Isobaric Vapor−Liquid Equilibrium for Binary Mixtures of 3-Methyl-1-butanol + 3-Methyl-1-butyl Ethanoate and 1-Pentanol + Pentyl Ethanoate at 101.3 kPa

Emilio A. Cepeda*

Departamento de Ingeniería Química, Facultad de Farmacia, Universidad del País Vasco, Paseo de la Universidad 7, 01006 Vitoria, Álava, Spain

---

Isobaric vapor−liquid equilibrium data at 101.325 kPa have been determined for the binary systems 3-methyl-1-butanol + 3-methyl-1-butyl ethanoate and 1-pentanol + pentyl ethanoate. The data were obtained using a vapor recirculating-type equilibrium still. Vapor pressures of 3-methyl-1-butanol and 3-methyl-1-butyl ethanoate were measured in a Swiestoslawski apparatus. Calculations of the nonideality of the vapor phase were made with the second virial coefficients evaluated from the Hayden−O'Connell method. The activity coefficients and boiling points of the solutions were well-correlated with the mole fraction using the Wilson, nonrandom two-liquid (NRTL), and universal quasichemical activity coefficient (UNIQUAC) equations. The mixtures do not present an azeotrope.

Introduction

The esters 3-methyl-1-butyl ethanoate (3-methyl-1-butyl ethanoate, isoamyl acetate) and pentyl ethanoate (pentyl acetate, amyl acetate) are ingredients widely used in the food and beverage industries to modify flavor and fragrance. They are also used as solvents in the industry of lacquers and paints. They are synthesized from acetic acid and the alcohols 3-methyl-1-butanol and 1-pentanol, respectively. The reaction is usually catalyzed by sulphuric acid, *p*-toluene sulphonic acid or other catalysts.[1] Because of the low values of the equilibrium constant of the esterification reaction, it is well-known that, to obtain higher yield of esters, the reaction must be forced to completion by removing the water which is formed during the course of reaction and/or by operating with an excess of one of the two reactants (acid or alcohol). The final product is a mixture of catalyst, alcohol, ester, and water which must be separated to obtain the pure ester. The separation is carried out by distillation. A process accomplishing both reaction and separation is the reactive distillation.[2]

Vapor−liquid equilibrium data are needed in the design of the separation process by distillation. In this way, other authors have measured the vapor−liquid equilibrium of the systems 3-methyl-1-butanol + 3-methyl-1-butyl ethanoate and 1-pentanol + *n*-pentyl ethanoate previously. The system 3-methyl-1-butanol + 3-methyl-1-butyl ethanoate has been measured by Durrans,[3] Krokhin,[4] and Kudriavtseva et al.[5] The data of these authors are old, and the differences between them are significant. The system 1-pentanol + *n*-pentyl ethanoate has been measured by Holley,[6] Croil,[7] and Lewell,[8] and recently Lee and Liang[2] have done a study of the quaternary system 1-pentanol + pentyl ethanoate + water + acetic acid, where specific data of the binary system are not included for the 1-pentanol + pentyl ethanoate system, although they give parameters from the correlation equation. Therefore, as the data found in the literature for the two systems are old or no actual specific data were found, an additional study is needed.

The aim of this work was the study of the vapor−liquid equilibrium of the systems 3-methyl-1-butanol + 3-methyl-1-butyl ethanoate and 1-pentanol + pentyl ethanoate. The activity coefficients calculated from equilibrium data were fitted with the usual thermodynamic models. Because of the discrepancy between the values of the vapor pressures found in the literature for 3-methyl-1-butanol and 3-methyl-1-butyl ethanoate, new experimental measurements were made.

Experimental Procedure

Chemicals. 3-Methyl-1-butanol (CAS Registry No. 123-51-3; AR grade, ≥ 0.99 mass fraction), 3-methyl-1-butyl ethanoate (CAS Registry No. 123-92-2; extra pure, ≥ 0.99 mass fraction), 1-pentanol (CAS Registry No. 71-41-0; AR grade ≥ 0.985 mass fraction), and pentyl ethanoate (CAS Registry No. 628-63-7, PS grade ≥ 0.98 mass fraction) were obtained from Merck (Schuchardt, Germany). The chemicals were treated with potassium bicarbonate as the agent of neutralization and drying and next were vacuum-distilled in a 1 m height and 30 mm diameter adiabatic distillation column (packed with 2 mm × 2 mm stainless Dixon rings), working at a 1:100 reflux ratio. The purity of the materials was checked by gas chromatography and was found to be better than 0.998 mass fraction. The densities were measured using an all-glass standard bicapillary pycnometer submerged in a thermostatted bath controlled to ± 0.1 K, which had been calibrated at atmospheric pressure with twice-distilled water. Refractive indices were measured with a PZO (Poland) Abbe refractometer thermostatted with water from a bath controlled to ± 0.1 K.

The density, refractive indices, and normal boiling points for the pure compounds are listed in the Table 1 along with their literature values. The estimated uncertainties in the measurements were: ± 0.0005 in mole fraction, ± 0.2 $\text{kg}\cdot\text{m}^{-3}$ in density, ± 0.0002 in refractive index, ± 0.05 K in temperature, and 14 Pa in pressure.

Vapor Pressures. The vapor pressure data were obtained by using a modified Swiestoslawski ebulliometer[9] (Figure 1). The ebulliometer was constructed of pyrex glass. A nichrome wire heats the liquid electrically. The still consists of a boiling flask,

---

* Corresponding author. Fax: 34 945 013014; e-mail: emilio.cepeda@ehu.es.

10.1021/je900812v

Table 1. Physical Properties of the Pure Compounds: Densities, ρ (298.15 K), Refractive Indices, n_D (298.15 K), and Normal Boiling Points, T_b (101.3 kPa)

	ρ/kg·m^{-3}		n_D		T_b/K	
compound	expt	lit.	expt	lit.	expt	lit.
3-methyl-1-butanol	807.6	807.1[11]	1.4051	1.4052[11]	404.55	405.05[4]
						403.65[11]
						404.35[13]
						405.15[12]
3-methyl-1-butyl ethanoate	866.4	866.4[11]	1.39893	1.3981[11]	414.75	415.25[11]
						415.25[4]
						415.27[13]
						415.70[21]
						414.95[14]
						414.85[20]
1-pentanol	811.2	810.8[11]	1.4077	1.4080[11]	410.95	411.13[11]
						410.95[13]
						410.75[14]
n-pentyl ethanoate	872.3	871.9[11]	1.4005	1.4005[11]	421.55	422.35[11]
						422.15[13]
						421.55[22]

a Cottrell pump, an equilibrium chamber which was insulated with a vacuum air jacket, and a thermometer well. The vapor−liquid mixture generated in the boiling chamber is forced upward through the Cottrell tube and then flows to equilibrium chamber.

The experimental atmospheric pressure was measured with a Fortin barometer with an estimated uncertainty of ± 4 Pa.

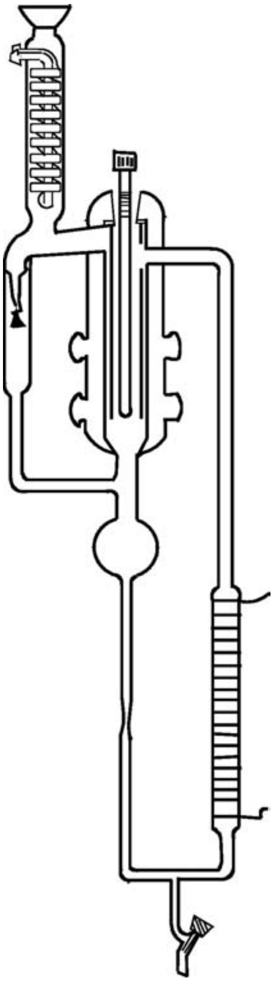

Figure 1. Swiestoslawski ebulliometer.

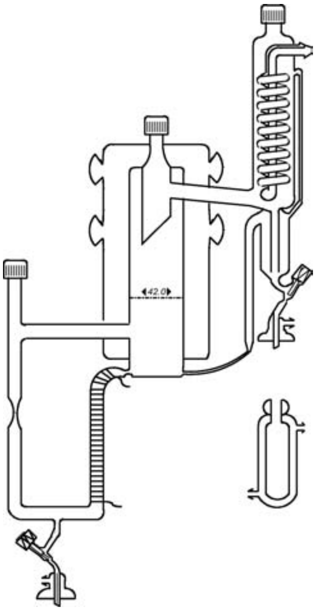

Figure 2. Equilibrium apparatus.

The pressure inside the measuring still was measured with a mercury manometer with an estimated uncertainty of 14 Pa. The temperatures were measured with a calibrated (ITS 90) mercury thermometer with an uncertainty of 0.1 K.

Apparatus and Procedure. The vapor−liquid equilibrium data were obtained by using a modified version of the equilibrium still.[10] The still was entirely constructed from borosilicate glass (Figure 2). The amount of solution required is about 65 cm^3 per determination. The ebullition takes place in the lateral pipe heated electrically by means a nichrome resistance. To avoid the backward movement of the vapor, the lateral pipe has a variable narrowing. The bubbles ascend to the equilibrium chamber and are distributed in the liquid by means of a magnetic stirrer. The vapor goes out from the liquid at the equilibrium temperature.

In each VLE experiment, the pressure was fixed and held constant by using a vacuum pump, and the heating and stirring systems of the liquid mixture were turned on. Equilibrium conditions were assumed when constant temperature and pressure were obtained for 60 min or longer. Then, samples of liquid and condensate were taken at the system pressure with the dispositive showed in the Figure 2. At least two analyses were made for each sample.

The estimated uncertainties in the measurements of temperature were ± 0.05 K and in pressure were 14 Pa.

Analysis. The compositions of the liquid and condensed-vapor samples from the *PTxy* experiments were analyzed by gas chromatography on a Perkin-Elmer 8700 with an flame ionization detector (FID). A stainless steel column of 2 m × 1/8 in. packed with Carbobax 20 M on Cromosorb W was used at 393.15 K with a helium flow rate of 30 cm^3·min^{-1} and a sample injection volume of 0.1 μL. Good separation was achieved under these conditions, and calibration analyses were carried out to convert the peak ratio to the mass composition of the sample. The pertinent polynomial fit had a correlation coefficient r^2 better than 0.99. At least three analyses were made of each sample. Mole fraction measurements had an estimated uncertainty of ± 0.0005. This estimate was done after to take several samples from the same phase at the same conditions and analyzing standards with the same analytical technique.

Table 2. Experimental Temperature−Vapor Pressure Data of 3-Methyl-1-butanol and 3-Methyl-1-butyl Ethanoate

3-methyl-1-butanol				3-methyl-1-butyl ethanoate			
T/K	P/kPa	T/K	P/kPa	T/K	P/kPa	T/K	P/kPa
336.35	5.27	381.65	43.64	368.15	22.4	401.85	70.1
346.9	9.25	389.6	59.58	369.35	23.4	403.35	73.3
354.2	12.96	391.35	64.30	370.65	24.6	407.15	81.9
354.3	13.24	392.65	66.58	371.85	25.7	409.55	87.8
356.85	14.83	395.55	74.19	372.45	26.3	410.95	91.3
359.75	17.09	396.9	77.47	380.65	35.3	412.85	96.3
360.65	17.61	398.25	81.46	381.75	36.7	414.15	99.8
363.55	20.13	403.05	96.21	387	43.9	414.85	101.7
364.05	20.81	403.75	99.99	387.9	45.2	415.35	103.1
365.45	21.98	404.55	101.33	390.95	50.0	416.45	106.2
368.3	25.18	405.15	103.46	392.75	52.9		
369.5	26.24	408.05	114.26	394.25	55.5		
371.5	28.64	410.95	125.72	395.65	58.0		
380.65	41.65	413.05	133.86	398.65	63.7		

Results and Discussion

Vapor Pressures. The vapor pressures were measured experimentally for pure 3-methyl-1-butanol and 3-methyl-1-butyl ethanoate, because important differences were found among the literature values. The experimental data are shown in Table 2.

The literature values for the normal boiling temperature of 3-methyl-1-butanol are between 403.15 K[11] and 405.15 K[12] (Table 1). The experimental normal boiling temperature is 404.55 K near to value of 404.35 K of Daubert and Danner.[13] The discrepancy of the experimental vapor pressures with those of other authors is shown in Figure 3.

Several equations and experimental data were found in the literature for the boiling point and vapor pressures of 3-methyl-1-butyl ethanoate (Table 1). The discrepancy of the experimental vapor pressures with the obtained data in this work is shown in Figure 4. The experimental data are coincident with the data given by Diaz et al.[14]

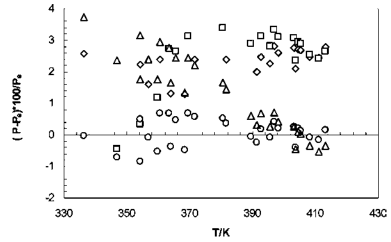

Figure 3. Discrepancy between experimental (P) and reported data (P_c) for the 3-methyl-1-butanol vapor pressure: ○, Antoine correlation; ◇, Daubert and Danner;[13] □, Riddick et al.;[11] △, Joo and Arlt.[24]

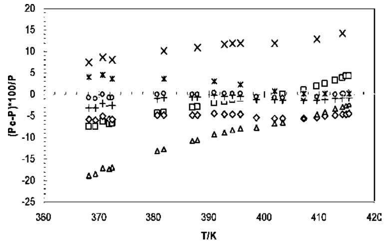

Figure 4. Discrepancy between experimental (P) and reported data (P_c) for 3-methyl-1-butyl ethanoate vapor pressure: ○, Antoine correlation: ×, Poling et al.;[21] □, Riddick et al.;[11] *, Chemcad;[20] ◇, Daubert and Danner;[13] △, Krokhin;[4] +, Diaz et al.[14]

Table 3. Vapor Pressure Parameters of the Antoine Equation (ln P/kPa) = A − B/((T/K) + C)

compound	A	B	C	σ/kPa	ref
3-methyl-1-butanol	14.7243	3002.04	−107.436	0.35	this work
3-methyl-1-butyl ethanoate	14.4851	3482.41	−61.6810	0.19	this work
1-pentanol	14.5133	2961.891	−111.843		11
pentyl ethanoate	13.4967	2888.5	−96.249		22

Table 4. Vapor−Liquid Equilibrium Data of the 3-Methyl-1-butanol + 3-Methyl-1-butyl Ethanoate System at 101.3 kPa

T/K	x_1	y_1	γ_1	γ_2
414.05	0.000	0.000		1.0000
413.15	0.025	0.044	1.3028	0.9997
411.95	0.059	0.098	1.2693	1.0007
410.55	0.108	0.169	1.2374	1.0045
410.05	0.185	0.265	1.1817	1.0102
408.85	0.218	0.303	1.1667	1.0117
408.45	0.299	0.388	1.1285	1.0249
407.45	0.330	0.418	1.1162	1.0308
406.75	0.424	0.504	1.0806	1.0512
406.15	0.504	0.574	1.0589	1.0692
405.75	0.578	0.636	1.0431	1.0919
405.15	0.650	0.695	1.0266	1.1162
405.05	0.768	0.794	1.0120	1.1574
404.95	0.794	0.815	1.0083	1.1729
404.85	0.838	0.855	1.0048	1.1759
404.75	0.863	0.876	1.0034	1.1896
404.75	0.891	0.900	1.0020	1.2069
404.65	0.904	0.912	1.0004	1.2093
404.55	0.923	0.929	1.0015	1.2169
404.55	0.959	0.961	1.0006	1.2503
414.05	1.000	1.000	1.000	

Table 5. Vapor−Liquid Equilibrium Data of the 1-Pentanol + *n*-Pentyl Ethanoate System at 101.3 kPa

T/K	x_1	y_1	γ_1	γ_2
421.55	0.000	0.000		1.0000
421.35	0.0089	0.016	1.2950	0.9990
420.85	0.0252	0.043	1.2689	1.0005
420.75	0.0265	0.045	1.2664	1.0024
419.65	0.0752	0.120	1.2284	1.0006
417.35	0.186	0.266	1.1820	1.0063
415.25	0.324	0.414	1.1254	1.0216
414.85	0.356	0.446	1.1188	1.0229
414.65	0.376	0.463	1.1061	1.0287
414.35	0.404	0.490	1.0923	1.0371
413.85	0.446	0.526	1.0885	1.0403
413.35	0.498	0.570	1.0699	1.0573
412.85	0.558	0.623	1.0574	1.0690
412.35	0.624	0.675	1.0444	1.0869
411.75	0.735	0.769	1.0199	1.1359
411.65	0.760	0.789	1.0151	1.1489
411.55	0.777	0.803	1.0178	1.1430
411.45	0.8001	0.824	1.0149	1.1519
411.4	0.809	0.830	1.0132	1.1572
411.3	0.844	0.860	1.0111	1.1709
411.15	0.900	0.908	1.0072	1.1847
410.95	0.9822	0.983	1.0018	1.2200
410.95	1	1	1.0000	

The temperature dependence of the pure component vapor pressure P^0 was calculated using the Antoine equation (Table 3). The root-mean-square deviation of pressure (σ) between experimental and calculated values was defined by the following equation,

$$\sigma = [\sum_{i=1}^{n} (P_i - P_i^{\text{cal}})^2/(n - 1)]^{1/2} \qquad (1)$$

where n is the number of experimental data, P_i is the experimental vapor pressure, and P_i^{cal} is the vapor pressure calculated at T_i temperature. The σ values are reported in Table 3.

Table 6. Properties of the Pure Compounds Used in Calculating the Second Virial Coefficients and UNIQUAC Parameters: Critical Temperature T_c, Critical Pressure P_c, Critical Volume V_c, Mean Gyration Radius R_D, Dipole Moment μ, Molar Volume MV (298 K), Structure Volume Parameter for the UNIQUAC Equation r, Structure Area Parameter for the UNIQUAC Equation q, Structure Volume Parameter for the Modified UNIQUAC Equation q', Association or Solvation Parameter η, and Acentric Factor ω

	3-methyl-1-butanol (1)	3-methy-1-butyl ethanoate (2)	1-pentanol (3)	pentyl ethanoate (4)
$T_c{}^a$/K	579.45	597.05	588.15	597.05
$P_c{}^a$/kPa	3920	2830	3910	2800
$V_c{}^a/\text{m}^3\cdot\text{kmol}^{-1}$	0.330	0.46	0.326	0.442
$R_D{}^a\cdot 10^{-10}$/m	3.684	4.656	3.679	4.772
$\mu^a\cdot 10^{-30}$/C·m	6.0042	6.0042	5.904	6.6742
$\text{MV}^a/\text{m}^3\cdot\text{kmol}^{-1}$	0.1092	0.1502	0.1085	0.1495
r^a	4.1279	5.5008	4.1287	5.5018
q^a	3.588	4.7319	3.592	4.736
q'^a	1.15	4.7319	1.15	4.736
$\eta_{\text{association}}{}^b$	1.55	0.53	2.2	0.53
$\eta_{\text{solvation}}{}^b$	(1) − (2), 1.3		(3) − (4), 1.3	
ω^a	0.5558	0.405	0.5738	0.4896

[a] Distil.[23] [b] Gess et al.[17]

Table 7. Correlation Parameters for Activity Coefficients and Average Mean Deviation of the Vapor Molar Fraction (Δy)

	Wilson			NRTL				UNIQUAC		
system	$A/\text{J}\cdot\text{mol}^{-1}$	$B/\text{J}\cdot\text{mol}^{-1}$	Δy	$A/\text{J}\cdot\text{mol}^{-1}$	$B/\text{J}\cdot\text{mol}^{-1}$	α	Δy	$A/\text{J}\cdot\text{mol}^{-1}$	$B/\text{J}\cdot\text{mol}^{-1}$	Δy
3-methyl-1-butanol + 3-methyl-1-butyl ethanoate	4518.06	−2897.26	0.008	−6518.62	8965.65	0.1041	0.008	−2656.04	4972.81	0.007
1-pentanol + pentyl ethanoate	3191.12	−1722.42	0.004	−1139.73	2623.61	0.3015	0.004	−2088.52	3818.61	0.006

Table 8. Results of the Thermodynamic Consistency Test

		Margules constants		
system	average deviation δ	A	B	D
3-methyl-1-butanol + 3-methyl-1-butyl ethanoate	0.0058	0.1304	−0.0684	−0.6472
1-pentanol + pentyl ethanoate	0.0052	0.5386	0.3788	0.5802

Vapor−Liquid Equilibrium. The isobaric vapor−liquid equilibrium data for the two systems have been obtained at 101.3 kPa and are shown in Tables 4 and 5. The liquid-phase activity coefficients of the components in the mixtures were calculated from:

$$\phi_i y_i P = \gamma_i x_i \phi_i^{\text{S}} \exp[v_i^{\text{L}}(P - P_i^{\text{S}})/RT] \tag{2}$$

where ϕ_i is the fugacity coefficient of component i in the vapor phase, y_i and x_i are the molar fractions in the vapor and liquid phases, respectively, γ_i is the activity coefficient of i with respect to the reference fugacity, $\phi_i{}^{\text{S}}$ is the fugacity coefficient of the pure saturated vapor of component i, $P_i{}^{\text{S}}$ is the vapor pressure of component i at temperature T, and $v_i{}^{\text{L}}$ is the molar volume of pure liquid. In the expression, it is assumed that the molar volume of component i is equal to the partial molar volume of component i at these conditions.

The fugacity coefficients were estimated by using the virial equation of state truncated after the second term. The second virial coefficients were obtained by using the method of Hayden and O'Connell.[15] The physical properties of the pure components required in this calculation are presented in Table 6. The Wilson, nonrandom two-liquid (NTRL), and universal quasichemical activity coefficient (UNIQUAC) models were used for the correlation of the activity coefficients. The values of R_k and Q_k were taken from Hansen et al.[16] in the UNIQUAC model.

The estimation of the parameters was done with the maximum likelihood technique, where the pressure, temperature, and liquid and vapor concentrations are considered simultaneously. The computer subroutines given by Gess et al.[17] were used. The fitted parameters along with the average mean deviations in vapor-phase mole fraction (Δy) are listed in Table 7. The best description of the equilibrium of the system 3-methyl-1-butanol + 3-methyl-1-butyl ethanoate was given by the UNIQUAC equation, with $\Delta y = 0.007$, with similar values for the other equations. The results of correlations for the system 1-pentanol + pentyl ethanoate by use of the Wilson and NTRL models present better correlations ($\Delta y = 0.004$) that those of the UNIQUAC model ($\Delta y = 0.006$). Considering the large differences in boiling points of the binary systems, the deviations are within an acceptable range.

The two systems satisfactorily passed the thermodynamic consistency test by using the Herrington analysis.[18] The values of D and J for 3-methyl-1-butanol + 3-methyl-1-butyl ethanoate were found to be 9.93 % and 3.52 % and for the 1-pentanol + pentyl ethanoate 9.19 % and 3.80 %. Also the consistency was checked by means of the modification of the Dechema test proposed by Gess et al.[17] for the prediction of the mole fraction in the vapor phase. In the method the activity coefficients were calculated with the four-suffix Margules equation

$$\ln \gamma_1 = x_2{}^2[A + 2(B - A - D)x_1 + 3Dx_1{}^2] \tag{3}$$

$$\ln \gamma_2 = x_1{}^2[B + 2(A - B - D)x_2 + 3Dx_2{}^2] \tag{4}$$

The pressure is calculated with the following equation,

$$P^* = \frac{x_1\gamma_1{}^* f_1{}^0}{\phi_1} + \frac{x_2\gamma_2{}^* f_2{}^0}{\phi_2} \tag{5}$$

Here the asterisk (*) denoted a calculated value. The parameters of Margules equation were calculated by minimization of ($P - P^*$). The values of y_1 were estimated by

$$y_1 = \frac{x_1\gamma_1 f_{1_1}{}^0}{P^*} \tag{6}$$

To pass the consistency test, a system must have an average deviation $\delta = \Sigma|y - y^*|/n$ lower than 0.01. The two systems have passed the test. The values of the constants A, B, D, and δ are shown in Table 8.

The system 3-methyl-1-butanol + 3-methyl-1-butyl ethanoate has been measured by several authors. Durrans[3] found an azeotrope at 101.3 kPa (393.25 K, $x = 0.98$), although its data

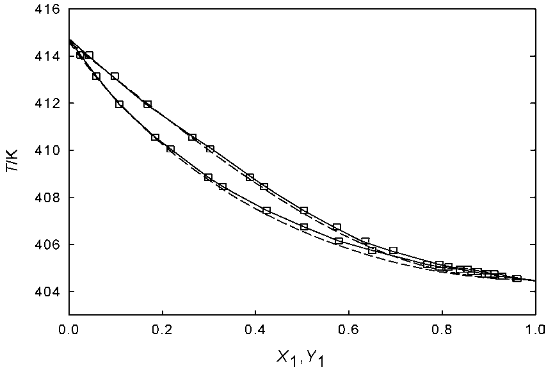

Figure 5. System of 3-methyl-1-butanol + 3-methyl-1-butyl ethanoate at 101.3 kPa. □, experimental data; —, smoothed using NRTL; ----, UNIFAC Dortmund prediction.[20]

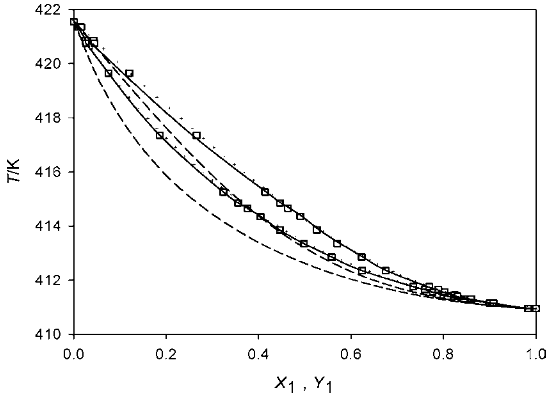

Figure 6. System of 1-pentanol + pentyl ethanoate at 101.3 kPa. □, experimental data; —, smoothed using NRTL model; ----, smoothed with the NRTL constants of Lee and Liang;[2] ++, predicted by UNIFAC method.

are old and obtained with impure products. Kudryavtseva et al.[5] found an azeotrope at 101.3 kPa (403.95 K, $x = 0.99$). Krokhin[4] also found an azeotrope at 101.3 kPa (403.15 K and $x = 0.93$). Experiments between 0.959 and 0.99 mole fraction were made, but because of little difference between the values of x and y in the composition range, the obtained data were not taken into account, because very small errors in the composition give high deviations in activity coefficients. When the experimental data were correlated with the models used, an azeotrope was not found. The UNIFAC[19] method predicted an azeotrope at $x = 0.72$ and $T = 403.05$ K, but the UNIFAC Dortmund method[20] predicted no azeotrope. Our data are coincident with those predicted by the UNIFAC Dortmund method in the $x-y$ diagram and are slightly different in the $T-x-y$ diagram (Figure 5).

The system 1-pentanol + *n*-pentyl ethanoate has been measured by Holley[6] using impure products. Croil[7] measured the system from $x = 0.4$ to $x = 1$ and did not find an azeotrope. Lewell[8] determined the system but indicates that the data were not precise. More recently, Lee and Liang[2] have done a study of the quaternary system pentanol + pentyl ethanoate + water + acetic acid, where specific data are not included for the system, although they give parameters for the correlation equation obtained from the data of the quaternary system (NRTL equation: $A_{12} = -932.67 \pm 698.31/\text{J}\cdot\text{mol}^{-1}$, $A_{21} = 1984.44 \pm 874.45/\text{J}\cdot\text{mol}^{-1}$, $\alpha = 0.30$). With these parameters, the equilibrium data were calculated with the vapor pressure equations used in this work and are shown in Figure 6. Our data are practically coincident with that calculated from the parameters given by Lee and Liang in the $x-y$ diagram, showing differences in $T-x-y$ diagram (Figure 6). No azeotrope was found. The UNIFAC[19] method predicts the vapor−liquid equilibrium poorly. Our data are coincident with those predicted by the UNIFAC Dortmund method in the $x-y$ diagram and are slightly different in the $T-x-y$ diagram (Figure 6). No azeotrope was predicted by the UNIFAC Dortmund method.

Conclusions

Sets of experimental VLE data were obtained for the binary 3-methyl-1-butanol + 3-methy-1-butyl ethanoate and 1-pentanol + *n*-pentyl ethanoate systems at 101.3 kPa in an Othmer modified equilibrium still. No azeotropes were observed. The experimental data were correlated satisfactorily with the Wilson, NRTL, and UNIQUAC models. Consistency of experimental data was proved on the basis of the Herrington as well as the point-to-point direct test of thermodynamic consistency. According to the later test, while omitting the most deviated points, the quality of measured data was classified to be good to excellent.

Literature Cited

(1) Liu, X. G.; Yin, Y. B.; Shi, M. C. Esterification of acetic acid with isoamyl alcohol over expandable graphite catalyst. *Chem. World* **1994**, *35*, 350–351.

(2) Lee, L. S.; Liang, S. J. Phase and reaction equilibria of acetic acid 1-pentanol water n-amyl acetate system at 760 mm Hg. *Fluid Phase Equilib.* **1998**, *149*, 57–74.

(3) Durrans, T. Treatise on distillation. *Perfum. Essent. Oil Rec.* **1920**, *11*, 154–198.

(4) Krokhin, N. G. Equiibrium liquid-vapor ratios in the system acetic acid-isoamyl alcohol-isoamyl acetate. II. Binary systems acetic acid-isoamyl acetate and isoamyl alcohol-isoamyl acetate. *Zh. Fiz. Khim.* **1967**, *41*, 1509–1511.

(5) Kudryavtseva, L. S.; Susarev, M. P.; Eisen, O. Concentration regions and thermal displacement of ternary azeotropes. VI. Repeated study of some azeotropes of ternary three-phase systems of the type water-alcohol-ester. *Zh. Fiz. Khim.* **1966**, *40*, 2637–2642.

(6) Holley, C. D. Liquid mixtures of minimum boiling-point. *J. Am. Chem. Soc.* **1902**, *24*, 448–457.

(7) Croil, T. A. B.A.Sc. Thesis, British Columbia University, Vancouver, BC Canada, 1957.

(8) Lewell, P. A.; Kristmanson, D. D. Vapor-liquid equilibriums in mixtures of n-alcohols and their esters. *AIChE J.* **1967**, *13*, 814–815.

(9) Swietoslawski, W.; Anderson, J. R. Determination of boiling and condensation temperatures. *Phys. Methods Org. Chem.* **1949**, *1*, 107–140.

(10) Mato, F.; Cepeda, E. Equilibrio líquido-vapor de mezclas binrias formadas por alcoholes y sus esteres del acido acetico. *An. Quim.* **1984**, *80*, 338–342.

(11) Riddick, J. A.; Bunger, W. B.; Sakano, T. K. *Organic solvents: physical properties and methods of purification*, 4th ed; New York: Wiley, 1986.

(12) Reddy, M. S.; Rao, C. V. Isothermal and Isobaric Vapor-Liquid Equilibrium Data System - Toulene-Isoamyl Alcohol. *J. Chem. Eng. Data* **1965**, *10*, 309–312.

(13) Daubert, T. E.; Danner, R. P. *Physical and thermodynamic properties of pure chemicals data compilation*; Hemisphere Pub. Corp: New York, 1984.

(14) Diaz, M. A. E.; Guetachew, T.; Landy, P.; Jose, J.; Voilley, A. Experimental and estimated saturated vapour pressures of aroma compounds. *Fluid Phase Equilib.* **1999**, *157*, 257–270.

(15) Hayden, J. G.; O'Connell, J. P. Generalized method for predicting second virial-coefficients. *Ind. Eng. Chem. Process Des. Dev.* **1975**, *14*, 209–216.

(16) Hansen, H. K.; Rasmussen, P.; Fredenslund, A.; Schiller, M.; Gmehling, J. Vapor-liquid-equilibria by Unifac group contribution. 5. Revision and extension. *Ind. Eng. Chem. Res.* **1991**, *30*, 2352–2355.

(17) Gess, M. A.; Danner, R. P.; Nagvekar, M. *Thermodynamic analysis of vapor-liquid equilibria: Recommended models and a standard data base*; AIChE: New York, 1991.

(18) Herrington, E. F. G. Tests of Consistency of Experimental Isobaric Vapor-Liquid Equilibrium Data. *J. Inst. Pet.* **1951**, *37*, 467–470.

(19) Fredenslund, A.; Gmehling, J. R.; Rasmussen, P. *Vapor-liquid equilibria using UNIFAC: a group-contribution method*; Elsevier: Amsterdam, 1977.

(20) *ChemCAD 5.2.0 Professional*; Chemstations, Inc.: Houston, TX, 2002.

(21) Poling, B. E.; Reid, R. C.; Prausnitz, J. M.; O'Connell, J. P. *The properties of gases and liquids*, 5th ed.; McGraw-Hill: New York, 2001.

(22) Brozena, A. *Vapor Pressure of n-Amyl Acetate: Literature Review and Experimental Determination*; Chemical Research Development and Engineering Center, Aberdeen Proving Grounds: Aberdeen, MD, 1992; pp 1−47.

(23) *Distil 5.0*; Hyprotech Ltd.: Calgary, Alberta, Canada, 2001.

(24) Joo, H. J.; Arlt, W. Vapor-liquid equilibrium for the binary systems ethylene glycol-n-amyl alcohol and ethylene glycol-isoamyl alcohol. *J. Chem. Eng. Data* **1981**, *26*, 138–140.

Received for review October 7, 2009. Accepted January 22, 2010.

JE900812V