Vapor−Liquid Equilibria Data for Methanol + 2-Propanol+ 2-Methyl-2-butanol and Constituent Binary Systems at 101.3 kPa

Gengxin Zhang,*,† Brandon L. Weeks,† and Jianhua Wei‡

Chemical Engineering Department, Texas Tech University, Lubbock, Texas 79409, and Shanghai Research Institute of Chemical Industry, Shanghai 200062, People's Republic of China

Isobaric vapor−liquid equilibria (VLE) were measured at atmospheric pressure for the ternary system methanol + 2-propanol + 2-methyl-2-butanol and its constituent binary system 2-propanol + 2-methyl-2-butanol. Parameters for the Wilson, NRTL, and UNIQUAC equations were determined from the binary VLE data, and the prediction for ternary VLE system was compared with experimental results. For both binary and ternary systems, the NRTL and UNIQUAC models gave good predictions.

Introduction

Methanol, 2-propanol, and 2-methyl-2-butanol mixtures are often produced in petroleum catalytic processes. Distillation is a simple and straightforward way to recover these products. In this work, the experimental vapor−liquid equilibria (VLE) data for the ternary system containing methanol, 2-propanol, and 2-methyl-2-butanol at 101.3 kPa is investigated. In order to qualify the experimental arrangement, the methanol + 2-propanol system was also investigated since there is suitable data available to compare.

Methanol and 2-propanol VLE have been previously reported at 1 bar.[1−12] However, the work presented used slightly different experimental apparatus, and the analysis methods were not consistent with that used in this work. Methanol + 2-methyl-2-butanol has also been reported at isobaric condition (94 kPa)[13] and isothermal condition (313.15 K).[14] The binary system 2-propanol and 2-methyl-2-butanol and the ternary system methanol, 2-propanol, and 2-methyl-2-butanol are new in this work. The quality of the measured data was verified by the Herington method.[15] The VLE data of the measured systems are also correlated by the NRTL, Wilson, and UNIQUAC equations.

Experimental Section

Materials. Methanol, 2-propanol, and 2-methyl-2-butanol were supplied by Shanghai Reagent Co. Ltd. The mass fraction purities of the chemicals were greater than 99.5 %. No further purification was needed as confirmed by a gas chromatograph (GC) equipped with a thermal conductivity detector (TCD), which failed to observe any significant impurities. The specifications and physical properties of the chemicals used in this study are shown in Table 1 and compared with the literature values of Yaws.[16] The refractive index of the chemicals used in this study was measured by a WAY-2S digital Abbe refractometer. Boiling point was measured by a Cottrell-type boiling point apparatus.

Table 1. Physical Property of Chemicals Used in This Study, Boiling Temperature T_b, and Reflection Index, n_D

chemicals and mass fraction purity	n_D(298.15 K) exp[a]	n_D(298.15 K) lit[b]	T_b(101.3 kPa)/K exp[a]	T_b(101.3 kPa)/K lit[b]
methanol (> 99.5 %)	1.3261	1.3265	337.68	337.696
2-propanol (> 99.5 %)	1.3750	1.3752	355.50	355.41
2-methyl-2-butanol (> 99.5 %)	1.4018	1.4024	375.01	375.15

[a] Measured. [b] Ref 2.

***Apparatus and Procedure*.** The VLE measurements were carried out with a modified William−Rose still[17] shown in Figure 1A. The heated fluid (containing liquid and vapor) rises along the vapor riser in the droplet separators, and the liquid recycles back to the reservoir. The vapor phase is collected in vapor-phase cell and attains the VLE. The vapor phase then goes through the bridge and rises along the water condenser forming a liquid that is collected. Excess liquid recycles to the sample reservoir. The thermometer was enclosed in the liquid chamber of the still and filled with a high-boiling mineral oil to maintain a stable temperature. The pressure was maintained at 101.3 kPa by an outside, constant-pressure, air source applied to the system. The feedback system is shown in Figure 1B. Air pressure at the top part of the tank was maintained at 101.3 kPa by adjusting the magnetic valve. If the pressure in the tank was higher than 101.3 kPa, the plug in the salt U-type tube will touch the liquid surface, the magnetic valve will open, and the pressure in the tank will decrease. The air was passed through a filter and a calcium chloride drying bottle before entering the system.

All the equilibria compositions were determined by GC model SP2000 supplied by Shandong Jingpu Instruments Co. Ltd, which was equipped with TCD. The GC column was a 4 m long and 3.025 mm in diameter stainless steel tube packed with GDX-403.[18] The column injector and detector temperature were 463.15 and 483.15 K, respectively. Very good separation was achieved under these conditions. The area of the concentration measured as a function of time is calculated automatically using standard routines supplied with the equipment. The precision of concentration measurements was better than ± 0.001 mole fraction. In this work, a TJ-800 (Mercury) U-type pressure gauge was used; the precision of pressure measurement was within ± 0.133 kPa with an estimated uncertainty of ± 0.065 kPa. A WLB-21 standard thermometer (provided by Nanjing Detair Appearance Machine Electricity Equipments Co. Ltd) was used

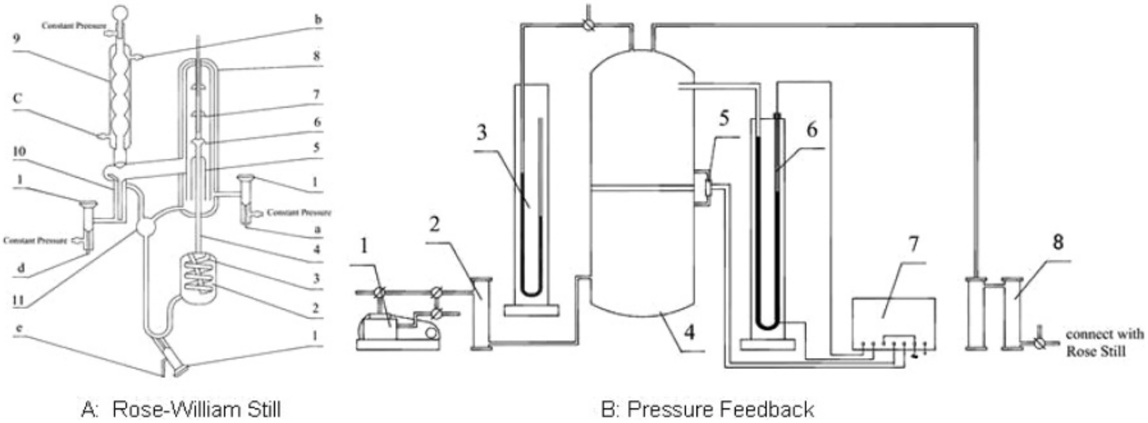
---

* Corresponding author. E-mail: Gengxin.zhang@ttu.edu.

† Texas Tech University.

‡ Shanghai Research Institute of Chemical Industry.

10.1021/je060476j CCC: $37.00



A: Rose-William Still

B: Pressure Feedback

Figure 1. (A) Modified Rose−William still: a, connect with liquid-phase sample collector; b and c, cooling water inlet/outlet; d, connect with vapor-phase sample collector; e, excess liquid outlet; 1, PTFE cork; 2, liquid-phase sample; 3, heater; 4, riser; 5, vapor-phase cell; 6, droplet separator; 7, thermometer well; 8, vacuum heat preservation jacket; 9, vapor-phase condenser; 10, vapor-phase collector; 11, mixing cell. (B) Feedback pressure control system: 1, vacuum pump; 2, $CaCl_2$ desiccant; 3, Hg pressure gauge; 4, constant pressure tank (0.75 m^3); 5, magnetic valve; 6, NaCl solution U tube; 7, electromagnetic delay; 8, $CaCl_2$ desiccant.

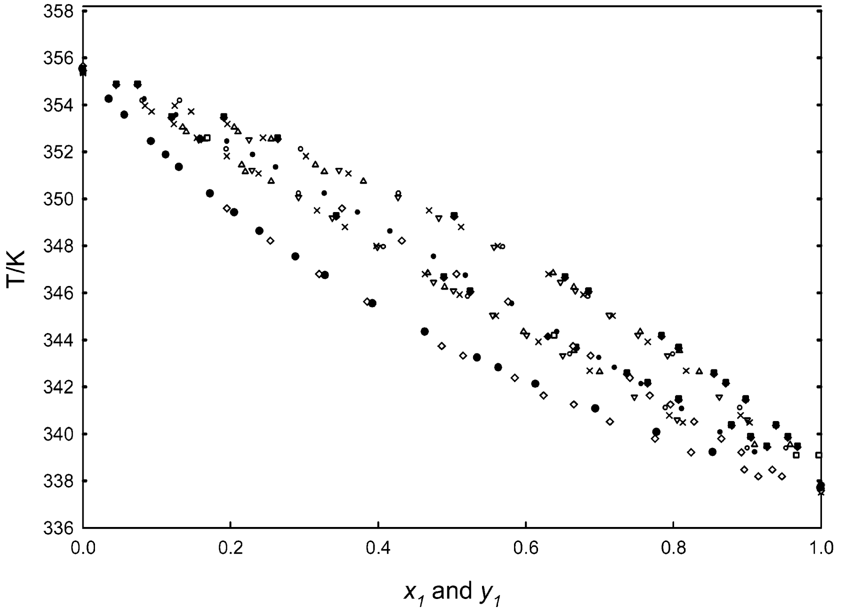


Figure 2. $T-x_1-y_1$ diagram for methanol (1) + 2-propanol (2) at 101.3 kPa. To compare this work to previous studies[1−5,8,9] gives confidence in our experimental apparatus and analysis: ○, ref 1; △, ref 2; □, ref 3; ▽, ref 4; ♦, ref 5; ◇, ref 8; ×, ref 9; ●, this work.

to measure the temperature, which was calibrated using ice and steam points, the accuracy of measurement was within ± 0.05 K.

Results and Discussion

The experimental arrangement was first benchmarked by investigating the methanol + 2-propanol binary system. The results are shown in Figure 2. Although there is a large amount of data available on the methanol + 2-propanol VLE, there is some inconsistency with the measured values. Differences in the literature are likely due to slightly different experimental arrangements and accuracy in measurements. In any event, our results match extremely well with those presented by Gultekin, who had a very similar experimental arrangement, giving us confidence is our experiment.[8] Details of the analysis are described as follows.

The VLE was measured at 101.3 kPa for the methanol + 2-propanol, methanol + 2-methyl-2-butanol, and 2-propanol + 2-methyl-2-butanol binary systems and the methanol + 2-propanol + 2-methyl-2-butanol ternary system at 101.3 kPa. The experimental data are shown in Tables 3 and 4 with the precision ± 0.001. The activity of pure liquid *i* in nonideal mixture at temperature *T* and pressure *P* was calculated according to

Table 2. Coefficients of the Antoine Equation, Minimum Temperature T_{min}, and Maximum Temperature T_{max}

compound	A_i	B_i	C_i	T_{min}/K	T_{max}/K
methanol	7.02052	1582.99	−33.439	175.47	512.58
2-propanol	18.6929	3640.20	−53.54	273.15	345.15
2-methyl-2-butanol	15.0113	1988.08	−137.80	264.35	545.15

$$y_i \Phi_i P = \gamma_i x_i P_i^{sat} \tag{1}$$

where y_i is the vapor-phase mole fraction of species *i*, x_i is the liquid-phase mole fraction of species *i*, γ_i is the activity coefficient of species *i*, the vapor correction term Φ_i was calculated from the truncated (two terms) virial equation of state. The second virial coefficients (data not shown) were calculated by means of the chemical theory with the correlation of Hayden and O'Connell[19] as reported by Resa et al.[20] *P* is the total

Table 3. Vapor−Liquid Equilibria Data for the Methanol (1) + 2-Propanol (2), Methanol (1) + 2-Methyl-2-butanol (2), and 2-Propanol (1) + 2-Methyl-2-butanol (2) Systems[a]

T/K	x_1	y_1	γ_1	γ_2	T/K	x_1	y_1	γ_1	γ_2	T/K	x_1	y_1	γ_1	γ_2
					Methanol (1) + 2-Propanol (2)									
337.68	1.000	1.000	1.000	1.202	344.32	0.464	0.643	1.075	1.037	351.32	0.131	0.262	1.197	1.003
339.20	0.854	0.911	1.006	1.163	345.52	0.393	0.582	1.096	1.026	351.85	0.113	0.231	1.205	1.002
340.05	0.778	0.864	1.013	1.126	346.72	0.329	0.519	1.117	1.019	352.42	0.093	0.196	1.214	1.001
341.05	0.695	0.812	1.025	1.096	347.52	0.289	0.476	1.132	1.013	353.54	0.057	0.127	1.232	1.000
342.10	0.614	0.757	1.039	1.080	348.60	0.240	0.417	1.150	1.010	354.22	0.036	0.084	1.242	1.000
342.80	0.564	0.721	1.050	1.071	349.40	0.206	0.373	1.164	1.007	355.50	0.000	0.000	1.000	1.202
343.22	0.535	0.700	1.0570	1.052	350.20	0.173	0.328	1.178	1.004					
					Methanol (1) + 2-Methyl-2-butanol (2)									
337.68	1.000	1.000	1.001	1.000	352.25	0.450	0.778	1.003	1.000	366.05	0.140	0.389	1.000	1.000
340.10	0.886	0.973	1.000	1.001	354.2	0.397	0.735	1.000	1.000	367.5	0.115	0.335	1.000	1.000
340.52	0.867	0.968	1.000	1.001	355.42	0.366	0.706	1.000	1.000	368.45	0.100	0.298	1.000	1.000
341.84	0.810	0.952	1.000	1.000	356.85	0.330	0.671	1.000	1.000	370.05	0.074	0.232	1.000	0.999
343.02	0.762	0.936	1.000	1.000	358.05	0.302	0.640	1.000	1.000	371.32	0.054	0.178	1.001	1.000
344.52	0.703	0.915	1.000	1.000	360.52	0.248	0.570	1.000	1.000	372.5	0.037	0.126	0.999	1.000
346.05	0.647	0.895	1.000	1.000	362.44	0.208	0.512	1.000	1.000	373.42	0.024	0.083	1.001	1.000
347.25	0.606	0.872	1.000	1.000	363.54	0.187	0.476	1.000	1.000	375.14	0.000	0.000	1.001	1.000
350.25	0.507	0.817	1.000	1.003	364.85	0.162	0.431	1.000	1.000					
					2-Propanol (1)+ 2-Methyl-2-butanol (2)									
355.50	1.000	1.000	1.009	0.000	363.75	0.484	0.665	0.993	0.999	370.02	0.192	0.331	0.980	1.004
356.22	0.947	0.975	1.008	0.992	364.42	0.448	0.631	0.993	1.000	371.15	0.146	0.263	0.978	1.005
357.45	0.862	0.930	1.005	0.993	365.10	0.415	0.599	0.991	1.000	372.05	0.111	0.206	0.976	1.006
358.60	0.785	0.887	1.003	0.994	366.45	0.350	0.530	0.988	1.001	372.75	0.085	0.162	0.975	1.006
360.10	0.691	0.826	1.000	0.995	367.60	0.296	0.469	0.986	1.002	373.12	0.071	0.137	0.974	1.007
361.25	0.623	0.778	0.998	0.996	368.32	0.264	0.429	0.984	1.003	374.00	0.041	0.082	0.970	1.006
362.42	0.556	0.726	0.996	0.997	368.85	0.241	0.399	0.983	1.003	375.14	0.000	0.000	0.000	1.008

[a] Liquid-phase mole fraction x_1, Vapor-phase mole fraction y_1, equilibria temperature T, and activity coefficients γ_1 and γ_2 at 101.3 kPa.

Table 4. Experimental Vapor−Liquid Equilibria Data for Methanol (1) + 2-propanol (2) + 2-Methyl-2-butanol (3) Ternary Components Systems at 101.3 kPa[a]

T/K	x_1	x_2	y_1	y_2	γ_1	γ_2	γ_3
			Methanol (1) + 2-Propanol (2) + 2-Methyl-2-butanol (3)				
345.15	0.495	0.391	0.693	0.275	1.051	1.075	0.954
346.76	0.453	0.360	0.673	0.270	1.051	1.072	0.959
348.45	0.407	0.341	0.643	0.273	1.051	1.066	0.966
349.24	0.389	0.326	0.633	0.269	1.050	1.064	0.969
350.46	0.358	0.318	0.608	0.273	1.051	1.060	0.973
352.45	0.307	0.304	0.562	0.283	1.052	1.052	0.978
354.15	0.266	0.301	0.516	0.298	1.053	1.042	0.979
355.32	0.238	0.298	0.483	0.307	1.055	1.040	0.983
359.10	0.160	0.279	0.371	0.329	1.056	1.027	0.990
361.00	0.125	0.271	0.309	0.342	1.056	1.021	0.992
362.51	0.104	0.251	0.269	0.335	1.053	1.018	0.994

[a] Liquid-phase mole fraction x_1 and x_2, vapor-phase mole fraction y_1 and y_2, equilibria temperature T, and activity coefficients γ_1, γ_2, and γ_3.

Table 5. Binary Components Thermodynamic Consistent Result Summary and Area Parameters *D* and *J*

binary mixtures	D	J	$\lvert D-J \rvert$
methanol + 2-propanol	1.049	6.640	5.231
methanol + 2-methyl-2-butanol	19.639	14.978	4.661
2-propanol + 2-methyl-2-butanol	4.654	7.850	3.196

Table 6. Correlation Parameters and Absolute Mean Deviations in Equilibria Temperatures and Vapor-Phase Mole Fractions for the Binary Systems at 101.3 kPa

	A_{12}[a]	A_{21}[a]		ΔT	
	J·mol^{-1}	J·mol^{-1}	α	K	Δy_1
	Methanol (1) + 2-Propanol (2) at 101.3 kPa				
Wilson	−190.847	−539.716		0.122	0.00541
NRTL	641.033	82.958	0.30	0. 105	0.0086
UNIQUAC	617.842	−1450.50		0. 118	0.00526
	Methanol (1) + 2-Methyl-2-butanol (2) at 101.3 kPa				
Wilson	−3.870	4.3854		0.167	0.00277
NRTL	−11.883	11.372	0.30	0.084	0.0001
UNIQUAC	581.770	−1393.74		0.128	0.0003
	2-Propanol (1) + 2-Methyl-2-butanol (2) at 101.3 kPa				
Wilson	−13.532	14.664		0.244	0.0022
NRTL	773.301	−719.38	0.30	0.237	0.0014
UNIQUAC	319.414	−418.483		0.236	0.008

[a] The binary adjustable parameters for various models are as follows: Wilson, $A_{ij} = (\lambda_{ij} - \lambda_{jj})$; NRTL, $A_{ij} = (g_{ij} - g_{jj})$; UNIQUAC, $A_{ij} = (u_{ij} - u_{jj})$.

pressure in kPa, and P_i^{sat} is the saturated vapor pressure of component i. The saturated vapor pressures were calculated from the Antoine equation (eq 2); the constants A_i, B_i, and C_i listed in Table 2 were obtained from Reid et al.[21] (temperature in K):

$$\log(P_i^{\text{sat}}) = A_i - B_i/(T + C_i) \tag{2}$$

The thermodynamic consistency was checked according to the Herington method. This method involves determining essentially two parameters (D and J) using the area obtained from plots of the logarithm of the activity coefficient ratio against the mole fraction of one of the components. If the quantity ($D - J$) is less than 10, the data pass the thermodynamic consistency test. The experimental data in Table 3 were checked by this method, and the results are reported in Table 5 showing that the experimental data are fit to this criterion appropriately.

The activity coefficients were correlated with the Wilson,[22] NRTL,[23] and UNIQUAC[24] equations. Estimation of the parameters for the equations were based on the iterative solution, using maximum likelihood[25] regression of the objective function (OF), with the active coefficients obtained from the calculations (γ_{cal}) with the equations and the experimental values (γ_{exp}):

$$\text{OF} = \sum\left(\frac{\gamma_{\text{exp}} - \gamma_{\text{cal}}}{\gamma_{\text{exp}}}\right)^2 \tag{3}$$

In eq 3, γ_{exp} are the activity coefficients calculated from experimental data and γ_{cal} are the coefficients calculated

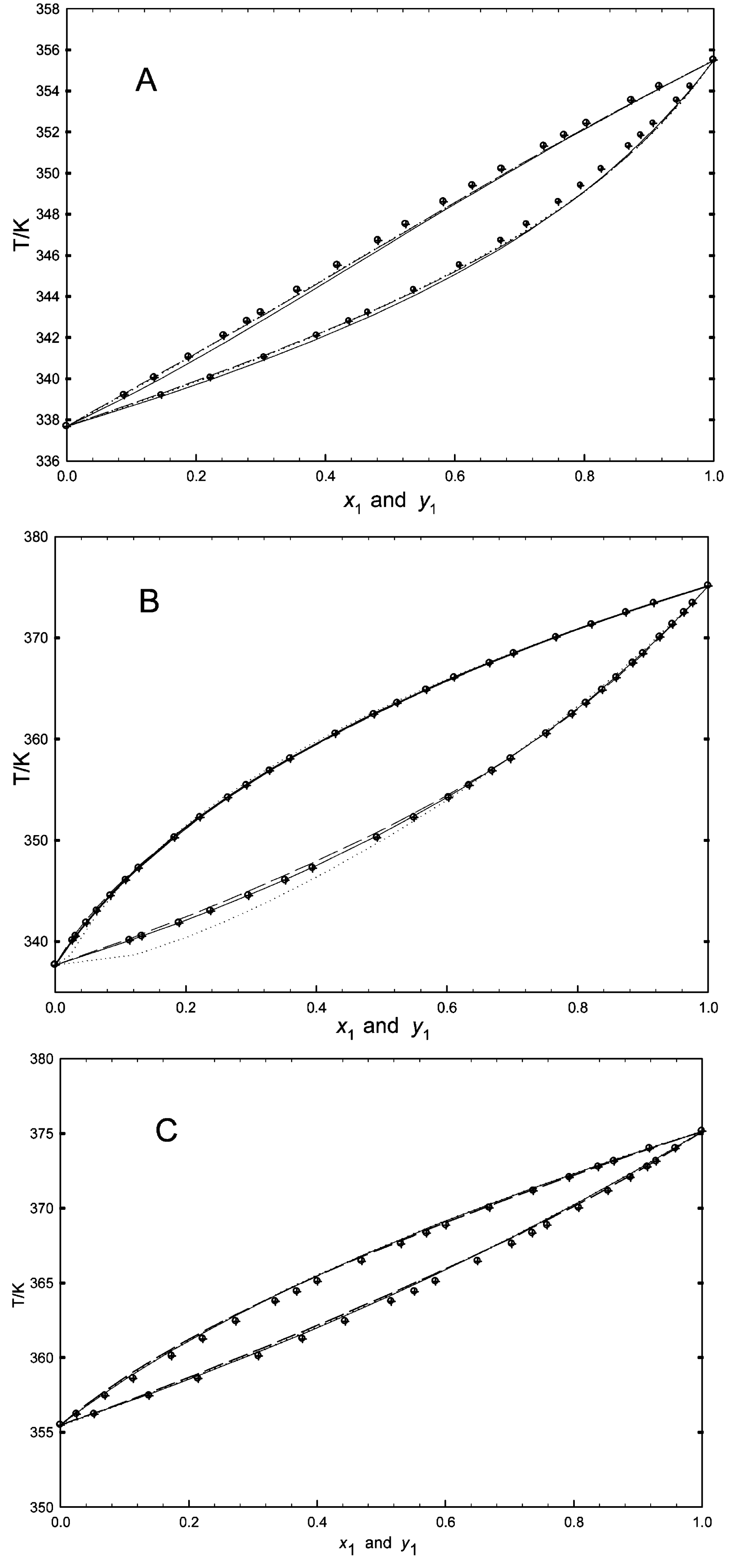


Figure 3. $T-x_1-y_1$ diagram for (A) methanol (1) + 2-propanol (2); (B) methanol (1) + 2-methyl-2-butanol (2); (C) 2-propanol (1) + 2-methyl-2-butanol (2) at 101.3 kPa. ⊗, experimental data; —, NRTL correlation; - - -, UNIQUAC correlation; · · ·, Wilson correlation.

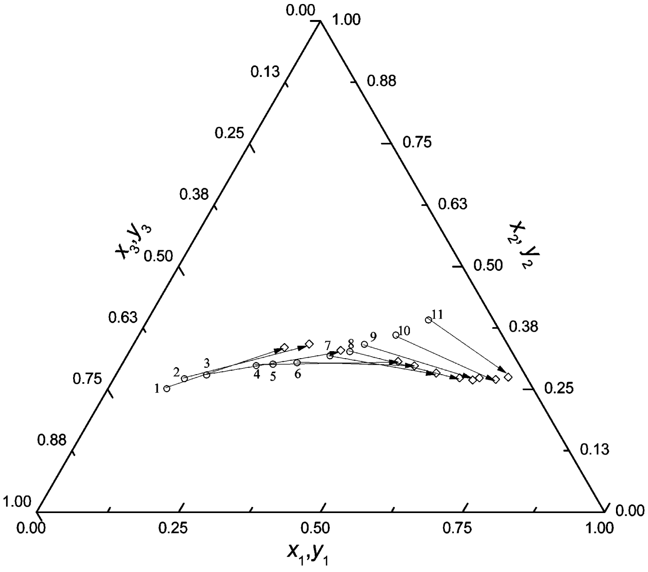


Figure 4. Experimental ternary VLE data for methanol (1) + 2-propanol (2) + 2-methyl-2-butanol (3) at 101.3 kPa. ○, liquid phase. ◇, vapor phase: 1, 345.15 K; 2, 346.76 K; 3, 348.45 K; 4, 349.24 K; 5, 350.46 K; 6, 352.45 K; 7, 354.15K; 8, 355.32 K; 9, 359.10 K; 10, 361.00 K; 11, 362.51 K.

with the y and T values of the correlations. The parameters along with the average deviation in $T(\Delta T)$ and the average deviation in $y(\Delta y)$ are listed in Table 6. The calculations from the Wilson, NRTL, and UNIQUAC equations are shown in Figure 3.

Ternary Mixtures. Experimental isobaric VLE for the ternary mixture containing methanol, 2-propanol, and 2-methyl-2-butanol are given in Table 4 and Figure 4. The thermodynamic consistency of ternary system was checked by the McDermott−Ellis method[26] modified by Wisniak and Tamir.[27] By comparing local difference D and maximum deviation $D_{\max}$ of the two adjacent experimental points a and b, it was considered thermodynamically consistent if following condition is satisfied:

$$D < D_{\max} \tag{4}$$

where D is the local deviation given by

$$D = \sum_{i=1}^{N} (x_{ia} - x_{ib})(\ln \gamma_{ia} - \ln \gamma_{ib}) \tag{5}$$

The maximum deviation $D_{\max}$ is given by

$$D_{\max} = \sum_{i=1}^{N}(x_{ia} - x_{ib})\left(\frac{1}{x_{ia}} + \frac{1}{y_{ia}} + \frac{1}{x_{ib}} + \frac{1}{y_{ib}}\right)\Delta x + \sum_{i=1}^{N}(x_{ia} - x_{ib})\frac{\Delta P}{P} + 2\sum_{i=1}^{N}|\ln \gamma_{ia} - \ln \gamma_{ib}|\Delta x + \sum_{i=1}^{N}(x_{ia} - x_{ib})B_j\{(T_a + C_j)^{-2} + (T_b + C_j)^{-2}\}\Delta T \tag{6}$$

In eq 6, the first term is dominate (the other terms can be neglected since they do not contribute under these conditions). Where N is the number of components, Δx, ΔP, and ΔT are the experimental average errors (the measurement error of liquid mole fraction x, pressure P, and temperature T are 0.002, 0.065, and 0.05, respectively). For the ternary system, experimental data are listed in Table 4 (note: the D value never exceeds 0.00059, while the smallest $D_{\max}$ is 0.00070).

Theoretical predictions of ternary equilibria using the Wilson, NRTL, and UNIQUAC equations with binary interaction parameters were made. The results are given in Table 6, Figure 5, and Figure 6. The NRTL and UNIQUAC equations gave good correlation to the experimental observations.

Conclusion

In this study, we measured the VLE data for methanol + 2-propanol to verify the reliability of our apparatus, which gave consistent VLE data as compared to the current literature. The binary systems methanol + 2-methyl-2-butanol and 2-propanol

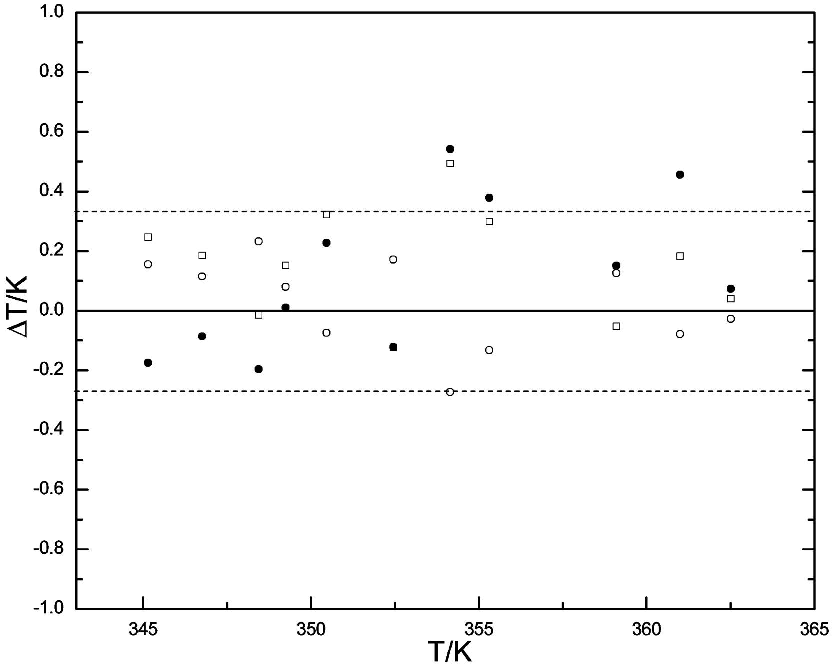


Figure 5. Temperature deviation of the ternary system: ○, NRTL prediction deviation from the experimental data; □, UNIQUAC equation prediction deviation from experimental data; ●, Wilson prediction deviation from the experimental data.

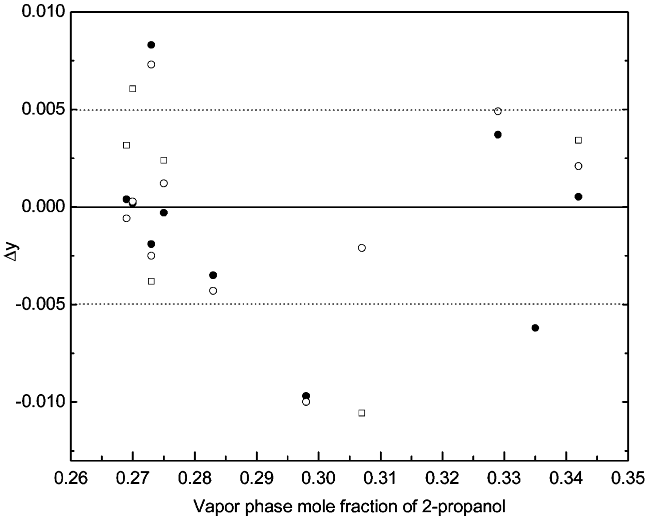


Figure 6. Vapor phase of 2-propanol deviation from the experimental of the ternary system; ○, NRTL prediction deviation from the experimental data; □, UNIQUAC equation prediction deviation from experimental data; ●, Wilson prediction deviation from the experimental data.

+ 2-methyl-2-butanol and the ternary system methanol + 2-propanol + 2-methyl-2-butanol VLE were also measured at 101.3 kPa with this system. The experimental data pass the thermodynamic consistency test and show that the experimental data are reliable. By comparing the experimental data and the correlated results with the NRTL, UNIQUAC, and Wilson equations, good predictions to the binary system and ternary system involving alcohols are given.

Literature Cited

(1) Ballard, L. H.; Winkle, M. V. Vapor−liquid equilibria at 760 mm pressures. *Ind. Eng. Chem.* **1952**, *44*, 2450−2453.
(2) Ochi, K.; Kojima, K. Vapor−liquid equilibrium for ternary system consisting of alcohols and water. *Kagaku Kogaku* **1969**, *33*, 352−357.
(3) Kohoutova, J.; Suska, J.; Novak, J. P.; Pick, J. Liquid−vapor equilibrium. XLV. System methanol−2-propanol−water. *Collect. Czech. Chem. Commun.* **1970**, *35*, 3210−3222.
(4) Verhoeye, L.; Herman, D. S. Vapor−liquid equilibriums of the binary, ternary, and quaternary systems formed by acetone, methanol, 2-propanol and water. *J. Appl. Chem. Biotechnol.* **1973**, *23*, 607−619.
(5) Wisniak, J.; Tamir, A. Vapor−liquid equilibria at 760 mmHg in the system methanol−2-propanol−propyl bromide and its binaries. *J. Chem. Eng. Data* **1985**, *30*, 339−344.
(6) Nagata, I. Vapor−liquid equilibrium of mixtures formed by methanol, 2-propanol, and chlorobenzene. *J. Chem. Eng. Data* **1986**, *31*, 413−416.
(7) Allen, P.; Pike, K. A. Experimental determination of the vapor−liquid equilibrium data for the system acetone−methanol−2-propanol. *Ind. Chem. Chem. Manuf.* **1964**, *40*, 260−266.
(8) Gultekin, N. Vapor−liquid equilibria at 1 atm for ternary and quaternary systems composed of acetone, methanol, 2-propanol, and 1-propanol. *J. Chem. Eng. Data* **1990**, *35*, 132−136.
(9) Lenka, M.; Persson, O.; Rasmussen, P. A modified Dvorak−Boublik (vapor + liquid) recirculating still with continuous analysis of the compositions of phases. *J. Chem. Thermodyn.* **1991**, *23*, 851−858.
(10) Nagata, I.; Fukushima, Y.; Miyazaki, K. Vapor−liquid equilibrium in the quaternary system methanol−2-propanol−acetonitrile−benzene at 55 °C. *Fluid Phase Equilib.* **1992**, *71*, 17−27.
(11) Jan, D. S.; Shiau, H. Y.; Tsai, F. N. Isobaric vapor−liquid-equilibria for methanol plus ethanol plus 2-propanol and the 3 constituent binary-systems. *J. Chin. Inst. Chem. Eng.* **1994**, *25*, 137−141.
(12) Nagata, I.; Tamura, K.; Miyai, K. Isothermal vapor−liquid equilibria of mixtures of (methanol + ethanol + 1-propanol or 2-propanol) at 333.15 K. *Fluid Phase Equilib.* **2000**, *170*, 37−48.
(13) Wisniak, J.; Yardeni, B.; Sling, T.; Segura, H. Isobaric vapor−liquid equilibria in the systems methyl acetate + 2,2′-oxybis[propane], 2,2′-oxybis[propane] + toluene, and methanol + 2-methyl-2-butanol. *J. Chem. Eng. Data* **2001**, *46*, 223−228.
(14) Barton, D. P.; Bhethanabotla, V. R.; Cambell, S. W. Binary total pressure measure for methanol with 1-pentanol, 2-pentanol, 3-pentanol, 2-methyl-1-butanol, 2-methyl-2-butanol, 3-methyl-1-butanol, and 3-mehyl-2-butanol at 313.15 K. *J. Chem. Eng. Data* **1996**, *41*, 1138−1140.
(15) Herington, E. F. G. Test of experimental isobaric vapor−liquid equilibrium data. *J. Inst. Petrol.* **1951**, *37*, 467−470.
(16) Yaws, C. L. *Chemical Properties Handbook*; McGraw Hill: New York, 1999.
(17) Chen, Z. X.; Hu, W. M.; Wang, L. H.; et al. Isobaric vapor−liquid equilibrium of tert-butyl alcohol cyclohexanol system. *Fluid Phase Equilib.* **1985**, *70*, 227−238.
(18) Dean, J. A. *Analytical Chemistry Handbook*; McGraw-Hill: New York, 1995.
(19) Hayden, J. G.; O'Connell, J. P. A generalized method for predicting second virial coefficients. *Ind. Eng. Chem., Process Des. Dev.* **1975**, *14*, 209−216.
(20) Resa, J. M.; Gonzalez, C.; De Landaluce, S. O. Vapor−liquid equilibrium of binary mixtures containing methanol plus propyl acetate, methanol plus isopropyl acetate, vinyl acetate plus propyl acetate, and vinyl acetate plus isopropyl acetate at 101.3 kPa. *J. Chem. Eng. Data* **2001**, *46*, 1338−1343.
(21) Reid, R. C.; Prausnitz, J. M.; Aherwood, T. K. *The Properties of Gases and Liquids*, 3rd ed.; McGraw-Hill: New York, 1977.
(22) Wilson, G. M. Vapor−liquid. XI. A new expression for the excess free energy of mixing. *J. Am. Chem. Soc.* **1964**, *86*, 127−130.
(23) Renon, H.; Prausnitz, J. M. Estimation of parameters for the NRTL equation for excess Gibbs energy of strongly non-ideal liquid mixtures. *Ind. Eng. Chem. Process. Des. Dev.* **1969**, *8*, 413−419.
(24) Abrams, D. S.; Pransnitz, J. M. Statistical thermodynamics of liquid mixtures: a new expression for the excess Gibbs energy of partially or completely miscible systems. *AIChE J.* **1975**, *21*, 116−128.
(25) Patino-Leal, H.; Reilly, P. Statistical estimation of parameters in vapor−liquid equilibrium. *AIChE J.* **1982**, *28*, 580−584.
(26) McDermott, C.; Ellis, S. R. M. A multicomonent consistency test. *Chem. Eng. Sci.* **1965**, *20*, 293−296.
(27) Wisniak, J.; Tamir, A. Vapor−liquid equilibria in the ternary system water−formic acid−acetic acid and water−acetic acid−propionic acid. *J. Chem. Eng. Data* **1977**, *22*, 253−260.

Received for review October 27, 2006. Accepted January 31, 2007.

JE060476J