for the vapor phase (mole fraction y, on a hydrogen-free basis) was less than 0.004, slightly larger than normal because of the presence of H_2 in the vapor phase.

The temperature fluctuation of the bubble-still was ±0.1 °C. The fluctuation of 0.1 °C may cause about 0.5% relative change of the saturated vapor pressure. The y value is equal to $p_i/\sum p_i$ ($i \neq H_2$), that is, the ratio of p_i to $\sum p_i$, if the nonideality of the vapor phase was negligible for the low-pressure system. For this situation, a fluctuation of 0.1 °C may only cause 0.01 to 0.02% relative change of the y.

Carrier gas, hydrogen, may entrain a minimal amount of liquid phase into the vapor phase. It may cause the inaccuracy in the determination of y. However, no detectable difference existed among the values of y determined under different flow rates of the hydrogen ranging from (30 to 200) $mL \cdot min^{-1}$. That means the entrained liquid phase was not notable as long as the flow rate of the hydrogen was appropriate. The error introduced by the entrained liquid phase was negligible compared to the analytical error of y.

Because the carrier gas, hydrogen, passed through the liquid phase within a rather short period, it may be in doubt whether the mass transfer of the components can be nearly completed and a vapor phase can be formed which was very approximate to the true equilibrium. To clarify this problem, instead of one still, two stills charged with the same liquid phase were connected in series. The vapor-phase samples from both stills were gathered and analyzed, respectively. Results showed that there was no notable difference between vapor-phase samples from both stills.

To eliminate any possible condensation of the vapor phase in the outlet tube (the vapor-phase sampling site) and in the injector for gathering the vapor-phase sample, an infrared heater was used. The experimental data were repeatable. This showed that the heater was effective for the elimination of the condensation.

What was mentioned above shows that this apparatus was reliable for VLE determination. The possible error for the determination is about 0.002 for x and 0.004 for y. To reduce the error further, each sample point was measured at least three times in this work and the mean value was reported.

Table 1. VLE Data for Ethanol (1) + Water (2)

$x_{1,exp}$	$y_{1,exp}$	$\ln(\gamma_1/\gamma_2)$	$x_{1,exp}$	$y_{1,exp}$	$\ln(\gamma_1/\gamma_2)$
0.0429	0.2982	1.4228	0.4356	0.6278	−0.0419
0.0654	0.3821	1.3049	0.5049	0.6664	−0.2017
0.1545	0.5132	0.8863	0.6400	0.7303	−0.4556
0.1825	0.5462	0.7693	0.6527	0.7322	−0.4760
0.2421	0.5679	0.5405	0.8056	0.8265	−0.6830
0.4081	0.6176	0.0280	0.9006	0.8996	−0.7804

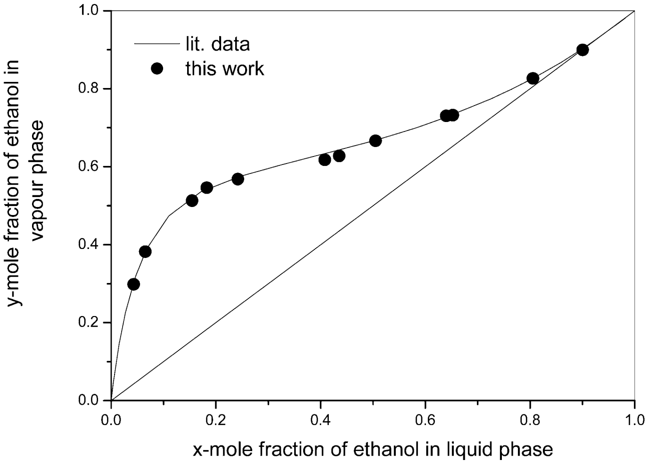

Figure 3. Comparison of experimental data with literature data: ●, this work; —, lit. data.[9]

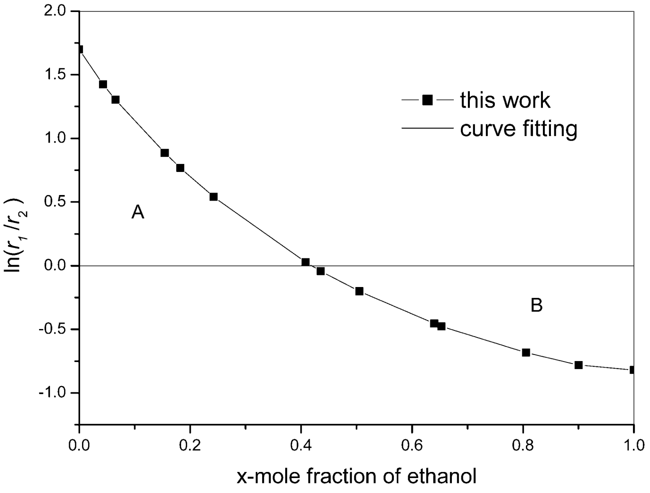

Figure 4. Integral test of thermodynamic consistency: ■, this work; —, curve fitting.

Verification Experiment. The apparatus was checked by measurement of the VLE for the system ethanol + water at 50 °C (Table 1), and a comparison was done between this work and the literature[9] (Figure 3). The literature data were considered to be of the very highest quality.

The experimental data were also tested by the method proposed in the literature[10] (Figure 4).

In Figure 4,

$$\int_0^1 \ln\left(\frac{\gamma_1}{\gamma_2}\right) \mathrm{d}x_1 = \frac{|A_{\mathrm{area}} - B_{\mathrm{area}}|}{A_{\mathrm{area}} + B_{\mathrm{area}}} = \frac{|0.3048 - 0.2968|}{0.3048 + 0.2968} = 0.013 < 0.02$$

The thermodynamic consistency test indicated that the experimental data were reliable. From the above results it can be seen that the experimental data fit well with the

Table 2. VLE Data for the Ethanol (1) + Cyclohexane (2) + Water (3) System

	mole fraction in liquid phase			mole fraction in vapor phase		
t/°C	x_1	x_2	x_3	y_1	y_2	y_3
35	0.5096	0.4257	0.0646	0.2948	0.6352	0.0700
	0.5776	0.3814	0.041	0.3269	0.6251	0.0480
	0.5972	0.3589	0.0439	0.3201	0.6325	0.0474
	0.6675	0.2752	0.0573	0.3381	0.6116	0.0504
	0.7155	0.2137	0.0708	0.3369	0.6095	0.0536
	0.7066	0.1073	0.1862	0.3213	0.5809	0.0979
	0.8100	0.0973	0.0927	0.4101	0.5302	0.0597
	0.8457	0.0678	0.0864	0.4795	0.4640	0.0565
	0.4790	0.0046	0.5164	0.4651	0.2965	0.2384
50	0.4902	0.4886	0.0212	0.3887	0.5754	0.0359
	0.5542	0.4095	0.0363	0.3881	0.5668	0.0451
	0.5825	0.3746	0.0429	0.3861	0.5588	0.0551
	0.6411	0.3065	0.0524	0.3957	0.5503	0.0540
	0.6885	0.2439	0.0676	0.4043	0.5344	0.0613
	0.7703	0.1121	0.1176	0.4274	0.4915	0.0811
	0.8324	0.0766	0.0910	0.5229	0.4075	0.0696
	0.6749	0.1437	0.1814	0.3603	0.5513	0.0883
	0.6753	0.0682	0.2565	0.4049	0.4525	0.1426
	0.5982	0.0263	0.3755	0.4332	0.3647	0.2021
	0.4644	0.0103	0.5253	0.3796	0.4190	0.2014
65	0.8276	0.0786	0.0938	0.5584	0.3672	0.0744
	0.6822	0.0603	0.2575	0.4141	0.4379	0.1480
	0.8650	0.0405	0.0945	0.6221	0.3027	0.0752
	0.8060	0.1113	0.0827	0.5175	0.4174	0.0651
	0.8098	0.1288	0.0614	0.5057	0.4418	0.0525
	0.7160	0.2370	0.0470	0.4572	0.4957	0.0471
	0.6124	0.3523	0.0352	0.4271	0.5244	0.0485
	0.5653	0.4041	0.0306	0.4204	0.5327	0.0468

Table 3. VLE Data for the Isobutanol (1) + Cyclohexane (2) + Water (3) System

	mole fraction in liquid phase			mole fraction in vapor phase		
t/°C	x_1	x_2	x_3	y_1	y_2	y_3
40	0.5966	0.0400	0.3634	0.1417	0.4487	0.4097
	0.5472	0.1368	0.3160	0.0961	0.5890	0.3170
	0.5695	0.1315	0.2990	0.0897	0.5870	0.3233
	0.5409	0.2592	0.1999	0.0660	0.6846	0.2495
	0.5009	0.3145	0.1846	0.0723	0.6549	0.2728
	0.7104	0.1089	0.1807	0.1208	0.5959	0.2834
	0.4650	0.3695	0.1655	0.0603	0.6772	0.2625
	0.3985	0.4750	0.1265	0.0641	0.6788	0.2570
	0.3068	0.6125	0.0807	0.0632	0.6536	0.2833
	0.0866	0.9050	0.0084	0.0590	0.7649	0.1761
	0.0449	0.9514	0.0034	0.0431	0.8665	0.0904
	0.1690	0.7553	0.0757	0.0689	0.7241	0.2070
60	0.5185	0.1247	0.3568	0.1163	0.5210	0.3628
	0.5916	0.0998	0.3086	0.2014	0.4211	0.3752
	0.5133	0.1846	0.3021	0.1160	0.5300	0.3544
	0.5024	0.2275	0.2701	0.1006	0.5721	0.3273
	0.5139	0.2442	0.2419	0.1077	0.5486	0.3439
	0.4973	0.2635	0.2392	0.1059	0.5733	0.3208
	0.4381	0.3794	0.1825	0.0943	0.5791	0.3267
	0.4876	0.3382	0.1742	0.1454	0.5656	0.2890
	0.4431	0.4208	0.1361	0.0889	0.5849	0.3263
	0.3914	0.4784	0.1302	0.0869	0.6009	0.3122
	0.4027	0.4938	0.1035	0.1003	0.6010	0.2987
	0.3872	0.5557	0.0771	0.1138	0.6321	0.2541
	0.2872	0.6443	0.0685	0.0878	0.6179	0.2943
	0.2737	0.6958	0.3050	0.1077	0.6926	0.2005
	0.0788	0.9092	0.0120	0.0723	0.7124	0.2153
	0.0797	0.9093	0.0110	0.0667	0.7460	0.1874

Table 4. Antoine Equation Constants[2]

	A_i	B_i	C_i
ethanol	8.112 2	1592.864	226.184
isobutanol	8.535 16	1950.94	237.147
cyclohexane	6.851 46	1206.47	223.136
water	8.071 31	1730.63	233.426

literature data. The apparatus was reliable when used in VLE measurements.

Results and Discussion

VLE Data for Ternary Systems. The mole fraction compositions of the liquid phase x and the vapor phase y (hydrogen-free basis) in equilibrium were shown in Table 2 for the system ethanol + cyclohexane + water and in Table 3 for the system isobutanol + cyclohexane + water.

Correlation. Because the nonideality of the vapor phase is negligible at low pressure,[2] the equilibrium equation could be simplified as

$$p_i = \gamma_i x_i p_i^{\mathrm{s}} \tag{1}$$

where p_i is the partial pressure of alcohol (i = 1), cyclohexane (i = 2), and water (i = 3) and p_i^{s} is the saturated vapor pressure of component i, which can be calculated according to the Antoine equation,

$$\log(p_i^{\mathrm{s}}/\mathrm{mmHg}) = A_i - \frac{B_i}{t + C_i} \tag{2}$$

where A_i, B_i, and C_i are the Antoine constants which are listed in Table 4, and t is temperature in °C,

$$y_i = p_i / \sum p_i \tag{3}$$

for an alcohol (1) + cyclohexane (2) + water (3) ternary system, i = 1, 2, 3.

Binary Model Parameters of Cyclohexane + Water. On the basis of the ternary equilibrium data measured in this work (Tables 2 and 3) and parameters for ethanol + water, ethanol + cyclohexane, isobutanol + water, and isobutanol + cyclohexane, the binary model parameters of cyclohexane + water can be acquired by an optimization method. The objective function selected was

$$F = \sum_j^N \sum_i^C |y_{i,\mathrm{cal}} - y_{i,\mathrm{exp}}| \tag{4}$$

where i = 1, 2, 3; j = 1, 2, ..., N; N is the number of experimental points; and C is the number of components.

The correlation equation used is the NRTL equation.

The related binary NRTL model parameters for ethanol + water and ethanol + cyclohexane were the recommended data in the literature.[2] The parameters for isobutanol + water and for isobutanol + cyclohexane were obtained by optimizing the data published in the literature.[2] They all are shown in Table 5.

Because the third parameter α in the NRTL equation was not sensitive to correlation results, in this work, α was constantly set to 0.3.

The obtained binary model parameters of cyclohexane + water by optimization were also listed in Table 5.

Correlation Results. Using the binary parameters listed in Table 5, the liquid activity coefficients γ_i and then the vapor phase molar fraction $y_{i,\mathrm{cal}}$ for ternary systems could be calculated with the NRTL equation. The deviation dy_i between y_{cal} and y_{exp} for both systems was separately shown in Tables 6 and 7. The average value of the mean correlation deviations was 0.0207 and 0.0229, respectively.

Prediction. Different equilibrium data may result in different NRTL parameters. There were two sets of parameters for cyclohexane + water before this work. One was obtained from the literature[2] by optimization of the VLE data for 2-propanol + cyclohexane + water. Another was obtained from the liquid−liquid equilibrium (LLE) data for the system cyclohexane + water.[12]

Table 5. Related Binary NRTL Parameters for the Alcohol (1) + Cyclohexane (2) + Water (3) System

system	Δg_{12}[a]	Δg_{21}[a]	a_{12}	ref
cyclohexane (1) + water (2)	9729.86	12871.23	0.3	this work
ethanol (1) + water (2)	−2918.642 + 4.085*T*	3409.355 + 8.400*T*	0.1803	2, Vol. 1, part 1a, pp 156−157
ethanol (1) + cyclohexane (2)	3668.289	5817.161	0.4485	2, Vol. 1, part 2c, p 419
isobutanol (1) + water (2)	2868.184	10169.262	0.4599	2, Vol. 1, part 1a, p 345 2, Vol. 1, part 1, pp 438−441
isobutanol (1) + cyclohexane (2)	287.392	4014.61	0.3958	2, Vol. 1, part 2d, p 368 2, Vol. 1, part 2b, p 288

[a] $\Delta g_{ij} = g_{ij} - g_{jj}$ energy parameters (J·mol^{-1}). *T* = temperature (in K).

Table 6. Comparison between y_{exp} and y_{cal} for the Ethanol (1) + Cyclohexane (2) + Water (3) System

t/°C	$y_{1,\mathrm{cal}}$	$y_{2,\mathrm{cal}}$	$y_{3,\mathrm{cal}}$	dy_1[a]	dy_2[a]	dy_3[a]
35	0.3276	0.6153	0.0572	0.0328	−0.0199	−0.0128
	0.3542	0.6109	0.0350	0.0273	−0.0142	−0.0130
	0.3561	0.6081	0.0358	0.0360	−0.0244	−0.0116
	0.3656	0.5943	0.0401	0.0275	−0.0173	−0.0103
	0.3770	0.5781	0.0449	0.0401	−0.0314	−0.0087
	0.3680	0.5394	0.0925	0.0467	−0.0415	−0.0054
	0.4509	0.4951	0.0540	0.0408	−0.0351	−0.0057
	0.5107	0.4364	0.0529	0.0312	−0.0276	−0.0036
	0.5407	0.1841	0.2752	0.0756	−0.1124	0.0368
50	0.3946	0.5781	0.0274	0.0059	0.0027	−0.0085
	0.3915	0.5700	0.0385	0.0034	0.0032	−0.0066
	0.3921	0.5658	0.0421	0.0060	0.0070	−0.0130
	0.3999	0.5550	0.0452	0.0042	0.0047	−0.0088
	0.4075	0.5406	0.0519	0.0032	0.0062	−0.0094
	0.4552	0.4695	0.0752	0.0278	−0.0220	−0.0059
	0.5334	0.4044	0.0622	0.0105	−0.0031	−0.0074
	0.3769	0.5183	0.1047	0.0166	−0.0330	0.0164
	0.4148	0.4502	0.1349	0.0099	−0.0023	−0.0077
	0.4598	0.3484	0.1918	0.0266	−0.0163	−0.0103
	0.4729	0.2728	0.2542	0.0933	−0.1462	0.0528
65	0.5667	0.3619	0.0714	0.0083	−0.0053	−0.0030
	0.4663	0.3804	0.1533	0.0522	−0.0575	0.0053
	0.6670	0.2563	0.0768	0.0449	−0.0464	0.0016
	0.5259	0.4109	0.0632	0.0084	−0.0065	−0.0019
	0.5255	0.4257	0.0488	0.0198	−0.0161	−0.0037
	0.4657	0.4921	0.0422	0.0085	−0.0036	−0.0049
	0.4403	0.5210	0.0386	0.0132	−0.0034	−0.0099
	0.4340	0.5287	0.0372	0.0136	−0.0040	−0.0096
	mean deviation[b]			0.0262	0.0255	0.0105
	maximum deviation			0.0933	0.1462	0.0528

[a] $dy = y_{\mathrm{cal}} - y_{\mathrm{exp}}$. [b] Mean deviation $= (1/NC)\sum_j^N \sum_i^C |y_{i,\mathrm{cal}} - y_{i,\mathrm{exp}}|$ with $i = 1, 2, 3$; $j = 1, 2, ..., N$; *N* is the number of experimental points; and *C* is the number of components.

Table 7. Comparison between y_{exp} and y_{cal} for the Isobutanol (1) + Cyclohexane (2) + Water (3) System

t/°C	$y_{1,\mathrm{cal}}$	$y_{2,\mathrm{cal}}$	$y_{3,\mathrm{cal}}$	dy_1	dy_2	dy_3
40	0.2000	0.3638	0.4362	0.0583	−0.0849	0.0265
	0.1120	0.5891	0.2989	0.0159	0.0001	−0.0181
	0.1199	0.5770	0.3031	0.0302	−0.0100	−0.0202
	0.0929	0.6477	0.2593	0.0269	−0.0369	0.0098
	0.0823	0.6620	0.2557	0.0100	0.0071	−0.0171
	0.1819	0.5125	0.3055	0.0611	−0.0834	0.0221
	0.0753	0.6692	0.2555	0.0150	−0.0080	−0.0070
	0.0665	0.6728	0.2607	0.0024	−0.0060	0.0037
	0.0588	0.6693	0.2720	−0.0044	0.0157	−0.0113
	0.0410	0.8032	0.1558	−0.0180	0.0383	−0.0203
	0.0281	0.8825	0.0894	−0.0150	0.0160	−0.0010
	0.0403	0.6300	0.3297	−0.0286	−0.0941	0.1227
60	0.1372	0.5108	0.3520	0.0209	−0.0102	−0.0108
	0.1744	0.4513	0.3743	−0.0270	0.0302	−0.0009
	0.1198	0.5544	0.3257	0.0038	0.0244	−0.0287
	0.1110	0.5733	0.3157	0.0104	0.0012	−0.0116
	0.1128	0.5755	0.3117	0.0051	0.0269	−0.0322
	0.1070	0.5831	0.3100	0.0011	0.0098	−0.0108
	0.0910	0.6025	0.3065	−0.0033	0.0234	−0.0202
	0.1035	0.5970	0.2995	−0.0419	0.0314	0.0105
	0.0950	0.6079	0.2970	0.0061	0.0230	−0.0293
	0.0849	0.6078	0.3073	−0.0020	0.0069	−0.0049
	0.0905	0.6156	0.2938	−0.0098	0.0146	−0.0049
	0.0914	0.6286	0.2800	−0.0224	−0.0035	0.0259
	0.0754	0.6159	0.3087	−0.0124	−0.0020	0.0144
	0.0509	0.6070	0.3421	−0.0568	−0.0856	0.1416
	0.0462	0.7348	0.2190	−0.0261	0.0224	0.0037
	0.0475	0.7460	0.2065	−0.0192	0.0000	0.0191
	mean deviation			0.0198	0.0256	0.0232
	maximum deviation			0.0611	0.0941	0.1416

Once the binary NRTL parameters of cyclohexane + water were obtained, it was reasonable to use them to predict the VLE of other multicomponent systems containing cyclohexane and water, such as the systems 2-propanol + cyclohexane + water and furanidine + cyclohexane + water. The comparison was made among three sets of parameters for cyclohexane + water.

The parameters are listed in Table 8. The mean prediction deviation result is shown in Table 9 for the systems 2-propanol + cyclohexane + water and furanidine + cyclohexane + water.

From Table 9, it can be seen that the binary NRTL parameters obtained from LLE[12] were not suitable for VLE prediction. The parameters obtained from this work had acceptable predictions of the vapor−liquid equilibrium for the systems 2-propanol + cyclohexane + water and furanidine + cyclohexane + water.

In addition, the binary parameters obtained from this work also had an acceptable prediction of the ternary azeotropic points, as shown in Table 10.

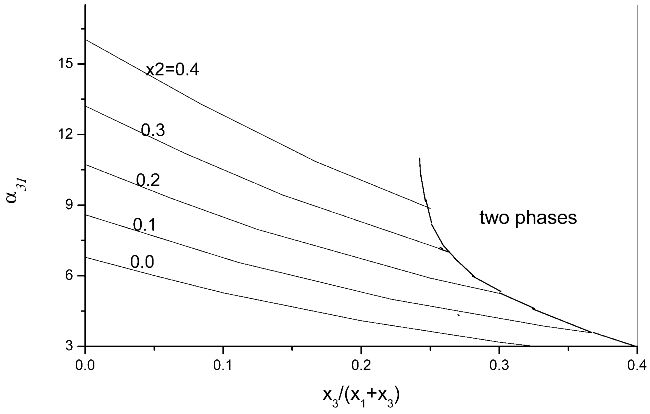

Figure 5. α_{31} − $x_3/(x_1 + x_3)$ for isobutanol (1) + cyclohexane (2) + water (3) (isopleth x_2).

Relationship between α and x. Using the binary parameters listed in Table 5, the relation between relative volatility α and *x* for the isobutanol (1) + cyclohexane (2) + water (3) system can be drawn as shown in Figures 5 and 6. The relationship between absolute temperature (*T*/K) and *x* was shown in Figure 7 (data for liquid−liquid equilibrium were cited from ref 14). Those figures for the system ethanol (1) + cyclohexane (2) + water (3) were similar (Figures 8−10). The LLE data were obtained from the literature.[12] They are helpful for designing the alcohol dewater facilities using cyclohexane as water-entrainer.

Table 8. Binary NRTL Parameters for Prediction

system	Δg_{12}	Δg_{21}	a_{12}	ref
cyclohexane (1) + water (2)	9729.86	12871.23	0.3	this work
	12047.9	18205.65	0.26	2, Vol. 1, part 1a, pp 626
	15019.24	23618.41	0.2	12, Vol. 5, part 1, p 384
2-propanol (1) + cyclohexane (2)	2898.55	5544.97	0.5542	2, Vol. 1, part 2d, p 73
2-propanol (1) + water (2)	−109.945	6565.543	0.2879	2, Vol. 1, part 1a, p 251
furanidine (1) + water (2)	3588.323	5677.356	0.415	11
furanidine (1) + cyclohexane (2)	1363.444	158.933	0.3	11

Table 9. Mean Deviation of Predicted Results Obtained by Use of Different Binary Parameters

	parameters for cyclohexane−water from		
	this work	lit.[2]	lit.[12]
2-propanol + cyclohexane + water	0.0149	0.0238	0.0600
furanidine + cyclohexane + water	0.0110	0.0077	0.0128

Table 10. Ternary Azeotropic Points of Alcohol (1) + Cyclohexane (2) + Water (3) at 101.33 kPa

	predicted		lit.[13] report
	isobutanol system at 71.4 °C	ethanol system at 62.8 °C	ethanol system at 62.6 °C
x_1	0.110	0.269	0.2685
x_2	0.579	0.530	0.5639
x_3	0.311	0.201	0.1670

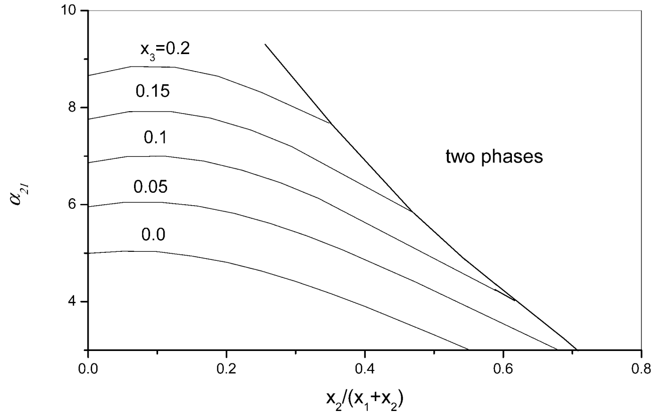

Figure 6. α_{21} − $x_2/(x_1 + x_2)$ for isobutanol (1) + cyclohexane (2) + water (3) (isopleth x_3).

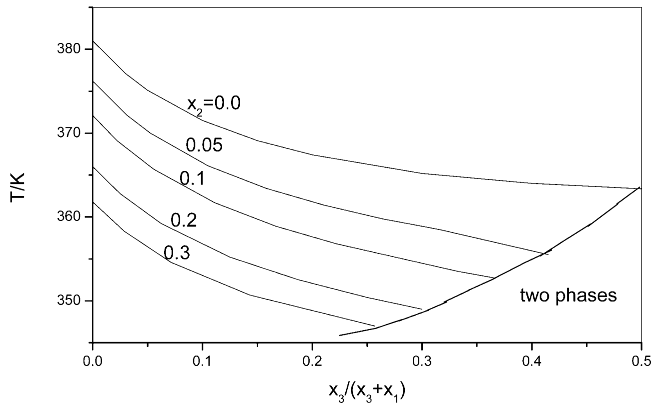

Figure 7. T − $x_3/(x_1 + x_3)$ for isobutanol (1) + cyclohexane (2) + water (3) (isopleth x_2).

Conclusions

1. The VLE data for the ternary system ethanol + cyclohexane + water at (35, 50, and 65) °C and the system isobutanol + cyclohexane + water at (40 and 60) °C were measured using an equilibrium still. The binary NRTL parameters for the cyclohexane + water system were

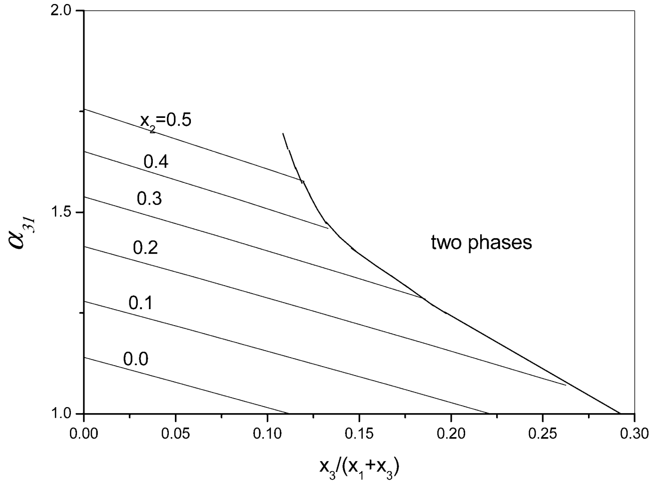

Figure 8. α_{31} − $x_3/(x_1 + x_3)$ for ethanol (1) + cyclohexane (2) + water (3) (isopleth x_2).

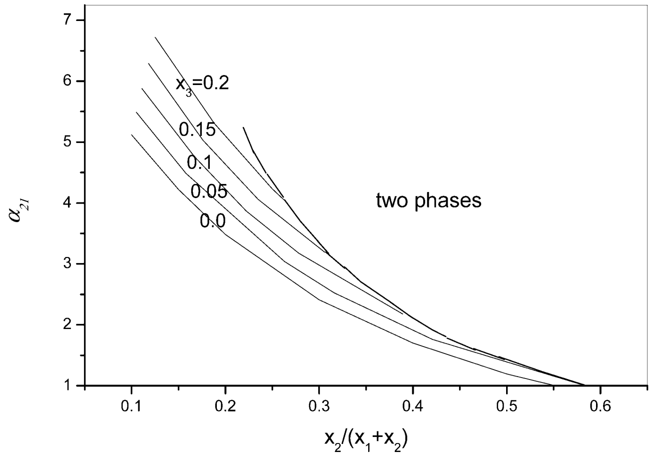

Figure 9. α_{21} − $x_2/(x_1 + x)$ for ethanol (1) + cyclohexane (2) + water (3) (isopleth x_3).

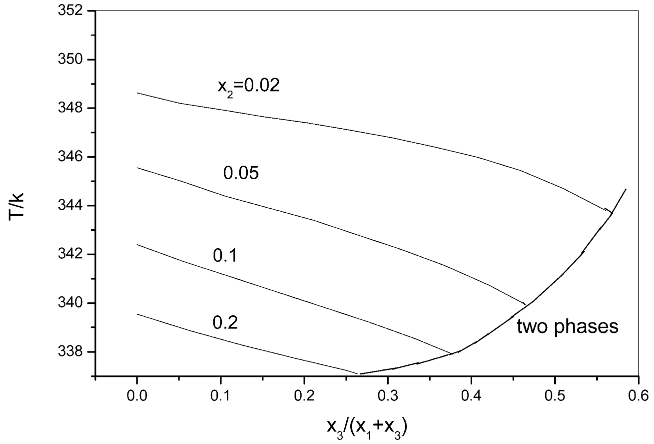

Figure 10. T − $x_3/(x_1 + x_3)$ for ethanol (1) + cyclohexane (2) + water (3) (isopleth x_2).

obtained by optimizing the measured ternary VLE data.

2. The VLE data were correlated with NRTL model. The mean deviation for the correlated data is 0.0207 for the ethanol + cyclohexane + water system and is 0.0229 for the isobutanol + cyclohexane + water system.

3. Using the obtained binary NRTL parameters for the cyclohexane + water system to predict the VLE of the 2-propanol + cyclohexane + water system and the furanidine + cyclohexane + water system, the mean deviation for the predicted data is 0.0149 and 0.0110. The predicted ternary azeotropic composition and temperature were close to those reported.

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