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Isobaric Vapor−Liquid Equilibria for Water + Acetic Acid + (*n*-Pentyl Acetate or Isopropyl Acetate)

Weixian Chang, Guofeng Guan,* Xinli Li, and Huqing Yao

College of Chemistry and Chemical Engineering, Nanjing University of Technology,
Nanjing 210009, People's Republic of China

Isobaric vapor−liquid equilibria (VLE) data for water + acetic acid, acetic acid + isopropyl acetate, acetic acid + *n*-pentyl acetate, water + acetic acid + isopropyl acetate, and water + acetic acid + *n*-pentyl acetate systems have been measured at 101.33 kPa using a recirculating still. The nonideality of the vapor phase caused by the association of the acetic acid has been corrected by the Hayden−O'Connell method. The three experimental binary data have been correlated by the NRTL and UNIQUAC models. The obtained NRTL model parameters from binary data have been used to predict ternary VLE data. The ternary predicted values obtained in this way agree well with the experimental values.

Introduction

The separation of organic acids from aqueous solutions is industrially important, and azeotropic distillation is an attractive process for such separation. Several acetates, such as isopropyl acetate,[1] butyl acetate,[2] isobutyl acetate,[3] and so on have been used as entrainers for the separation of acetic acid. It is known that vapor−liquid equilibria data is vital to the simulation and design of the azeotropic distillation process. Unfortunately, little work has been done on the vapor−liquid equilibria of the water + acetic acid + entrainer system.

No experimental study of the vapor−liquid phase equilibria of acetic acid + (*n*-pentyl acetate or isopropyl acetate) system at 101.33 kPa has been found. The aim of this article is mainly to investigate the vapor−liquid phase equilibria of acetic acid + isopropyl acetate, acetic acid + *n*-pentyl acetate, water + acetic acid + isopropyl acetate, and water + acetic acid + *n*-pentyl acetate systems at 101.33 kPa and supply basic data for the simulation and design of the azeotropic distillation process.

The water + acetic acid + ester systems are reactive systems because of the hydrolysis of the ester. However, acetic acid can hold down the hydrolytic reaction, and the reaction rate is very slow. Therefore, the hydrolysis of the ester is neglected.

It is known that the acetic acid molecules associate with each other to form stable dimers in both the liquid and vapor phases. In the present study, the deviation from ideal gas behavior, caused by the dimerization of acetic acid molecules and interaction between two molecules in the vapor phase, is described with the Hayden−O'Connell[4] (HOC) equation. This theory has been commonly used to calculate the vapor−liquid equilibria of systems with associating components. The nonidealities caused by water + acetic acid interaction and the dimerization effect of acetic acid molecules in the liquid phase are considered by the nonrandom two-liquids model (NRTL)[5] and the universal quasi-chemical theory (UNIQUAC).[6] In this work, both the NRTL and UNIQUAC models were used in combination with the HOC method for correlating the vapor−liquid equilibria of binary systems and predicting the vapor−liquid equilibria of the ternary systems containing the associating component acetic acid.

Table 1. Refractive Index of the Experimental Materials at 293.15 K

	water	acetic acid	isopropyl acetate	*n*-pentyl acetate
n_D[a]	1.3330	1.3716	1.3773	1.4023
n_D[b]	1.3330	1.3719	1.3772	1.4021

[a] Taken from Robert et al.[7] [b] This work.

Experimental Section

Materials. The chemicals used were acetic acid (glacial) (PA grade) with a stated minimum purity of 99.5 mass % supplied by Shanghai Lingfeng Chemical Reagents Limited, deionized water (PA grade) supplied by the membrane science technology research laboratory of Nanjing University of Technology, and isopropyl acetate (≥98.5 mass %) and *n*-pentyl acetate (≥98.5 mass %) both supplied by Shanghai Chemical Reagents Co. All of the solvents except water were distilled in a glass column and further purified before use.

Apparatus and Procedure. Refractive indices were measured by a refractometer, model WZS-I-79040 with a precision of ±0.0001. The measured refractive indices of the pure liquids were compared with published values in Table 1.

Different types of VLE apparatuses have been designed to obtain VLE data. In this work, the apparatus used was a recirculating still of the modified Rose type.[8] Gu and Zhang[9] have applied this apparatus to obtain VLE data for the *N*-methylpiperazine + piperazine and water + *N*-methylpiperazine binary systems. Gu[10] has used this apparatus to measure VLE data for water + *N*-ethylpiperazine. During the measurements, temperature was measured by using a mercury thermometer. The uncertainty of the temperature measurements was ±0.01 K. The uncertainty of the measured vapor-phase mole fraction was 0.001. The pressure was obtained at (101.33 ± 0.04) kPa with the help of a pressure control system, which consisted of one water manometer, one mercury manometer, three

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* Corresponding author. E-mail: njutggf@163.com.

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Table 2. Experimental VLE Data for the Binary Systems at 101.33 kPa

	water (1) + acetic acid (2)			isopropyl acetate (1) + acetic acid (2)			acetic acid (1) + *n*-pentyl acetate (2)		
no.	T/K	x_1	y_1	T/K	x_1	y_1	T/K	x_1	y_1
1	388.49	0.0738	0.1203	386.43	0.0661	0.1314	415.94	0.0981	0.2323
2	386.52	0.1273	0.1924	385.74	0.0835	0.1599	414.12	0.1753	0.3460
3	385.81	0.1426	0.2208	384.61	0.1035	0.2036	411.22	0.2407	0.4229
4	384.17	0.1900	0.2805	384.10	0.1127	0.2231	409.88	0.2731	0.4725
5	382.47	0.2448	0.3581	382.47	0.1325	0.2452	407.93	0.3330	0.5305
6	381.21	0.2980	0.4334	381.56	0.1623	0.3051	406.39	0.3814	0.6052
7	379.84	0.3731	0.5196	375.16	0.3157	0.5195	405.22	0.4322	0.6334
8	378.42	0.4780	0.6192	373.15	0.3723	0.5904	403.13	0.4947	0.7094
9	377.71	0.5279	0.6691	371.15	0.4252	0.6617	401.35	0.5696	0.7653
10	377.06	0.5871	0.7199	370.06	0.4751	0.7032	399.16	0.6501	0.8202
11	376.60	0.6294	0.7558	368.44	0.5512	0.7747	397.01	0.7248	0.8618
12	376.09	0.6788	0.7924	367.14	0.6153	0.8227	395.94	0.7765	0.8877
13	375.59	0.7366	0.8288	365.52	0.7433	0.8874	394.77	0.8314	0.9146
14	374.98	0.8080	0.8697	364.49	0.8178	0.9317	393.54	0.8827	0.9430
15	374.73	0.8434	0.8910				392.45	0.9289	0.9640
16	374.43	0.8751	0.9181						
17	374.02	0.9259	0.9530						
18	373.82	0.9813	0.9854						

Table 3. Experimental VLE Data for the Ternary Systems

	water (1) + acetic acid (2) + isopropyl acetate (3)					water (1) + acetic acid (2) + *n*-pentyl acetate (3)				
no.	T/K	x_1	x_2	y_1	y_2	T/K	x_1	x_2	y_1	y_2
1	370.52	0.5986	0.3774	0.6751	0.1677	376.30	0.4416	0.5010	0.6226	0.3210
2	371.69	0.5977	0.3837	0.6715	0.2061	376.50	0.4547	0.4997	0.6303	0.3184
3	371.94	0.6112	0.3734	0.6799	0.2082	376.71	0.4283	0.4807	0.6075	0.3230
4	372.65	0.5047	0.4682	0.6149	0.2655	377.01	0.4750	0.5091	0.6197	0.3558
5	372.91	0.4962	0.4726	0.6023	0.2688	377.82	0.3548	0.5609	0.5649	0.3750
6	372.95	0.6121	0.3772	0.6899	0.2257	378.02	0.3437	0.5646	0.5686	0.3677
7	373.31	0.4981	0.4764	0.6084	0.2817	381.72	0.2377	0.6329	0.4307	0.4912
8	374.18	0.2261	0.6580	0.3662	0.3948	385.03	0.2105	0.5522	0.4031	0.4787
9	374.73	0.2602	0.6539	0.3904	0.4184	385.79	0.1522	0.5593	0.3854	0.4993
10	374.87	0.6291	0.3672	0.6997	0.2740	386.39	0.1416	0.5437	0.3843	0.4806
11	375.44	0.2594	0.6634	0.3925	0.4213	386.65	0.1310	0.7195	0.2681	0.6587
12	375.58	0.6279	0.3701	0.7223	0.2651	387.71	0.1283	0.5263	0.3666	0.4792
13	375.95	0.2649	0.6701	0.3879	0.4562	389.09	0.1311	0.5237	0.3377	0.5032
14	377.15	0.3827	0.5987	0.4905	0.4455	389.24	0.1284	0.5054	0.3418	0.4891
15	378.03	0.3835	0.6069	0.5023	0.4595	390.71	0.1083	0.5339	0.3041	0.5200
16	382.27	0.1618	0.8115	0.2681	0.6703	391.11	0.1085	0.5771	0.2533	0.6038
17	382.69	0.1676	0.8131	0.2832	0.6699	391.68	0.1037	0.5663	0.2629	0.5833
18	383.30	0.1794	0.8095	0.2737	0.7013					

triple valves, one vacuum pump, two reservoirs, and one electromagnetic-type relay. The experimental procedures are almost the same as those described previously.[11]

Sample Analysis. Compositions of the water + acetic acid + *n*-pentyl acetate system were analyzed using an SP 6800A gas chromatograph with a thermal conductivity detector. The GC response was treated with a Zhejing Zhida chromatography station. A 2-m chromatographic column was packed with Porapak Q. The carrier gas was hydrogen flowing at 50 mL/min, and the column temperature was 473 K. The injector and detector temperatures were 428 K and 473 K, respectively. The detector current was 150 mA.

Compositions of water + acetic acid + isopropyl acetate system were also analyzed by a gas chromatograph with a TCD detector. A 1-m column was packed with GDX-102 on which isophthalic acid and polyglycol were loaded. The optimum operation conditions were the following: injection temperature, 433 K; oven temperature, 423 K; detector temperature, 433 K; detector current, 150 mA; and carrier gas, hydrogen with a flow rate of 50 mL/min.

Results and Discussion

Experimental Data. Vapor−liquid equilibria for the binary systems water (1) + acetic acid (2), acetic acid (2) + isopropyl acetate (3), and acetic acid (2) + *n*-pentyl acetate (3) have been obtained at 101.33 kPa. The results are reported in Table 2. Also, the vapor−liquid equilibria for the water (1) + acetic acid (2) + isopropyl acetate (3) and water (1) + acetic acid (2) + *n*-pentyl acetate (3) ternary systems were obtained at 101.33 kPa, and the results are reported in Table 3.

To test the equilibria apparatus and operation method, VLE data of water−acetic acid system were compared with the published data shown in Figure 1. It can be found that the experimental data of this work agreed well with the literature data. The test results show that the equilibrium apparatus and operation method are applicable.

The Herington method[13] was used to check the thermodynamic consistency, and the check results should be less than 10%. The check results for water (1) + acetic acid (2), acetic acid (2) + isopropyl acetate (3), and acetic acid (2) + *n*-pentyl acetate (3) systems were 4.35%, 0.10%, and −7.27%, respectively. All binary VLE data of this work were thermodynamically consistent.

Vapor−Liquid Equilibria Model. The vapor−liquid equilibria equation can be expressed by the following equation

$$\phi_i^{\hat{V}} y_i p = x_i \gamma_i \phi_i^{S}\, p_i^{S} \exp\left[\frac{V_i^{L}(p - p_i^{S})}{RT}\right] \qquad (1)$$

where $\phi_i^{\hat{V}}$ is the fugacity coefficient of component i in the mixture, ϕ_i^{S} is the fugacity coefficient at the saturated

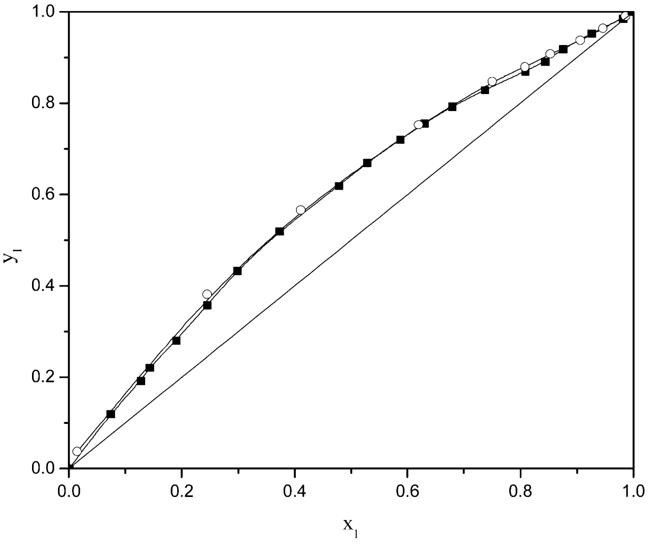

Figure 1. VLE data of water (1) + acetic acid (2) at 101.33 kPa: ■, this work; ○, Gilmont et al.[12]

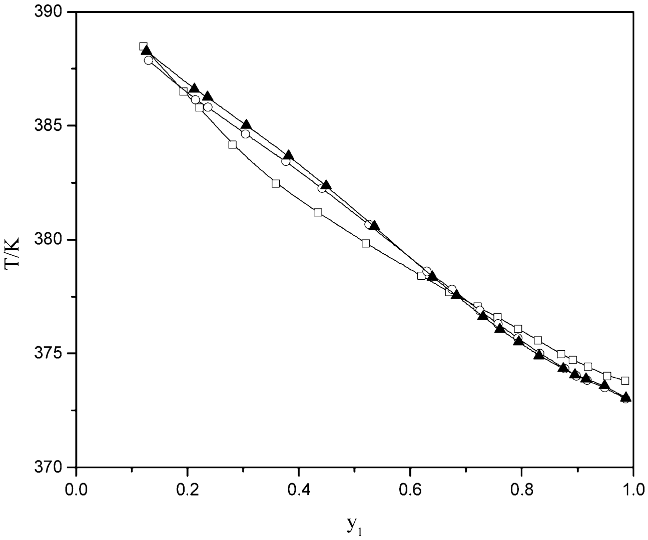

Figure 2. Experimental and calculated $T-y_1$ diagram for water (1) + acetic acid (2) at 101.33 kPa: □, $T-y_1$ experimental; ○, $T-y_1$ calculated (calculation based on the NRTL model; ▲, $T-y_1$ calculated (calculation based on the UNIQUAC model).

vapor pressure, y_i is the apparent mole fraction in the vapor phase, x_i is the mole fraction in the liquid phase, γ_i is the activity coefficient in the liquid phase, p is the system pressure, and p_i^{S} is the saturated vapor pressure.

At low pressure, the term $\exp[V_i^{\mathrm{L}}(p - p_i^{\mathrm{S}})/RT]$ is approximately equal to 1, thus eq 1 can be rewritten as

$$\hat{\phi}_i^{\mathrm{V}} y_i p = x_i \gamma_i \phi_i^{S} p_i^{\mathrm{S}} \quad (2)$$

In the present work, the vapor-phase fugacity coefficients are computed by using the chemical theory.[14] The second virial coefficient B is calculated with Hayden−O'Connell equation. The liquid-phase activity coefficient is calculated by the solution models for the excess Gibbs free energy such as UNIQUAC and NRTL, and the relationship is

$$\ln \gamma_i = \left[\frac{\partial\left(\frac{nG^{\mathrm{E}}}{RT}\right)}{\partial n_i}\right]_{T,P,nj\neq i} \quad (3)$$

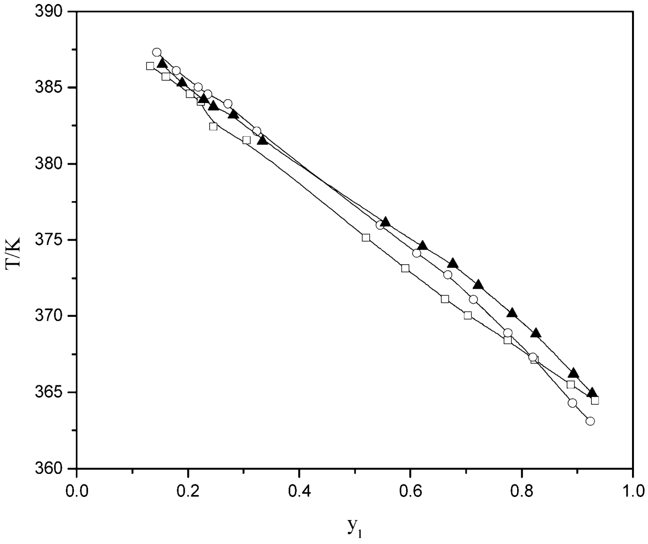

Figure 3. Experimental and calculated $T-y_1$ diagram for isopropyl acetate (1) + acetic acid (2) at 101.33 kPa: □, $T-y_1$ experimental; ○, $T-y_1$ calculated (calculation based on the NRTL model); ▲, $T-y_1$ calculated (calculation based on the UNIQUAC model).

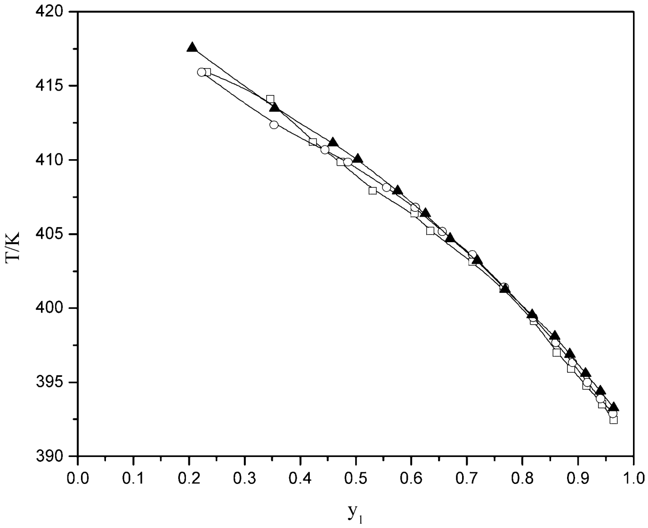

Figure 4. Experimental and calculated $T-y_1$ diagram for acetic acid (1) + n-pentyl acetate (2) at 101.33 kPa: □, $T-y_1$ experimental; ○, $T-y_1$ calculated (calculation based on the NRTL model; ▲, $T-y_1$ calculated (calculation based on the UNIQUAC model).

Calculation of Binary Vapor−Liquid Equilibria. To predict the VLE of the water + acetic acid + entrainer system, it is very necessary to determine the binary adjustable parameters for each two components in the system. For each binary system, the three corresponding parameters were estimated by the minimization of the objective function

$$F = \sum_{K=1}^{N}\{(\gamma_{1,\mathrm{calcd}} - \gamma_{1,\mathrm{exptl}})_{\mathrm{K}}^2 + (\gamma_{2,\mathrm{calcd}} - \gamma_{2,\mathrm{exptl}})_{\mathrm{K}}^2\} \quad (4)$$

where N represents the number of experimental data points and the indices exptl and calcd represent the experimental and calculated values. The summations are extended over all data points.

Figures 2 to 4 show the correlation deviations of the vapor-phase composition and deviations of temperature between the experimental and calculated values. Table 4 shows the calculated second virial coefficients for binary systems. The estimated binary parameters and the average

Table 4. Calculated Second Virial Coefficients for the Binary Systems

	water (1) + acetic acid (2)				isopropyl acetate (1) + acetic acid (2)				acetic acid (1) + n-pentyl acetate (2)			
	NRTL		UNIQUAC		NRTL		UNIQUAC		NRTL		UNIQUAC	
no.	B_1	B_2	B_1	B_2	B_1	B_2	B_1	B_2	B_1	B_2	B_1	B_2
						cm^3·mol^{-1}						
1	−7.87	19.96	−7.73	20.17	−71.28	19.66	−71.67	19.23	33.43	−87.40	34.13	−87.66
2	−8.49	19.03	−8.33	19.28	−71.87	19.02	−72.28	18.57	31.88	−87.47	32.38	−88.82
3	−8.61	18.85	−8.45	19.10	−72.40	18.43	−72.80	17.98	31.12	−88.93	31.34	−89.39
4	−9.05	18.21	−8.91	18.42	−72.63	18.17	−73.02	17.73	30.76	−89.13	30.84	−89.64
5	−9.50	17.55	−9.40	17.69	−72.94	17.82	−73.29	17.41	29.97	−89.53	29.87	−90.06
6	−9.94	16.90	−9.90	16.96	−73.79	16.83	−74.10	16.47	29.35	−89.82	29.16	−90.33
7	−10.56	16.00	−10.59	15.96	−76.61	13.31	−76.55	13.40	28.60	−90.13	28.38	−90.58
8	−11.38	14.83	−11.48	14.69	−77.41	12.22	−77.23	12.48	27.87	−90.40	27.68	−90.76
9	−11.69	14.38	−11.80	14.23	−78.01	11.38	−77.72	11.80	26.82	−90.70	26.75	−90.95
10	−12.07	13.84	−12.18	13.69	−78.68	10.40	−78.30	10.96	25.82	−90.92	25.91	−91.06
11	−12.32	13.50	−12.41	13.37	−79.55	9.06	−79.06	9.83	24.99	−91.04	25.21	−91.12
12	−12.57	13.14	−12.64	13.04	−80.17	8.06	−79.58	9.01	24.32	−91.11	24.61	−91.13
13	−12.85	12.74	−12.90	12.68	−81.28	6.15	−80.58	7.37	23.65	−91.14	23.95	−91.12
14	−13.14	12.34	−13.14	12.35	−81.70	5.37	−81.05	6.56	23.09	−91.14	23.35	−91.08
15	13.27	12.16	−13.25	12.19					22.59	−91.12	22.78	−91.02
16	−13.36	12.04	−13.33	12.08								
17	−13.50	11.85	−13.46	11.90								
18	−13.71	11.55	−13.69	11.58								

Table 5. Correlation Parameters and the Average Absolute Deviations for Binary Systems

model	A_{12}[a] J·mol^{-1}	A_{21} J·mol^{-1}	α_{12}	Δy[b]	ΔT[c]
Water (1) + Acetic Acid (2)					
NRTL	3042.92	730.34	1.33	0.0088	0.52
UNIQUAC	2383.76	−1592.81		0.0108	0.57
Isopropyl Acetate (1) + Acetic Acid (2)					
NRTL	4293.86	798.79	1.20	0.0104	0.65
UNIQUAC	22320.46	−12411.26		0.0206	0.94
Acetic Acid (1) + n-Pentyl Acetate (2)					
NRTL	1873.99	2332.01	1.65	0.0076	0.38
UNIQUAC	−1022.62	2634.54		0.0154	0.54
Water (1) + Isopropyl Acetate (2)[d]					
NRTL	121.07	3894.12	1.26		
Water (1) + n-Pentyl Acetate (2)[e]					
NRTL	3134.65	203.76	0.20		

[a] The binary adjustable parameters for various models are as follows: NRTL, $Aij = (gij - gjj)$; UNIQUAC, $Aij = (uij - ujj)$. [b] $\Delta y = (1/N)|y_{\text{calcd}} - y_{\text{exptl}}|$. [c] $\Delta T = (1/N)|T_{\text{calcd}} - T_{\text{exptl}}|$. [d] Taken from Teodorescu et al.[15] [e] Taken from Lee et al.[16]

absolute deviation (AAD) between the calculated values and experimental values are reported in Table 5.

From the average absolute deviation between calculated and experimental values, it can be seen that there is good agreement between the experimental and the calculated data by both the NRTL and UNIQUAC models. The NRTL model is better than the UNIQUAC model on the basis of the average absolute deviations.

Prediction of Ternary Vapor−Liquid Equilibria. In this work, no research was done on the phase equilibria of the water + acetate system. The parameters of the water + isopropyl acetate and water + n-pentyl acetate systems are from published documents[15,16] shown in Table 5. The NRTL interaction parameters obtained from the binary systems were used to predict the vapor−liquid equilibria of the water (1) + acetic acid (2) + entrainer (3) ternary system. The predictive deviations and the calculated second virial coefficients are shown in Table 6.

For the water + acetic acid + isopropyl acetate system, the average absolute deviation of the vapor-phase mole fractions of water and acetic acid were 0.0399 and 0.0190, and the average absolute deviation of the equilibrium temperature was 0.72 K. For the water + acetic acid + n-pentyl acetate system, the average absolute deviations (AAD) of the vapor-phase mole fractions of water and acetic acid were 0.0325 and 0.0223, and the average absolute

Table 6. Predictive Deviations and Calculated Second Virial Coefficients for the Ternary Systems[a]

	water (1) + acetic acid (2) + isopropyl acetate (3)						water (1) + acetic acid (2) + n-pentyl acetate (3					
no.	ΔT/K	Δy_1	Δy_2	B_1	B_2	B_3	ΔT/K	Δy_1	Δy_2	B_1	B_2	B_3
1	−0.87	−0.0807	0.0070	−15.40	7.83	−79.15	1.73	0.0037	0.0022	−11.78	13.68	−87.38
2	−0.47	−0.0535	−0.0138	−14.70	8.79	−78.51	1.51	−0.0014	0.0079	−11.79	13.67	−87.37
3	−0.17	−0.0422	−0.0170	−14.46	9.13	−78.28	0.98	0.0347	−0.0298	−11.92	13.49	−87.24
4	−0.39	−0.0594	−0.0115	−14.24	9.43	−78.08	1.45	0.0017	0.0016	−11.60	13.93	−87.56
5	−1.18	−0.0597	−0.0184	−14.47	9.11	−78.30	1.76	−0.0106	0.0149	−11.15	14.57	−87.99
6	0.40	−0.0245	−0.0177	−13.77	10.09	−77.62	1.75	−0.0210	0.0268	−11.08	14.68	−88.06
7	−0.49	−0.0522	−0.0157	−14.00	9.77	−77.84	0.82	0.0064	0.0071	−10.00	16.23	−88.99
8	−1.86	−0.0529	−0.0111	−14.21	9.46	−78.05	−0.95	0.0742	−0.0542	−9.41	17.08	−89.42
9	−1.38	−0.0451	−0.0222	−13.77	10.09	−77.62	0.19	0.0219	−0.0204	−8.71	18.12	−89.88
10	0.83	0.0247	−0.0510	−12.77	11.49	−76.60	0.27	0.0191	−0.0069	−8.46	18.48	−90.02
11	−1.27	−0.0474	−0.0046	−13.41	10.58	−77.27	0.02	0.0065	0.0014	−8.46	18.49	−90.03
12	0.93	0.0163	−0.0323	−12.43	11.97	−76.24	−0.08	0.0285	−0.0088	−8.11	19.00	−90.21
13	−0.82	−0.0366	−0.0181	−13.01	11.15	−76.85	−0.66	0.0639	−0.0395	−7.82	19.43	−90.35
14	0.30	−0.0085	−0.0248	−12.04	12.52	−75.82	−0.57	0.0679	−0.0412	−7.74	19.56	−90.39
15	1.03	−0.0095	−0.0057	−11.39	13.45	−75.09	−0.50	0.0516	−0.0171	−7.20	20.37	−90.61
16	0.10	−0.0371	0.0229	−10.09	15.33	−73.54	−1.15	0.0754	−0.0575	−7.29	20.24	−90.57
17	0.25	−0.0456	0.0358	−9.87	15.65	−73.26	−1.25	0.0638	−0.0413	−7.12	20.48	−90.63
18	0.21	−0.0216	0.0125	−9.65	15.97	−72.99						

[a] B_1, B_2, and B_3 are given in units of cm^3·mol^{-1}.

deviation of the equilibria temperature was 0.92 K. The values of AAD show that the NRTL model gives a good representation of the experimental data.

Conclusions

The NRTL and UNIQUAC model can both satisfactorily correlate the vapor−liquid equilibria data of binary systems. But the NRTL model is more accurate than the UNIQUAC model in correlating the equilibria compositions of binary systems. The obtained NRTL interaction parameters were used to predict the vapor−liquid equilibria of the water + acetic acid + (isopropyl acetate or *n*-pentyl acetate) systems. Ternary predicted values agree well with the experimental data in the experimental range of compositions. It can be said that NRTL−HOC model is suitable for correlating the vapor−liquid equilibria of binary systems and the NRTL interaction parameters are good enough to represent the two ternary systems.

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