Vapor−Liquid Equilibria for the Ternary System Acetonitrile + 1-Propanol + Dimethyl Sulfoxide and the Corresponding Binary Systems at 101.3 kPa

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Isobaric vapor−liquid equilibrium (VLE) data were measured at 101.3 kPa by using an improved Rose equilibrium still for three binary systems, acetonitrile (1) + 1-propanol (2), acetonitrile (1) + dimethyl sulfoxide (DMSO) (3), and 1-propanol (2) + DMSO (3), and for one ternary system, acetonitrile (1) + 1-propanol (2) + DMSO (3). The VLE data of the binary systems were examined by thermodynamic consistency tests and satisfactorily correlated by Wilson and NRTL models. The parameters of two models obtained from the binary data were used to predict the ternary VLE data. The prediction yielded reasonable results for the ternary system.

Introduction

Acetonitrile and 1-propanol have been used extensively as solvents or as important fine chemicals in the chemical and pharmaceutical production process[1,2] as well as in chromatography separation.[3,4] A large volume of acetonitrile and 1-propanol solution is generated continuously in the relative processes. A suitable and efficient method to recover the acetonitrile and 1-propanol is necessary. Separation of them with a conventional distillation process is very difficult due to the azeotropic system.[5] Extractive distillation is a preferable way to improve the separation of azeotropic systems and approximate boiling point systems[6,7] and was successfully used in the recovery of alcohol and 1,3-butadiene in related industries.[8,9]

Dimethyl sulfoxide (DMSO), as the third component, was employed as the extractive solvent in the distillation to improve the separation of acetonitrile and 1-propanol in this work. To simulate and design the separation process, it is essential to determine the vapor−liquid equilibrium (VLE) data for the binary and ternary systems and to study their correlating models. The VLE data of the binary system acetonitrile (1) + 1-propanol (2) at atmospheric pressure were reported by Prasad et al.[5] However, the VLE data for the binary systems acetonitrile (1) + DMSO (3) and 1-propanol (2) + DMSO (3) and the ternary system acetonitrile (1) + 1-propanol (2) + DMSO (3) at 101.3 kPa have not been available up to now.

This work was carried out to provide fundamental data for the separation of acetonitrile and 1-propanol by extractive distillation using DMSO as extractant. The isobaric VLE data for the binary and ternary systems at 101.3 kPa were measured in this work. Moreover, the VLE correlation for the binary systems and the prediction for the ternary with the Wilson and NRTL models were studied and discussed.

Experimental Section

Materials. Acetonitrile, 1-propanol, and DMSO (analytical grade, 99 % mass) were obtained commercially and were purified by redistillation. The purities of the reagents were checked by measuring their physical properties and further confirmed by gas chromatography with more than 99.5 % mass. Good agreement of the properties was found between the measured values and literature ones as shown in Table 1. Refractive indices were measured by a WZS-I Abbe refractometer (Shanghai Optical Instruments Factory, China), with an uncertainty of ± 0.0001. Densities were measured by a DMA-4100 densimeter (AntonPaar GmbH, Germany), with an uncertainty of ± 0.0001 $g\cdot cm^{-3}$. Boiling temperatures were measured using a mercury-in-glass thermometer accurate to ± 0.01 K.

Apparatus and Procedure. The modified Rose-type still and auxiliary equipment, the same as in the previous work,[11] were employed to measure isobaric VLE data at 101.3 kPa, and the favorable performance of the apparatus was verified in the previous measurement.

The experiments were accomplished under a dried inert atmosphere at a constant pressure of 101.3 kPa. The pressure was automatically adjusted to the desired value by an electric contact pressure adjuster (DYT01, Yangzhong Mechanical Instrument Factory, China) with an uncertainty of ± 1 mmHg. The inert air in the isobaric bottle would be heated to maintain the pressure at 101.3 kPa when pressure variation was detected by the pressure adjuster. The liquid phase was kept boiling until the system reached constant temperature and pressure for 15 min or longer to ensure completed VLE. The temperature was recorded by a mercury-in-glass thermometer with an uncertainty of ± 0.01 K, and about 1.5 mL of the vapor and liquid samples was taken simultaneously with two syringes from the liquid outlet and the condensate outlet.

Sample Analysis. The equilibrium compositions of the liquid and vapor phases were analyzed by a gas chromatograph GC7890II with a flame ionization detector (FID), a capillary column (30 m by 0.25 mm i.d.) of the AT.FFAP stationary phase, and a chromatographic workstation N2000. High purity nitrogen was used as the carrier gas at a constant flow rate of 50 $mL\cdot min^{-1}$. The injector, detectors, and oven temperature were kept at (483.15, 493.15, and 473.15) K, respectively. The gas chromatograph was calibrated with a set of mixtures of known compositions that were prepared gravimetrically by an electronic balance (uncertainty of ± 0.0001 g). The reproducibility of concentration measurement was better than ± 0.0003

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Table 1. Physical Properties of Pure Reagents

	n_D		ρ/g·cm^{-3}		T_b/K	
substance	exptl	lit.[10]	exptl	lit.[10]	exptl	lit.[10]
acetonitrile	1.3449	1.3441 (293.15 K)	0.7831	0.7822 (293.15 K)	354.65	354.60
1-propanol	1.3860	1.3856 (293.15 K)	0.8040	0.8036 (293.15 K)	370.24	370.20
DMSO	1.4775	1.4773 (298.15 K)	1.0961	1.0958 (298.15 K)	462.06	462.15

Table 2. Antoine Coefficients *A*, *B*, and *C*

		Antoine constants		
components	*T* range/K	A_i	B_i	C_i
acetonitrile[12,a]	354 to 462	15.2851[c]	3652.381[c]	12.292[c]
1-propanol[13,a]	303 to 369	16.0353	3415.56	70.733
1-propanol[14,a]	369 to 402	16.01787	3415.557	70.657
1-propanol[15,a]	402 to 463	14.6132[d]	2587.343[d]	111.913[d]
DMSO[16,b]	356 to 462	6.66676	1952.13	45.35

[a] $\ln(P_i^s) = A_i - B_i/(T - C_i)$. Units: P_i^s/kPa, *T*/K. [b] $\log(P_i^s) = A_i - B_i/(T - C_i)$. Units: P_i^{ss}/kPa, *T*/K. [c] Calculated from the vapor pressure in ref 12. [d] Calculated from the vapor pressure in ref 15.

Table 3. Intrinsic Properties of the Pure Liquids

compound	P_c kPa	T_c K	V_c cm^3·mol	ω	Z_{RA}
acetonitrile	4830[a]	548.0[a]	173.0[a]	0.3270[a]	0.184[a]
1-propanol	5180[a]	536.8[a]	219.0[a]	0.6290[a]	0.254[a]
DMSO	5845[a]	707.0[a]	276.1[a]	0.3627[b]	0.274[a]

[a] Ref 19. [b] Calculated from our experimental data with the Lee−Kesler equation.[19]

mass fractions, and the maximum uncertainty for the measurements was ± 0.0002.

Results and Discussion

Fundamental Equation. The activity coefficient γ_i of the component *i* in the mixtures was calculated from the following equation

$$\phi_i^{\mathrm{v}} y_i P = \gamma_i x_i \phi_i^{\mathrm{s}} P_i^{\mathrm{s}} \exp\left(\frac{\nu_i^{\mathrm{L}}(P - P_i^{\mathrm{s}})}{RT}\right) \qquad (1)$$

where x_i and y_i are the mole fractions of the liquid and vapor phases in equilibrium, respectively; ϕ_i^{v} is the fugacity coefficient of vapor component *i*; ϕ_i^{s} is the fugacity coefficient of component *i* at saturation; *R* is the universal gas constant; *T* is the experimental temperature; *P* is total pressure of the system, 101.3 kPa, in this study; and P_i^{s} is the vapor pressure for the pure component calculated by an Antoine equation. The Antoine equation and its constants (A_i, B_i, and C_i) are listed in Table 2, and the molar liquid volumes, ν_i^{L}, of pure compounds were estimated using the modified Rackett equation.[17] The fugacity coefficients were calculated by using the virial equation of state truncated after the second term. The second virial coefficients were obtained from the Tsonopoulos[18] empirical equation. All the required parameters are listed in Table 3. In this way, the liquid-phase activity coefficients can be calculated by experimental results through eq 1 as given in Table 4.

Experimental Data. Experimental VLE data of the binary systems acetonitrile + 1-propanol, acetonitrile + DMSO, and 1-propanol + DMSO and the ternary system acetonitrile + 1-propanol + DMSO were measured at 101.3 kPa. The results are listed in Tables 4 and 6. The comparison between the measured VLE data of acetonitrile + 1-propanol with the literature[5] is shown in Figure 1, with good agreement. The figure also suggests that the binary system acetonitrile and 1-propanol is an azeotropic system with minimum azeotropic temperature (352.92 K), and the mole fractions of the liquid and vapor phases of azeotrope are 0.7792 and 0.7739, respectively. The unequal mole fractions in the two phases may be caused by experimental error.

The experimental binary VLE data were found to be thermodynamically consistent by means of the point-to-point test of Van Ness,[20] modified by Fredenslund et al.[21] A Legendre polynomial was used for the excess Gibbs energy. According to this method, isobaric data would pass the consistency test if the mean absolute deviation between calculated and measured mole fractions of component 1 in the vapor phase, δy, was less than 0.01. The parameters of the Legendre polynomial and results of the tests for the binary systems are listed in Table 5. Each δy_1 of the three binary systems is less than 0.01. Therefore, all binary VLE data of this work could pass the thermodynamic consistency test.

Calculation of Binary Vapor−Liquid Equilibrium. The activity coefficients were correlated with the Wilson[22] and NRTL[23] models in this work. The parameters of these models are given in Table 7, which were obtained by minimizing the following objective function (OF)

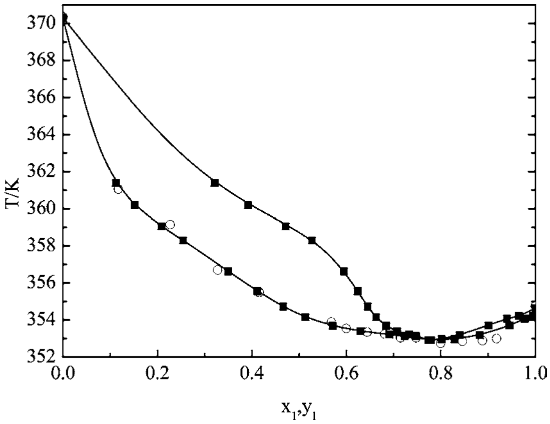

Figure 1. VLE relation for acetonitrile (1) + 1-propanol (2) at 101.3 kPa: ■, this work; ○, the literature data.[5]

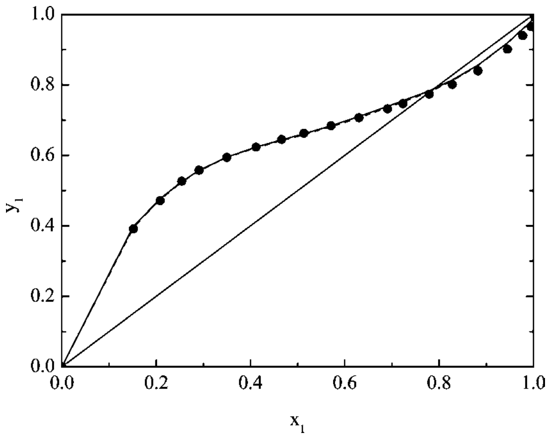

Figure 2. Equilibrium diagram for the system acetonitrile (1) + 1-propanol (2) at 101.3 kPa: ■, experimental data; —, calculation based on the Wilson model; - -, calculation based on the NRTL model.

Table 4. Experimental VLE Data and Correlated Results of Binary Systems at 101.3 kPa

						calculated by Wilson			calculated by NRTL		
no.	T/K	x_1	y_1	γ_1	γ_2	ΔT^a	$\Delta y_1{}^b$	$\Delta y_2{}^b$	ΔT^a	$\Delta y_1{}^b$	$\Delta y_2{}^b$
					Acetonitrile (1) + 1-Propanol (2)						
1	361.38	0.1121	0.3210	2.3342	1.0683	0.73	0.0078	0.0358	0.88	0.0032	0.0348
2	360.19	0.1519	0.3916	2.1780	1.0518	0.22	0.0060	0.0163	0.36	0.0025	0.0154
3	359.06	0.2086	0.4712	1.9748	1.0260	0.50	0.0044	0.0105	0.40	0.0025	0.0115
4	358.30	0.2539	0.527	1.8571	1.0045	0.87	0.0032	0.0311	0.80	0.0041	0.0321
5	356.64	0.3498	0.5945	1.6000	1.0587	0.93	0.0015	0.0308	0.88	0.0014	0.0323
6	355.56	0.4115	0.6237	1.4753	1.1357	0.64	0.0022	0.0206	0.59	0.0022	0.0225
7	354.73	0.4661	0.6454	1.3830	1.2218	0.36	0.0031	0.0114	0.30	0.0034	0.0137
8	354.15	0.5132	0.6629	1.3137	1.3056	0.17	0.0034	0.0049	0.11	0.0042	0.0078
9	353.68	0.5707	0.6842	1.2373	1.4150	0.09	0.0016	0.0003	0.03	0.0031	0.0037
10	353.40	0.6300	0.7072	1.1688	1.5405	0.12	0.0019	0.0021	0.06	0.0001	0.0019
11	353.22	0.6907	0.7324	1.1103	1.6972	0.18	0.0059	0.0044	0.11	0.0036	0.0001
12	353.13	0.7235	0.7470	1.0842	1.8019	0.18	0.0076	0.0062	0.11	0.0053	0.0019
13	352.92	0.7792	0.7739	1.0498	2.0348	0.04	0.0082	0.0114	0.04	0.0060	0.0075
14	352.97	0.8283	0.8014	1.0211	2.2934	0.04	0.0125	0.0153	0.03	0.0108	0.0120
15	353.18	0.8824	0.8399	0.9979	2.6752	0.04	0.0165	0.0188	0.03	0.0154	0.0166
16	353.69	0.9451	0.9010	0.9836	3.4671	0.98	0.0184	0.0215	0.08	0.0181	0.0208
17	354.07	0.9776	0.9398	0.9801	5.0842	0.15	0.0194	0.0254	0.18	0.0194	0.0253
18	354.22	0.9953	0.9654	0.9843	13.8383	0.36	0.0152	0.0269	0.37	0.0152	0.0269
					Acetonitrile (1) + DMSO (3)						
1	439.01	0.0295	0.5056	2.0828	1.0112	0.21	0.0003	0.0190	0.24	0.0005	0.0055
2	421.43	0.0603	0.7008	2.0400	1.0778	0.47	0.0098	0.0370	0.70	0.0043	0.0213
3	409.64	0.0911	0.8156	2.0481	1.0111	0.18	0.0031	0.0170	0.51	0.0111	0.0016
4	400.63	0.1215	0.8662	2.0186	1.0379	0.37	0.0053	0.0188	0.71	0.0138	0.0043
5	389.11	0.1801	0.9198	1.9277	1.0186	0.01	0.0004	0.0136	0.20	0.005	0.0005
6	384.56	0.2123	0.9398	1.8810	0.9484	0.22	0.0009	0.0081	0.10	0.0018	0.0044
7	379.48	0.2556	0.9531	1.8148	0.9564	0.26	0.0029	0.0082	0.28	0.004	0.0035
8	376.98	0.2803	0.959	1.7827	0.9570	0.18	0.0010	0.0079	0.28	0.0042	0.0033
9	372.81	0.3314	0.9675	1.7080	0.9704	0.17	0.0014	0.0077	0.40	0.0084	0.0028
10	370.01	0.3727	0.9722	1.6520	0.9960	0.08	0.0004	0.0079	0.39	0.0087	0.0021
11	367.35	0.4237	0.9766	1.5758	1.0231	0.17	0.0024	0.0077	0.52	0.0129	0.0019
12	363.87	0.5032	0.9816	1.4765	1.0870	0.02	0.0027	0.0075	0.28	0.0066	0.0015
13	362.92	0.5319	0.9829	1.4387	1.1183	0.01	0.0023	0.0075	0.25	0.0055	0.0014
14	361.58	0.5800	0.9848	1.3758	1.1764	0.03	0.0008	0.0073	0.18	0.0038	0.0014
15	360.32	0.6331	0.9865	1.3113	1.2660	0.04	0.0004	0.0072	0.04	0.0006	0.0014
16	358.99	0.7000	0.9883	1.2369	1.4256	0.00	0.0017	0.0070	0.22	0.0084	0.0014
17	358.62	0.7222	0.9888	1.2131	1.4989	0.01	0.0018	0.0069	0.30	0.0106	0.0014
18	357.61	0.7918	0.9903	1.1429	1.8144	0.04	0.0024	0.0067	0.49	0.0163	0.0014
19	357.11	0.8309	0.9911	1.1068	2.0975	0.06	0.0029	0.0065	0.54	0.0179	0.0013
20	356.45	0.8876	0.9925	1.0588	2.7418	0.05	0.0027	0.0059	0.47	0.0158	0.0010
21	356.01	0.9204	0.9935	1.0361	3.4248	0.09	0.0036	0.0053	0.40	0.0133	0.0006
22	355.29	0.9700	0.9962	1.0081	5.4941	0.05	0.0021	0.0033	0.15	0.0047	0.0002
					1-Propanol (2) + DMSO (3)						
1	458.68	0.0198	0.1267	0.5079	1.0271	0.26	0.0166	0.0178	0.61	0.0075	0.0236
2	449.78	0.0611	0.3394	0.5367	1.0305	0.68	0.0393	0.0079	0.05	0.0205	0.0220
3	439.47	0.1136	0.5456	0.5905	1.0041	1.14	0.0373	0.0117	0.37	0.0176	0.0076
4	433.86	0.1448	0.6373	0.6209	0.9794	1.16	0.0301	0.0207	0.48	0.0133	0.0001
5	425.94	0.1927	0.7435	0.6666	0.9335	0.92	0.0152	0.0295	0.49	0.0053	0.0087
6	422.43	0.2157	0.7864	0.6914	0.8931	0.75	0.0039	0.0356	0.44	0.0024	0.0152
7	416.98	0.2519	0.8329	0.7277	0.8724	0.15	0.0117	0.0326	0.04	0.0124	0.0133
8	410.51	0.3013	0.8782	0.7708	0.8436	0.39	0.0257	0.0284	0.27	0.0195	0.0110
9	402.97	0.3709	0.9196	0.8207	0.8017	0.26	0.0335	0.0230	0.36	0.0199	0.0083
10	398.33	0.4200	0.9378	0.8414	0.7936	0.53	0.0243	0.0177	0.06	0.0073	0.0051
11	394.01	0.4715	0.9532	0.8756	0.7673	0.74	0.0299	0.0145	0.21	0.0111	0.0038
12	388.94	0.5439	0.9685	0.9126	0.7238	0.73	0.029	0.0111	0.21	0.0101	0.0028
13	385.99	0.5908	0.9752	0.9353	0.7114	0.78	0.0295	0.0086	0.29	0.0119	0.0018
14	383.79	0.6337	0.9803	0.9458	0.6878	0.55	0.0215	0.0072	0.11	0.0056	0.0015
15	381.45	0.6806	0.9849	0.9605	0.6632	0.46	0.0182	0.0057	0.09	0.0046	0.0011
16	378.89	0.7417	0.9895	0.9701	0.6319	0.18	0.0079	0.0042	0.09	0.0022	0.0008
17	377.59	0.7722	0.9913	0.9783	0.6258	0.19	0.0078	0.0033	0.04	0.0005	0.0005
18	376.05	0.8134	0.9935	0.9846	0.6079	0.10	0.0043	0.0025	0.06	0.0016	0.0004
19	374.65	0.8536	0.9953	0.9896	0.5936	0.04	0.0018	0.0018	0.07	0.0021	0.0003
20	373.35	0.8925	0.9968	0.9947	0.5810	0.03	0.0014	0.0012	0.03	0.0008	0.0001
21	372.28	0.9309	0.9980	0.9938	0.5908	0.09	0.0033	0.0006	0.12	0.0042	0.0000
22	371.51	0.9594	0.9988	0.9935	0.6233	0.14	0.0054	0.0002	0.16	0.0057	0.0001

[a] $\Delta T = |T^{\mathrm{exptl}} - T^{\mathrm{calcd}}|$. [b] $\Delta y_i = |y_i^{\mathrm{exptl}} - y_i^{\mathrm{calcd}}|$.

The calculated values from Wilson and NRTL models and the comparison between the experimental and the calculated values for the three binary systems are shown in Table 4 and Figures 2 to 4. It could be seen that in the acetonitrile + DMSO system the composition variations of the vapor and liquid phases with temperature were not obvious when the mole fraction of acetonitrile in the liquid phase was greater than 0.4 as shown in Figure 3, and a similar trend was found when the mole

Table 5. Results of the Thermodynamic Consistency Test

system	A_0[a]	A_1[a]	A_2[a]	A_3[a]	A_4[a]	δy_1[b]	δP[c]/kPa
acetonitrile (1) + 1-propanol (2)	1.1109	0.0035	0.0004	0.0221	0.0111	0.0056	1.17
acetonitrile (1) + DMSO (3)	1.2218	0.6413	0.2836	0.1399	0.0519	0.0075	0.81
1-propanol (2) + DMSO (3)	−0.5740	0.1429	0.0307	0.0189	0.0329	0.0046	0.91

[a] The parameters of the Legendre polynomial. [b] Average absolute deviation in vapor-phase composition. [c] Average absolute deviation in pressure.

Table 6. Experimental VLE Data and Correlated Results of the Ternary System at 101.3 kPa

acetonitrile (1) + 1-propanol (2) + DMSO (3)						calculated by Wilson				calculated by NRTL			
no.	T/K	x_1	x_2	y_1	y_2	ΔT[a]	Δy_1[b]	Δy_2[b]	Δy_3[b]	ΔT[a]	Δy_1[b]	Δy_2[b]	Δy_3[b]
1	355.26	0.8148	0.1003	0.9108	0.0817	0.15	0.0050	0.0082	0.0032	0.22	0.0022	0.0031	0.0009
2	356.72	0.5042	0.3924	0.7186	0.2764	0.76	0.0006	0.0033	0.0027	0.49	0.0029	0.0067	0.0038
3	358.84	0.2827	0.6513	0.5605	0.4381	0.80	0.0034	0.0039	0.0005	0.43	0.0117	0.0132	0.0015
4	360.97	0.3160	0.5063	0.6342	0.3636	1.15	0.0011	0.0027	0.0016	0.31	0.0135	0.0156	0.0021
5	366.40	0.2348	0.4565	0.6133	0.3845	0.90	0.0086	0.0155	0.0069	0.77	0.0143	0.0163	0.0020
6	367.92	0.1069	0.7230	0.3554	0.6433	1.14	0.0026	0.0053	0.0027	0.33	0.0220	0.0233	0.0013
7	373.45	0.1285	0.5214	0.4391	0.5423	1.40	0.0304	0.0249	0.0055	0.40	0.0049	0.0235	0.0186
8	379.68	0.2301	0.1526	0.8460	0.1192	2.87	0.0160	0.0146	0.0014	0.72	0.0098	0.0100	0.0002
9	382.32	0.0441	0.5427	0.2027	0.7756	0.56	0.0294	0.0315	0.0021	0.76	0.0010	0.0206	0.0216
10	385.15	0.1021	0.3715	0.4667	0.5205	2.97	0.0268	0.0481	0.0213	0.17	0.0006	0.0122	0.0128
11	388.31	0.1298	0.2631	0.6234	0.3530	4.33	0.0060	0.0273	0.0213	0.11	0.0071	0.0160	0.0231
12	390.87	0.0907	0.3204	0.4735	0.5021	3.97	0.0230	0.0458	0.0228	0.14	0.0062	0.0182	0.0244
13	399.68	0.1219	0.0683	0.8121	0.0767	2.92	0.0161	0.0239	0.0078	1.49	0.0215	0.0142	0.0073
14	404.78	0.1023	0.0345	0.7970	0.0402	0.94	0.0005	0.0201	0.0206	1.57	0.0325	0.0097	0.0228
15	408.10	0.0923	0.0592	0.7648	0.0873	3.27	0.0199	0.0235	0.0036	1.54	0.0195	0.0151	0.0044

[a] $\Delta T = |T^{\text{exptl}} - T^{\text{calcd}}|$. [b] $\Delta y_i = |y_i^{\text{exptl}} - y_i^{\text{calcd}}|$.

Table 7. Parameters and Correlation Deviations of Wilson and NRTL Models

systems	$(\lambda_{12} - \lambda_{11})/R$[a] K	$(\lambda_{21} - \lambda_{22})/R$[a] K	α	AADy_1[b]	AADy_2[b]	AADy_3[b]	AADT[c] K
			Acetonitrile (1) + 1-Propanol (2)				
Wilson	357.56	117.84	-	0.0077	0.0163	-	0.38
NRTL	230.43	203.32	0.3	0.0067	0.0159	-	0.30
			Acetonitrile (1) + DMSO (3)				
Wilson	94.87	696.16	-	0.0023	0.0102	-	0.12
NRTL	827.84	−140.11	0.3	0.0081	0.0029	-	0.35
			1-Propanol (2) + DMSO (3)				
Wilson	−75.60	−153.11	-	0.0181	0.0130	-	0.47
NRTL	−490.59	374.33	0.3	0.0085	0.0058	-	0.21
			Acetonitrile (1) + 1-Propanol (2) + DMSO (3)				
Wilson	-	-	-	0.0126	0.0199	0.0083	1.88
NRTL	-	-	0.3	0.0113	0.0145	0.0098	0.63

[a] $(\lambda_{12} - \lambda_{11})/R$ and $(\lambda_{21} - \lambda_{22})/R$ are the parameters adjusted by using experimental VLE data. [b] $\text{AAD}y = (1/N)\sum_{i=1}^{N}|y^{\text{exptl}} - y^{\text{calcd}}|$. [c] $\text{AADT} = (1/N)\sum_{i=1}^{N}|T^{\text{exptl}} - T^{\text{calcd}}|$; N = number of data points.

$$\text{OF} = \sum_k \sum_i (y_i^{\text{exptl}} - y_i^{\text{calcd}})_k^2 \qquad (2)$$

fraction of 1-propanol in the liquid phase was greater than 0.6 in Figure 4. The average absolute deviations (AAD) in temperature and vapor mole fraction are listed in Table 7. It could be found from the above tables and figures that values correlated by the Wilson and NRTL models agree well with the experimental ones.

Predication of Ternary Vapor−Liquid Equilibria. In this study, the Wilson and NRTL models were used to predict the VLE data of the ternary system. The VLE data and the deviations in temperatures and vapor mole fraction are listed in Tables 6 and 7. The azeotrope and tie-lines of the ternary system are shown in Figure 5. These results suggest that the Wilson and NRTL models could give a good representation of the experimental data, and the NRTL model could be comparatively better in this work.

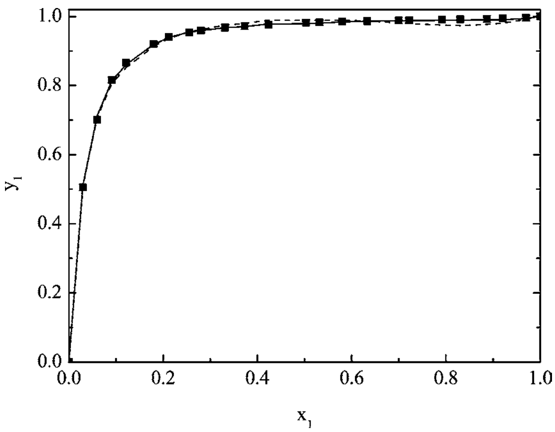

Figure 3. Equilibrium diagram for the system acetonitrile (1) + DMSO (3) at 101.3 kPa: ■, experimental data; —, calculation based on the Wilson model; - -, calculation based on the NRTL model.

Conclusions

The VLE data of the ternary system acetonitrile + 1-propanol + DMSO and the corresponding binary systems, acetonitrile + 1-propanol, acetonitrile + DMSO, and 1-propanol + DMSO, were measured, respectively, at 101.3 kPa by using an improved Rose equilibrium still. The thermodynamic consistency test was

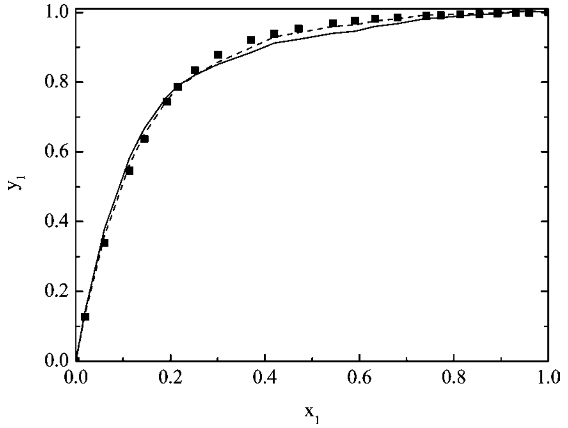

Figure 4. Equilibrium diagram for the system 1-propanol (2) + DMSO (3) at 101.3 kPa: ■, experimental data; —, calculation based on the Wilson model; - -, calculation based on the NRTL model.

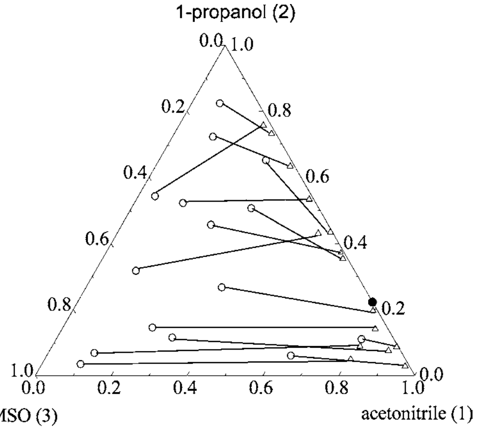

Figure 5. Tie-lines for the ternary system acetonitrile (1) + 1-propanol (2) + DMSO (3) at 101.3 kPa: ○, liquid-phase mole fraction; Δ, vapor-phase mole fraction; ●, azeotrope.

passed using the point-to-point method. The parameters of Wilson and NRTL models were obtained from the binary systems. Then, the VLE data of the ternary system were predicted with Wilson and NRTL models and agreed well with the experimental data. The Wilson and NRTL models could be adopted to correlate VLE of the present binary systems, and the NRTL model yielded more reasonable predictions for the ternary system.

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