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Vapor Liquid Equilibrium for the Binary Systems of 2-Methyl-2-propanol + 2,4,4-Trimethyl-1-pentene at 333 K and 348 K and 2-Butanol + 2,4,4-Trimethyl-1-pentene at 360 K

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Isothermal vapor liquid equilibrium data were measured for two binary systems, 2-methyl-2-propanol + 2,4,4-trimethyl-1-pentene at 333 K and 348 K and 2-butanol + 2,4,4-trimethyl-1-pentene at 360 K. The measurements were made with a recirculation still. The results were correlated with the Soave−Redlich−Kwong equation of state and the Wilson activity coefficient model.

Introduction

Vapor liquid equilibrium (VLE) data are necessary in distillation column design. Estimation methods such as UNIFAC or ASOG are useful when no data are available. Estimation methods do not provide enough accuracy for process design purposes, when the system shows major deviation from ideal behavior.

MTBE (2-methoxy-2-methylpropane) will be banned in California not later than 31 December 2002 due to groundwater pollution problems.[1] The consumption[2] of MTBE in California was about 4 million gallons per day during the first quarter of 2000. MTBE will have to be replaced with other fuel components. It is economically sound to convert existing MTBE plants in order to produce di-isobutylene (2,4,4-trimethyl-1-pentene and 2,4,4-trimethyl-2-pentene) or to hydrogenate the di-isobutylene to a high-quality fuel component: isooctane (2,2,4-trimethylpentane).[3] The systems measured have relevance in the design of the di-isobutylene processes. Data for the systems measured was not found in the literature.

Experimental Section

Materials. The 2-methyl-2-propanol (99.7%, by gas chromatography (GC)), 2-butanol (99.5%, GC), and 2,4,4-trimethyl-1-pentene (98+%, GC gave 99.4%) were provided by Fluka. The materials were used without further purification except for drying over molecular sieves (Merck3A).

Apparatus. A Yerazunis type apparatus[4] was build at the glass workshop of Helsinki University of Technology with minor modifications to the original design.[5] The liquid volume needed for running the apparatus was approximately 80 mL. The experimental setup is presented schematically in Figure 1. The apparatus was tested by measuring the vapor pressure of water and by measuring the isobaric system of toluene + *n*-heptane at 1 atm. Results compared well with literature data.[4,6] For temperature measurements a Thermolyzer S2541 (Frontec) temperature meter was used with a Pt-100 probe calibrated at the Finnish National Standards Laboratory. The resolution of the temperature measurement system was 0.005 K, and the calibration uncertainty was ±0.015 K; the uncertainty in the temperature measurement of the system is believed to be ±0.05 K. The Pt-100 probe was located at the bottom of the packed section of the equilibrium chamber in a thermometer well. The pressure measurement was done with a Druck pressure transducer (0−100 kPa) and a Red Lion panel meter. The uncertainty of the pressure measurement was ±0.07 kPa, according to the data provided by the manufacturer of the pressure measurement devices. The pressure measurement system was calibrated against a DHPPC-2 pressure calibrator. Including the calibration uncertainty, the uncertainty in the pressure measurement system is ±0.15 kPa.

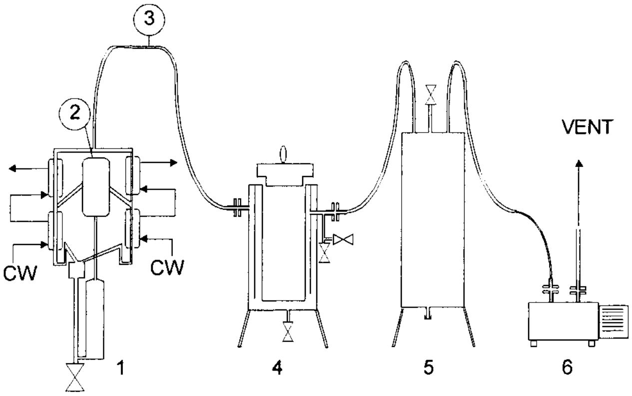

Figure 1. Experimental setup: (1) recirculation still; (2) temperature probe (Pt-100); (3) pressure transducer; (4) liquid nitrogen trap; (5) 30 dm^3 buffer tank; (6) vacuum pump.

Table 1. 2,4,4-Trimethyl-1-pentene Response Factor (*Q*), Number of Calibration Mixtures (*n*), and Average Deviation of the Response Factor (av dev *Q*) for the Systems 2-Methyl-2-propanol + 2,4,4-Trimethyl-1-pentene at 333 K and 348 K (System 1) and 2-Butanol + 2,4,4-Trimethyl-1-pentene at 360 K (System 2)

system	*Q*	*n*	av dev *Q*
1	0.722	6	0.016
2	0.616	6	0.007

Analysis and GC Calibration. The condensed vapor phase and the liquid phase were analyzed with a HP 6850A gas chromatograph with an autosampler and a flame ionization detector. The GC column used was a HP-1 (cross-linked methyl siloxane, length 30 m, column inner diameter 0.25 mm, film thickness 1.0 μm). Isooctane was used as a

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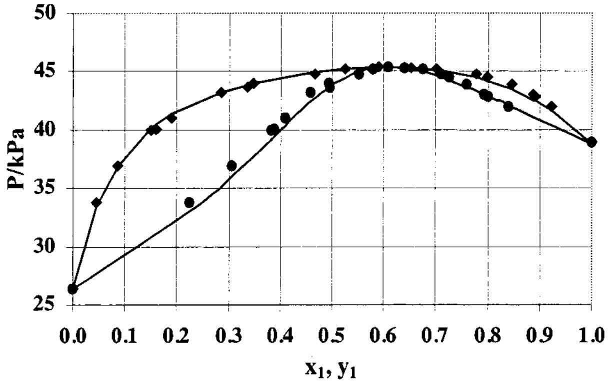

Figure 2. Pressure–composition diagram for the 2-methyl-2-propanol (1) + 2,4,4-trimethyl-1-pentene (2) system at 333 K: ◆, x_1; ●, y_1; —, x_1 calculated; —, y_1 calculated.

Table 2. VLE Data, Liquid Phase (x_1) and Vapor Phase (y_1) Mole Fractions, Pressure (P), Temperature (T), and Activity Coefficient (γ_i) for the 2-Methyl-2-propanol (1) + 2,4,4-Trimethyl-1-pentene (2) System at 333 K and 348 K

x_1	y_1	P/kPa	T/K	γ_1	γ_2
0.0000	0.0000	26.4	333.15		
0.0455	0.2244	33.8	333.15	1.04	4.32
0.0850	0.3058	36.9	333.14	1.05	3.44
0.1513	0.3830	40.0	333.15	1.09	2.62
0.1606	0.3880	40.1	333.15	1.10	2.50
0.1899	0.4101	41.0	333.14	1.12	2.29
0.2854	0.4592	43.2	333.13	1.23	1.79
0.3364	0.4952	43.6	333.13	1.24	1.66
0.3478	0.4935	44.0	333.14	1.28	1.61
0.4673	0.5535	44.8	333.12	1.41	1.37
0.5254	0.5796	45.2	333.15	1.50	1.29
0.5894	0.6094	45.4	333.13	1.62	1.21
0.6521	0.6411	45.3	333.13	1.75	1.15
0.7008	0.6755	45.2	333.14	1.84	1.12
0.7776	0.7104	44.8	333.14	2.19	1.06
0.7998	0.7265	44.5	333.14	2.28	1.04
0.8451	0.7590	43.9	333.15	2.56	1.02
0.8872	0.7921	43.0	333.13	2.97	0.99
0.8905	0.8001	42.9	333.14	2.94	0.99
0.9210	0.8396	42.0	333.15	3.20	0.99
1.0000	1.0000	38.9	333.17		
0.0000	0.0000	45.0	348.14		
0.0328	0.1752	53.9	348.14	1.02	3.85
0.0811	0.2936	62.3	348.16	1.06	3.00
0.1414	0.3859	68.8	348.17	1.08	2.49
0.1680	0.4159	70.3	348.15	1.08	2.31
0.2601	0.4723	75.5	348.13	1.18	1.82
0.3092	0.5084	76.8	348.15	1.19	1.67
0.3267	0.5102	77.7	348.13	1.24	1.61
0.4468	0.5747	80.4	348.14	1.35	1.37
0.5083	0.6077	81.4	348.14	1.42	1.29
0.5731	0.6399	82.3	347.93	1.52	1.23
0.6359	0.6729	82.8	348.15	1.62	1.16
0.7008	0.7059	83.1	348.16	1.78	1.11
0.7688	0.7429	83.0	348.16	2.01	1.06
0.7925	0.7570	82.8	348.17	2.11	1.04
0.8385	0.7900	82.1	348.15	2.33	1.02
0.8836	0.8310	81.0	348.14	2.57	1.01
0.8838	0.8304	81.0	348.14	2.58	1.01
0.9190	0.8672	79.8	348.16	2.86	1.00
0.9820	0.9654	76.6	348.17	3.22	1.00
1.0000	1.0000	75.7	348.13		

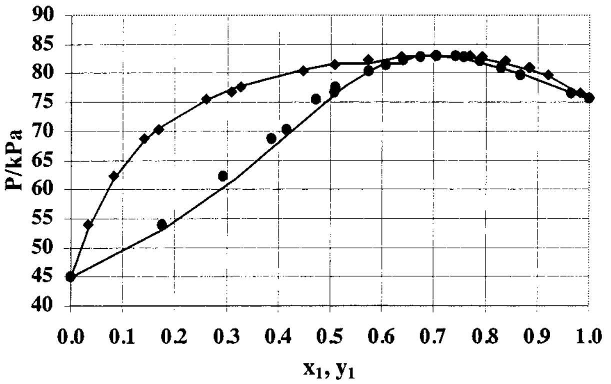

Figure 3. Pressure–composition diagram for the 2-methyl-2-propanol (1) + 2,4,4-trimethyl-1-pentene (2) system at 348 K: ◆, x_1; ●, y_1; —, x_1 calculated; —, y_1 calculated.

Table 3. VLE Data, Liquid Phase (x_1) and Vapor Phase (y_1) Mole Fractions, Pressure (P), Temperature (T), and Activity Coefficient (γ_i) for the 2-Butanol (1) + 2,4,4-Trimethyl-1-pentene (2) System at 360 K

x_1	y_1	P/kPa	T/K	γ_1	γ_2
0.0000	0.0000	62.8	360.16		
0.0511	0.1568	75.4	360.17	3.69	1.01
0.0533	0.1606	75.6	360.17	3.63	1.01
0.0587	0.1662	75.8	360.17	3.42	1.01
0.0929	0.2299	79.9	360.16	3.15	1.02
0.1288	0.2708	82.6	360.16	2.76	1.03
0.1792	0.3160	85.1	360.17	2.39	1.06
0.2322	0.3474	86.9	360.17	2.07	1.10
0.2814	0.3759	87.9	360.15	1.87	1.14
0.3330	0.3989	88.6	360.14	1.69	1.19
0.3905	0.4251	89.1	360.17	1.54	1.25
0.4579	0.4539	89.3	360.15	1.41	1.34
0.5150	0.4784	89.1	360.16	1.31	1.43
0.5831	0.5096	88.7	360.15	1.23	1.56
0.6454	0.5418	87.7	360.16	1.17	1.69
0.7008	0.5700	86.3	360.17	1.11	1.85
0.7529	0.6092	84.4	360.16	1.09	2.00
0.7815	0.6259	83.3	360.17	1.06	2.13
0.7875	0.6269	83.8	360.16	1.06	2.20
0.8235	0.6517	81.8	360.17	1.03	2.42
0.8595	0.6665	79.5	360.16	0.98	2.83
0.8877	0.7119	76.6	360.15	0.98	2.95
0.9140	0.7539	73.9	360.15	0.97	3.18
0.9322	0.7852	72.1	360.17	0.97	3.44
0.9517	0.8290	69.9	360.16	0.97	3.73
0.9675	0.8771	67.7	360.17	0.98	3.86
0.9807	0.9236	65.7	360.17	0.99	3.93
1.0000	1.0000	62.0	360.15		

solvent for the samples to avoid the precipitation of 2-methyl-2-propanol (its melting point is 298.97 K[7]) and to reduce the volume of the sample. Isooctane was also used as a solvent for the system 2-butanol + 2,4,4-trimethyl-1-pentene. Gravimetric calibration mixtures were prepared in 2 mL vials with approximately 1 mL of isooctane as a solvent. The alcohol response factors were set to the value 1; thus, it is possible to calculate the 2,4,4-trimethyl-1-pentene response factors for the binary systems with eq 1

$$Q = \frac{m_1 A_2}{m_2 A_1} \tag{1}$$

where m_1 is the mass of 2,4,4-trimethyl-1-pentene in the gravimetrically prepared sample, m_2 is the mass of the alcohol in the gravimetrically prepared sample, A_1 is the GC peak area of the 2,4,4-trimethyl-1-pentene, and A_2 is the GC peak area of the alcohol. The results obtained with these response factors were converted to mole fractions. The GC runs were repeated three times for each calibration mixture. GC response factors with average deviations of response factors for the systems measured are presented in Table 1.

Procedure. Pure component 1 was introduced to the recirculation still, and its vapor pressure was measured. After vapor pressure measurements, component 2 was added to the equilibrium still. The temperature was

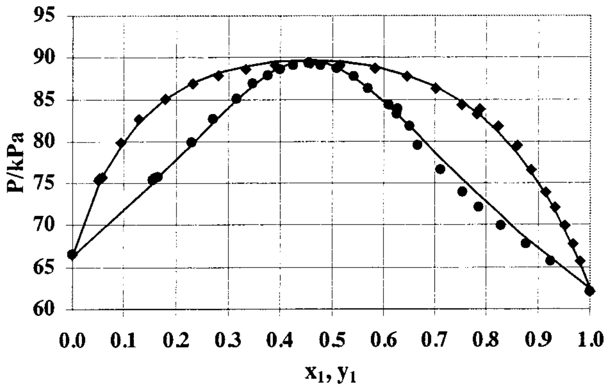

Figure 4. Pressure−composition diagram for the 2-butanol (1) + 2,4,4-trimethyl-1-pentene (2) system at 360 K: ◆, x_1; ●, y_1; —, x_1 calculated; —, y_1 calculated.

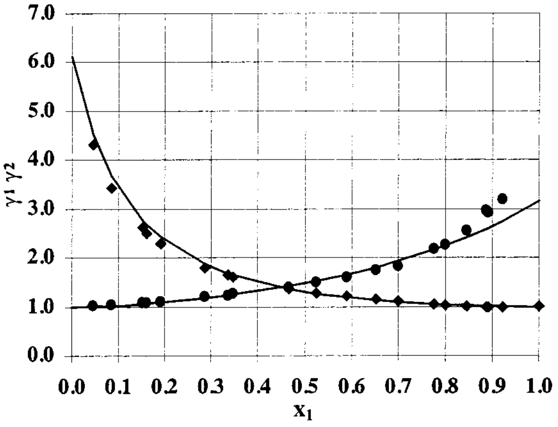

Figure 5. Activity coefficient−composition diagram for the 2-methyl-2-propanol (1) + 2,4,4-trimethyl-1-pentene system at 333 K: ◆, γ_1 from data; ●, γ_2 from data; —, γ_1 model; —, γ_2 model.

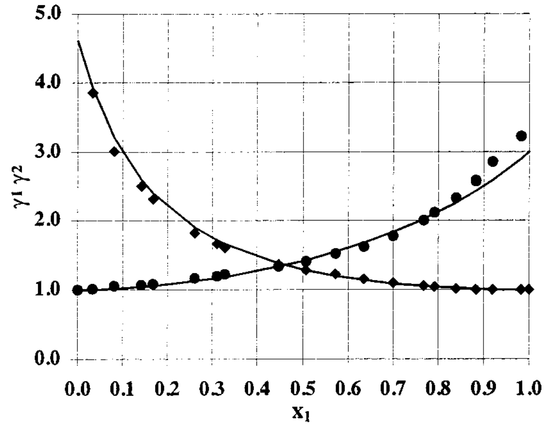

Figure 6. Activity coefficient−composition diagram for the 2-methyl-2-propanol (1) + 2,4,4-trimethyl-1-pentene (2) system at 348 K: ◆, γ_1 from data; ●, γ_2 from data; —, γ_1 model; —, γ_2 model.

Table 4. Azeotropic Pressure (*P*), Temperature (*T*), and Composition (x_1)

binary pair	*P*/kPa	*T*/K	x_1
2-methyl-2-propanol (1) + 2,4,4-trimethyl-1-pentene (2)	44.3 82.0	333.15 348.15	0.630 0.712
2-butanol (1) + 2,4,4-trimethyl-1-pentene (2)	89.3	360.15	0.451

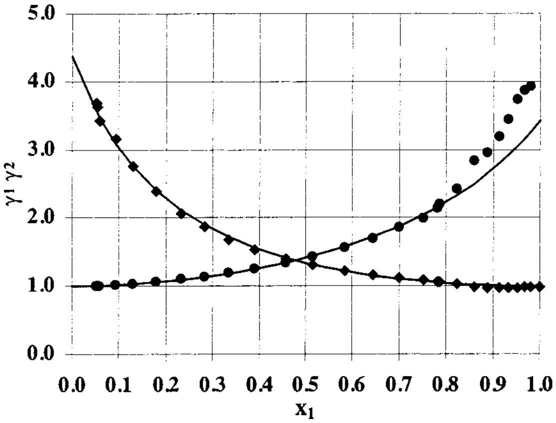

Figure 7. Activity coefficient−composition diagram for the 2-butanol (1) + 2,4,4-trimethyl-1-pentene (2) system at 360 K: ◆, γ_1 from data; ●, γ_2 from data; —, γ_1 model; —, γ_2 model.

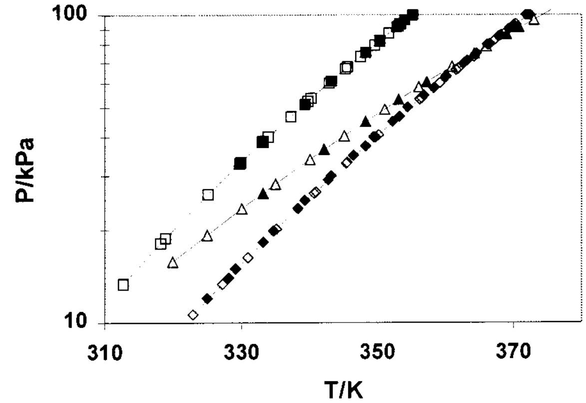

Figure 8. Vapor pressures of pure substances: ■, 2-methyl-2-propanol, measured, this work; ◆, 2-butanol, measured, this work; ▲, 2,4,4-trimethyl-1-pentene, measured, this work; □, 2-methyl-2-propanol, Boublik et al.;[13] ◇, 2-butanol, Boublik et al.;[13] △, 2,4,4-trimethyl-1-pentene, Smith and Shrivastava.[14]

Table 5. Critical Temperature (T_c), Critical Pressure (P_c), Critical Molar Volume (V_c), Acentric Factor (ω), Liquid Molar Volume (Used for Fitting the Wilson Equation Parameters) (v_i), Pure Component Vapor Pressure Equation Parameters (*A*, *B*, and *C*) for the Antoine Equation (Vapor Pressure Data Measured in this Work were Fitted), and Recommended Temperature Range of the Vapor Pressure Correlation (T_{min}, T_{max})

	2-methyl-2-propanol	2-butanol	2,4,4-trimethyl-1-pentene
T_c/K	506.2 ± 5[a]	536.01 ± 5[a]	553.0 ± 28[a]
P_c/MPa	3.9719 ± 0.12[a]	4.1938 ± 0.12[a]	2.630 ± 0.26[a]
V_c/cm^3·mol^{-1}	275 ± 11[a]	268 ± 13[a]	465 ± 116[a]
ω	0.6158[a]	0.5711[a]	0.2695[a]
v$_i$/cm^3·mol^{-1}	94.861 ± 2.8[a]	92.118 ± 0.9[a]	157.915 ± 4.7[a]
A	10.401	8.3640	6.9460
B	3982.9	3026.1	2999.3
C	-41.420	-88.316	-49.678
T_{min}/K	329.76	325.05	333.11
T_{max}/K	355.24	372.20	374.33

[a] Daubert and Danner.[7]

adjusted to the desired value by adjusting the pressure of the system. The temperature was held constant for approximately 35 min to further enhance the steady-state condition before sampling. Approximately 1 mL of isooctane was added to the 2 mL autosampler vials before sampling was carried out. Samples of the liquid and the vapor condensate were taken with a 1 mL Hamilton Sample Lock syringe after the steady-state condition was achieved. At first the syringe was flushed with 0.1 to 0.2 mL of sample, and then a 0.4 to 0.5 mL sample was taken and injected into the cooled 2 mL autosampler vial.

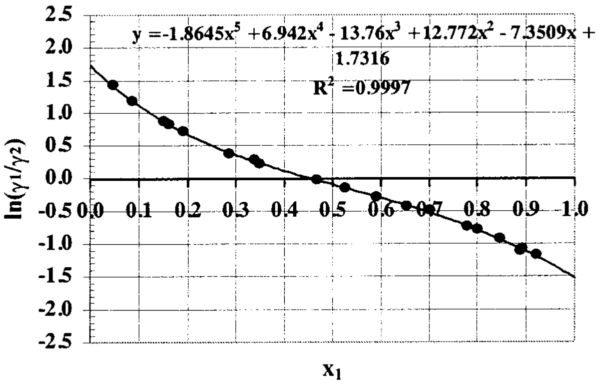

Figure 9. Integral test for the 2-methyl-2-propanol (1) + 2,4,4-trimethyl-1-pentene (2) system at 333 K.

Table 6. Pure Component Vapor Pressures for 2-Methyl-2-propanol, 2,4,4-Trimethyl-1-pentene, and 2-Butanol

2-methyl-2-propanol		2,4,4-trimethyl-1-pentene	
T/K	P/kPa	T/K	P/kPa
329.78	32.9	333.11	26.3
333.13	38.6	333.15	26.4
333.14	38.7	342.11	36.5
333.17	38.9	348.14	45.0
339.25	51.3	353.12	53.0
343.13	61.0	357.23	60.4
348.14	75.7	360.15	62.8
350.31	82.7	364.21	75.0
352.81	91.6	368.97	86.5
353.05	92.3	370.60	91.1
353.29	93.4	370.78	91.3
354.06	96.4	374.31	101.0
355.11	100.3		

2-butanol		2-butanol	
T/K	P/kPa	T/K	P/kPa
325.02	12.0	358.24	57.7
328.09	14.0	360.14	63.0
329.21	15.0	360.15	63.2
333.20	18.3	362.75	69.9
334.69	19.9	363.19	70.7
338.21	23.4	364.39	74.1
339.23	24.9	364.47	74.8
342.71	29.1	366.23	80.1
343.14	30.0	367.79	85.0
346.45	35.0	368.10	85.6
348.19	37.4	368.14	85.7
349.43	40.0	368.15	85.8
352.15	45.0	369.33	90.1
353.27	46.8	370.00	92.4
354.48	49.9	371.89	100.1
356.82	54.9	372.11	100.1

Results and Discussion

The data measured and calculated activity coefficients are reported in Tables 2 and 3 and Figures 2−7. Azeotropic behavior was observed for the 2-methyl-2-propanol + 2,4,4-trimethyl-1-pentene systems at both temperatures measured and also for the 2-butanol + 2,4,4-trimethyl-1-pentene system at the temperature measured. The azeotropic data for the systems measured are presented in Table 4. The azeotropic data were determined graphically from measured values.

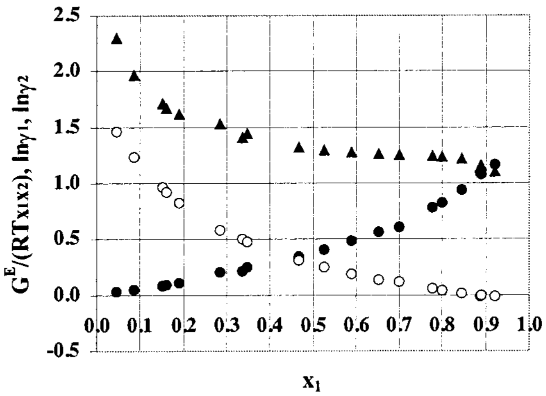

Figure 10. Infinite dilution test for the 2-methyl-2-propanol (1) + 2,4,4-trimethyl-1-pentene (2) system at 333 K: ▲, $G^E/(RTx_1x_2)$; ○, ln γ_1; ●, ln γ_2.

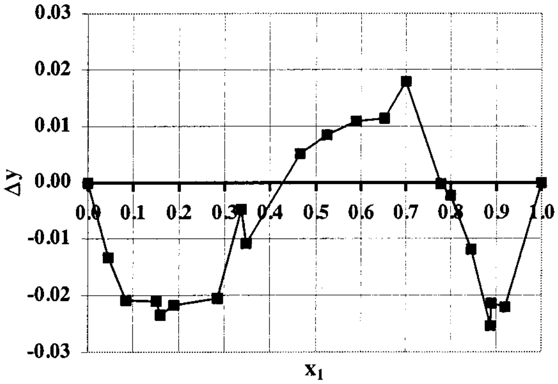

Figure 11. Point test for the 2-methyl-2-propanol (1) + 2,4,4-trimethyl-1-pentene (2) system at 333 K.

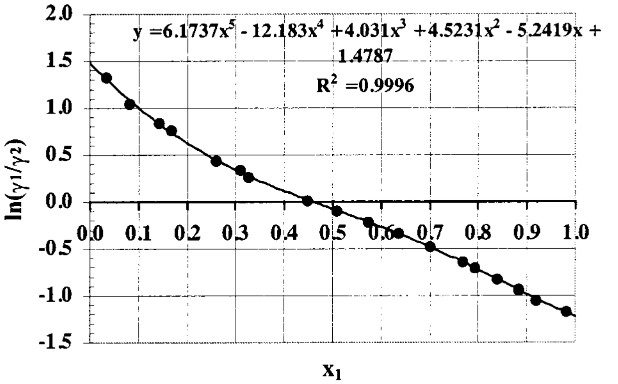

Figure 12. Integral test for the 2-methyl-2-propanol (1) + 2,4,4-trimethyl-1-pentene (2) system at 348 K.

The activity coefficients γ_i for the species i were calculated from eq 2

$$y_i P \phi_i = \gamma_i x_i P_{\mathrm{vp}i} \phi_i^{\mathrm{s}} \exp \int_{P_{\mathrm{vp}i}}^{P} \frac{V_i^{\mathrm{L}}\,\mathrm{d}P}{RT} \tag{2}$$

where y_i is the mole fraction of component i in the vapor phase, P is the system total pressure, ϕ_i is the fugacity coefficient of component i in the vapor phase, x_i is the mole

Table 7. Wilson Equation Parameters ($\lambda_{ij} - \lambda_{ii}$) for the Mixtures, Averages of the Absolute Vapor Fraction Residuals (Δy), and Averages of the Absolute Pressure Residuals (ΔP) for the Wilson Fit

system	$\lambda_{12} - \lambda_{11}$/J·mol^{-1}	$\lambda_{21} - \lambda_{22}$/J·mol^{-1}	Δy	ΔP/kPa
2-methyl-2-propanol (1) + 2,4,4-trimethyl-1-pentene (2), 333 K	5563.41	−374.34	0.0130	0.20
2-methyl-2-propanol (1) + 2,4,4-trimethyl-1-pentene (2), 348 K	4949.63	−327.40	0.0093	0.28
2-butanol (1) + 2,4,4-trimethyl-1-pentene (2), 360 K	4673.31	170.9	0.0097	0.37

Table 8. Results of Integral Test for the Binary Systems (A) 2-Methyl-2-propanol (1) + 2,4,4-Trimethyl-1-pentene (2) at 333 K, (B) 2-Methyl-2-propanol (1) + 2,4,4-Trimethyl-1-pentene (2) at 348 K, and (C) 2-Butanol (1) + 2,4,4-Trimethyl-1-pentene (2) at 360 K

system	D^a/%	test result
A	7.4	pass
B	5.9	pass
C	5.0	pass

[a] The criterion for passing the test is $D < 10\%$.[11]

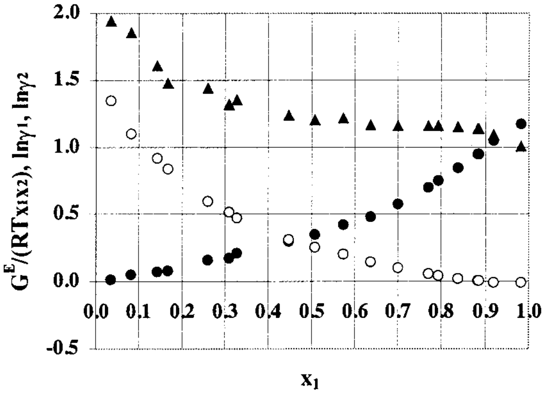

Figure 13. Infinite dilution test for the 2-methyl-2-propanol (1) + 2,4,4-trimethyl-1-pentene (2) system at 348 K: ▲, $G^E/(RTx_1x_2)$; ○, ln γ_1; ●, ln γ_2.

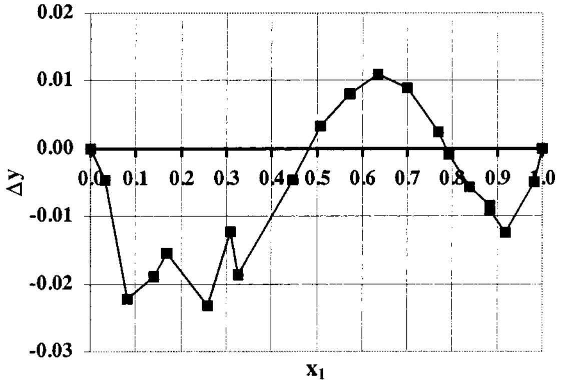

Figure 14. Point test for the 2-methyl-2-propanol (1) + 2,4,4-trimethyl-1-pentene (2) system at 348 K.

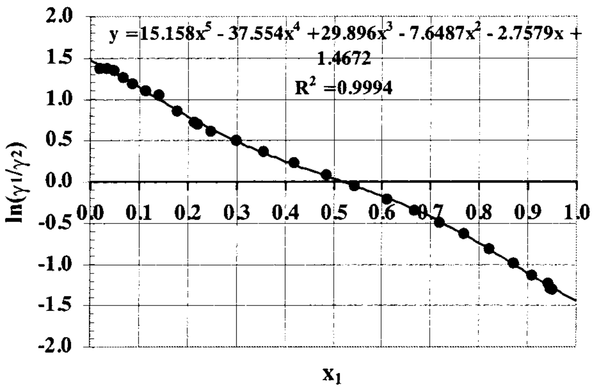

Figure 15. Integral test for the 2-butanol (1) + 2,4,4-trimethyl-1-pentene (2) system at 360 K.

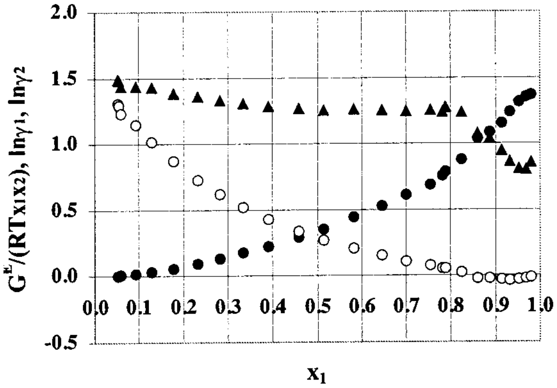

Figure 16. Infinite dilution test for the 2-butanol (1) + 2,4,4-trimethyl-1-pentene (2) system at 360 K: ▲, $G^E/(RTx_1x_2)$; ○, ln γ_1; ●, ln γ_2.

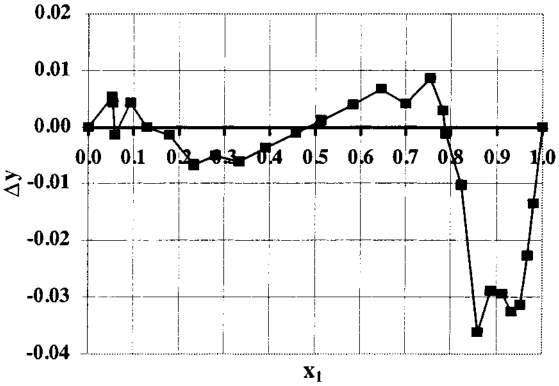

Figure 17. Point test for the 2-butanol (1) + 2,4,4-trimethyl-1-pentene (2) system at 360 K.

fraction of component i in the liquid phase, P_{vpi} is the vapor pressure of pure component i at the system temperature, ϕ_i^s is the pure component saturated liquid fugacity coefficient at the system temperature, v_i^L is the component i liquid-phase molar volume at the system temperature, T is temperature in Kelvin, and R is the universal gas constant (8.314 J·K^{-1}·mol^{-1}). The Soave−Redlich−Kwong equation of state, which has quadratic mixing rules in the attractive parameter and is linear in covolume, was used for vapor-phase calculation.[8] The liquid phase was modeled with the Wilson equation.[9] Critical temperatures, critical pressures, critical volumes, acentric factors, and the liquid molar volumes used in the calculations are presented in Table 5. The vapor pressures of the pure substances were calculated from the Antoine equation, eq 3. The vapor pressure equation parameters were fitted from data measured with the same apparatus that was used for the VLE measurements. The pure component vapor pressure equation parameters with the recommended temperature range of the vapor pressure equations are also presented in Table 5. Pure component vapor pressures for 2-methyl-2-propanol, 2-butanol, and 2,4,4-trimethyl-1-pentene are presented in Table 6 and Figure 8.

$$P/\text{MPa} = \exp\left(A - \frac{B}{(T/\text{K} + C)}\right) \tag{3}$$

The systems measured indicate positive deviations from Raoult's law. The objective function[10] O.F. used for fitting of the Wilson equation parameters is presented in eq 4. Wilson equation parameters for the mixtures with the averages of the absolute values of the residuals for the vapor phase and pressure are presented in Table 7

$$\text{O.F.} = \frac{1}{N}\sum_{i=1}^{N}(P^{\text{model}} - P^{\text{measured}})^2 \tag{4}$$

where N is the number of points used in the fit.

The results of the integral test are presented in Table 8. The data sets measured passed the integral test[11] (Figures 9, 12, and 15). The infinite dilution test plots[12] (Figures 10, 13, and 16) show that the data sets measured are not consistent in the dilute region, especially the measurement of 2-methyl-2-propanol + 2,4,4-trimethyl-1-pentene at 333 K. The reason for this behavior is believed to lie in the lack of mixing in the sampling chambers and in the mixing chamber of the condensed vapor phase and the liquid phase. In the point test a set of data is considered consistent[11] if the averages of the absolute values of the residuals for the vapor phase in mole fraction are smaller than 0.01 (Table 7 and Figures 11, 14, and 17). The 2-methyl-2-propanol + 2,4,4-trimethyl-1-pentene data set measured at 333 K did not satisfy the point test; the other data sets measured passed the point test.

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