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Isothermal Vapor−Liquid Equilibria for Water + 2-Aminoethanol + Dimethyl Sulfoxide and Its Constituent Three Binary Systems

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Isothermal vapor−liquid equilibria were measured for the ternary system water + 2-aminoethanol + dimethyl sulfoxide and its three constituent binary mixtures at 363.15 K. The apparatus used was a modified Rogalski−Malanoski equilibrium still. The experimental binary data were correlated by the NRTL equation. The ternary system was predicted using the binary NRTL parameters with good accuracy.

Introduction

The mixture of 2-aminoethanol and dimethyl sulfoxide has been used as alternatives of chlorofluorocarbons (CFCs) which had been utilized extensively for the cleaning of electronic components. The vapor−liquid equilibrium data for the mixtures containing 2-aminoethanol, dimethyl sulfoxide, and water are necessary for designing the distillation process as the treatment process of waste fluid.

This paper presents the vapor−liquid equilibria (VLE) for the ternary system of water + 2-aminoethanol + dimethyl sulfoxide and its constituent three binary mixtures at 363.15 K. For water + 2-aminoethanol, two isothermal VLE (343.15, 363.15 K) sets of data are available in the literature (Lenard et al., 1987), and for water + dimethyl sulfoxide, there are three sets of isobaric VLE (20.2, 46.6, and 73.8 kPa) data (Nishimura et al., 1972).

Experimental Section

Apparatus and Procedure. A modified Rogalski−Malanoski equilibrium still, with pressure control and analysis similar to those described in the literature (Hiaki et al., 1992; Kurihara et al., 1995), was used. The apparatus consisted of an equilibrium still, a Hewlett−Packard Model 3421A acquisition data/control unit, an NEC personal computer, six solenoid valves, three pressure transducers, three surge tanks, cold traps, a refrigerator, and a vacuum pump. An attractive feature of this apparatus is that the temperature of the system can be kept controlled very precisely using a computer in conjunction with the six solenoid valves and three pressure transducers.

The equilibrium temperature was measured with a calibrated platinum resistance thermometer with an accuracy of ±0.01 K. The pressure in the still was determined with a Druck multifunction pressure indicator DPI 145. The accuracy was estimated to be ±0.03 kPa.

Analysis. Vapor and liquid samples were analyzed with a Shimazu gas chromatograph type GC-8AIT equipped with a thermal conductivity detector. TENAX TA was used as the column packing and helium as carrier gas. The compositions were determined by the relative area method with an accuracy of ±0.7 mol %.

Table 1. Experimental Vapor Pressures for 2-Aminoethanol and Dimethyl Sulfoxide

T/K	P/kPa	T/K	P/kPa	T/K	P/kPa
		2-Aminoethanol			
439.69	90.71	414.51	37.94	376.74	7.85
434.89	77.50	409.40	31.32	372.84	6.53
432.22	70.91	403.58	25.00	369.07	5.45
429.33	64.31	396.15	18.38	363.98	4.23
426.17	57.71	385.73	11.78	363.15	4.02
422.70	51.12	383.06	10.46	357.63	3.07
418.92	44.55	380.12	9.17		
		Dimethyl Sulfoxide			
462.52	97.09	439.41	51.59	393.51	11.50
459.81	90.50	434.67	45.11	386.51	8.81
456.92	83.91	429.55	38.42	377.58	6.17
453.87	77.32	423.39	31.78	365.19	3.65
450.60	70.72	416.11	25.15	363.15	3.28
447.03	64.13	415.54	24.80	356.23	2.44
443.15	57.52	406.26	18.16		

Table 2. Antoine Equation Constants[a]

substance	A	B	C	ΔP^b/kPa
2-aminoethanol	7.380 81	2081.50	−55.79	0.19
dimethyl sulfoxide	6.666 76	1952.13	−45.35	0.13

[a] $\log P/\text{kPa} = A - B/((T/\text{K}) + C)$. [b] $\Delta P = \sum_k |(P_{\text{expt}} - P_{\text{calc}})/P_{\text{expt}}|_k / N \times 100$; N, number of data points.

Materials. 2-Aminoethanol and dimethyl sulfoxide were special grade pure reagents (Wako Pure Chemical Industry, Ltd.) and were used after removing traces of water with 3 Å molecular sieves. The water was passed through an ion exchanger and distilled. The purity of materials was checked by gas chromatography and found to be better than 99.6 mass % for 2-aminoethanol and 99.9 mass % for dimethyl sulfoxide.

Tables 1 and 2 show experimental vapor pressures and Antoine equation constants of 2-aminoethanol and dimethyl sulfoxide, respectively. The average deviations between the experimental and calculated values using the literature Antoine constants (Riddick and Bunger, 1970; Boublik et al., 1973) are 1.58% and 0.98% for 2-aminoethanol and dimethyl sulfoxide, respectively.

Experimental Results

Binary Systems. The experimental VLE data at 363.15 K for water + 2-aminoethanol, 2-aminoethanol + dimethyl

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Table 3. Experimental Vapor−Liquid Equilibria and Activity Coefficients γ_i for Water (1) + 2-Aminoethanol (2) at 363.15 K

P/kPa	x_1	y_1	γ_1	γ_2
4.02	0.000	0.000	−	1.000
8.03	0.112	0.560	0.575	0.990
14.05	0.240	0.796	0.666	0.938
18.59	0.326	0.869	0.707	0.898
26.82	0.466	0.931	0.765	0.864
32.02	0.529	0.952	0.822	0.806
40.90	0.645	0.975	0.883	0.705
54.13	0.795	0.991	0.964	0.564
57.90	0.841	0.994	0.977	0.518
68.15	0.974	0.999	0.998	0.387
70.07	1.000	1.000	1.000	−

Table 4. Experimental Vapor−Liquid Equilibria and Activity Coefficients γ_i for the 2-Aminoethanol (2) + Dimethyl Sulfoxide (3) System at 363.15 K

P/kPa	x_2	y_2	γ_2	γ_3
3.28	0.000	0.000	−	1.000
3.37	0.091	0.110	1.019	0.987
3.40	0.111	0.137	1.038	0.986
3.48	0.202	0.239	1.022	0.993
3.52	0.249	0.293	1.032	0.991
3.57	0.302	0.348	1.024	0.998
3.62	0.360	0.410	1.024	0.997
3.67	0.411	0.471	1.045	0.986
3.72	0.491	0.539	1.015	1.006
3.75	0.554	0.602	1.014	0.998
3.79	0.612	0.651	1.001	1.020
3.82	0.689	0.724	0.998	1.016
3.85	0.713	0.745	1.003	1.021
3.87	0.777	0.799	0.990	1.043
3.93	0.850	0.866	0.997	1.046
3.95	0.897	0.908	0.994	1.060
4.02	1.000	1.000	1.000	−

Table 5. Experimental Vapor−Liquid Equilibria and Activity Coefficients γ_i for the Water (1) + Dimethyl Sulfoxide (3) System at 363.15 K

P/kPa	x_1	y_1	γ_1	γ_3
3.28	0.000	0.000	−	1.000
6.06	0.123	0.538	0.377	0.975
8.51	0.202	0.702	0.421	0.971
11.23	0.266	0.799	0.482	0.939
13.09	0.310	0.840	0.505	0.929
15.58	0.364	0.882	0.539	0.884
19.63	0.439	0.923	0.589	0.824
23.79	0.497	0.944	0.645	0.807
27.86	0.550	0.962	0.696	0.710
33.89	0.634	0.978	0.746	0.611
39.24	0.676	0.987	0.818	0.487
43.49	0.732	0.992	0.842	0.375
51.18	0.799	0.996	0.910	0.311
54.98	0.837	0.997	0.935	0.288
59.35	0.871	0.998	0.970	0.239
62.03	0.898	0.999	0.985	0.203
65.99	0.945	0.9995	0.996	0.184
70.07	1.000	1.000	1.000	−

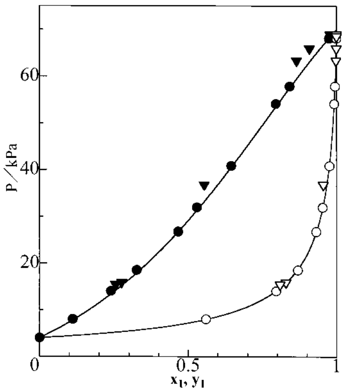

Figure 1. Pressure−composition diagram for the water (1) + 2-aminoethanol (2) system at 363.15 K: (●, ○) experiment; (▼, ▽) Lenard et al. (1987); (−) NRTL equation.

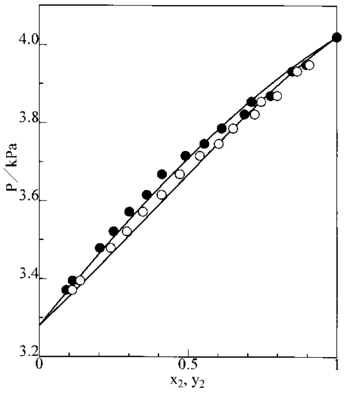

Figure 2. Pressure−composition diagram for the 2-aminoethanol (2) + dimethyl sulfoxide (3) system at 363.15 K: (●, ○) experiment; (−) NRTL equation.

Table 6. Experimental Vapor−Liquid Equilibria and Activity Coefficients γ_i for Water (1) + 2-Aminoethanol (2) + Dimethyl Sulfoxide (3) at 363.15 K

P/kPa	x_1	x_2	y_1	y_2	γ_1	γ_2	γ_3
4.70	0.029	0.886	0.2005	0.7381	0.475	1.002	1.043
4.21	0.031	0.280	0.1878	0.2667	0.340	1.043	0.999
5.01	0.039	0.755	0.2615	0.5977	0.443	1.009	1.020
5.20	0.050	0.620	0.3053	0.4803	0.416	1.019	1.004
6.57	0.089	0.473	0.5109	0.2823	0.408	1.037	0.983
7.48	0.100	0.763	0.5543	0.3875	0.493	1.007	0.985
7.06	0.125	0.158	0.5906	0.0971	0.371	1.078	0.979
9.74	0.197	0.278	0.7218	0.1176	0.438	1.069	0.940
13.28	0.307	0.076	0.8469	0.0227	0.471	1.106	0.901
24.38	0.446	0.495	0.9271	0.0672	0.725	0.900	0.651
34.95	0.590	0.356	0.9683	0.0288	0.820	0.803	0.493
41.81	0.688	0.179	0.9822	0.0126	0.851	0.775	0.427
43.91	0.696	0.256	0.9870	0.0118	0.886	0.713	0.382
46.75	0.720	0.211	0.9864	0.0117	0.892	0.706	0.368
48.46	0.743	0.200	0.9876	0.0108	0.909	0.675	0.340
49.58	0.762	0.127	0.9911	0.0064	0.902	0.694	0.345
50.04	0.773	0.121	0.9922	0.0056	0.909	0.682	0.334
50.28	0.780	0.118	0.9929	0.0053	0.914	0.673	0.326
50.50	0.785	0.043	0.9927	0.0026	0.896	0.717	0.352
51.67	0.789	0.082	0.9934	0.0040	0.910	0.683	0.330
54.93	0.819	0.130	0.9937	0.0054	0.948	0.598	0.270
54.78	0.820	0.045	0.9957	0.0020	0.925	0.659	0.305
55.60	0.828	0.082	0.9953	0.0033	0.941	0.617	0.278

sulfoxide, and water + dimethyl sulfoxide are shown in Tables 3−5 and Figures 1−3. The activity coefficients, γ_i, in Tables 3−5 were evaluated by the following equation:

$$\gamma_i = P y_i / P_i^{S} x_i \qquad (1)$$

where P_i^{S} is vapor pressure of pure component i. Here nonideality of the gas has been neglected, because the binary coefficients in Tsonopoulos's procedure (Tsonopoulos, 1974) have not been founded for 2-aminoethanol and dimethyl sulfoxide.

From Tables 3−5, the logarithm of activity coefficients of both components i of water-containing systems is negative. The experimental data are consistent from the area test of Redlich−Kister (1948), except the system 2-aminoethanol + dimethyl sulfoxide which is close to ideal. For the water + 2-aminoethanol system, one set of data is available in the literature (Lenard et al., 1987) at the temperature studied. Figure 4 shows the comparison of the

Table 7. NRTL Parameters and Deviations between Experimental and Calculated Values Using the NRTL Equation[a]

system	$[(g_{ji} - g_{ii})/R]$/K	$[(g_{ij} - g_{jj})/R]$/K	$\alpha_{ij} = \alpha_{ji}$	Δy_i	ΔP/%
water (1) + 2-aminoethanol (2)	−301.8	44.9	0.346	0.005	1.6
2-aminoethanol (2) + dimethyl sufoxide (3)	−145.7	193.2	0.300	0.004	0.4
water (1) + dimethyl sulfoxide (3)	−555.6	116.8	0.302	0.006	4.0

[a] $\gamma y_i = \sum_k |y_{i,\mathrm{expt}} - y_{i,\mathrm{calc}}|_k/N$; $\Delta P = \sum_k |(P_{\mathrm{expt}} - P_{\mathrm{calc}})/P_{\mathrm{expt}}|_k/N \times 100$; N, number of data points.

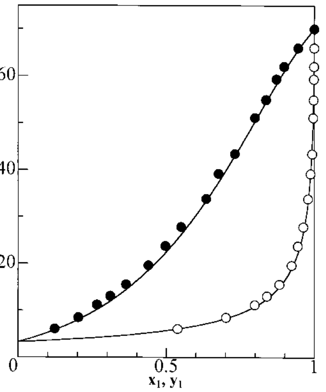

Figure 3. Pressure−composition diagram for the water (1) + dimethyl sulfoxide (3) system at 363.15 K: (●, ○) experiment; (—) NRTL equation.

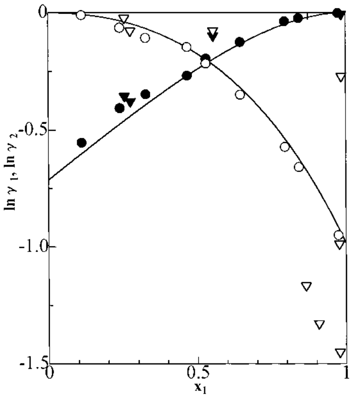

Figure 4. Activity coefficient−liquid composition diagram for the water (1) + 2-aminoethanol (2) system at 363.15 K: (●, ○) experiment; (▼, ▽) Lenard et al. (1987); (—) NRTL equation.

activity coefficients, though the literature data are inconsistent from the area test.

Ternary Systems. Table 6 and Figure 5 show the experimental VLE data for water + 2-aminoethanol + dimethyl sulfoxide at 363.15 K. The tails of solid arrows in Figure 5 represent experimental liquid compositions, and the heads of arrows show experimental vapor compositions on the same tie line.

Discussion

The activity coefficients of binary systems were correlated by the NRTL equation (Renon and Prausnitz, 1968) given by eq 2 for each system, where $(g_{ji} - g_{ii})$, $(g_{ij} - g_{jj})$, and α_{ij} are binary NRTL parameters.

$$\ln \gamma_i = \frac{\sum_j \tau_{ji} G_{ji} x_j}{\sum_l G_{li} x_l} + \sum_j \frac{x_j G_{ij}}{\sum_l G_{lj} x_l}\left(\tau_{ij} - \frac{\sum_n x_n \tau_{nj} G_{nj}}{\sum_l G_{lj} x_l}\right) \qquad (2)$$

$$\tau_{ji} = (g_{ji} - g_{ii})/RT \qquad (3)$$

$$G_{ji} = \exp(-\alpha_{ji}\tau_{ji}) \qquad (4)$$

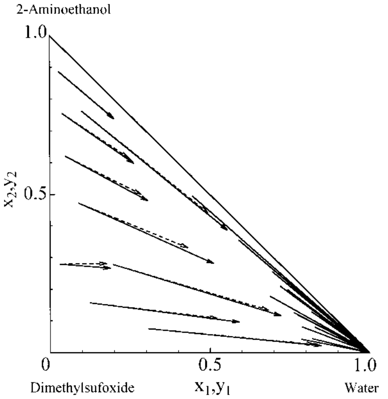

Figure 5. Vapor−liquid equilibria for the water (1) + 2-aminoethanol (2) + dimethyl sulfoxide (3) system at 363.15 K: (solid arrows) experiment; (dashed arrows) NRTL equation.

The correlation procedure for water-containing systems was based on the minimization of the following objective function:

$$F_{\mathrm{obj}} = \sum_N \sum_i \left| \frac{(\gamma_{i,expt} - \gamma_{i,calc})}{\gamma_{i,expt}} \right|_N \qquad (5)$$

where N is the number of data points. Table 7 lists estimated parameters of the binary systems and deviations between the calculated and experimental vapor-phase compositions and total pressures using the NRTL equation. Calculated results are shown by solid lines in Figures 1−4.

The VLE for the ternary water + 2-aminoethanol + dimethyl sulfoxide system was predicted using the binary NRTL parameters listed in Table 7 and the average deviations between the experimental and predicted vapor-phase composition and total pressure are 1.1 mol % and 2.94%, respectively.

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