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Vapor−Liquid Equilibrium for Binary Systems 2-Propanol + 2-Ethoxy-2-methylpropane and Ethyl Ethanoate + 2-Ethoxy-2-methylpropane at 333 K and 2-Propanone + 2-Ethoxy-2-methylpropane at 323 K

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Isothermal vapor−liquid equilibria were measured in a range of pressures from 38.8 kPa to 84.4 kPa for 2-propanol + 2-ethoxy-2-methylpropane and ethyl ethanoate + 2-ethoxy-2-methylpropane at 333 K and 2-propanone + 2-ethoxy-2-methylpropane at 323 K with a circulation still. The liquid- and condensed vapor-phase samples were analyzed by gas chromatography. The experimental data were correlated with the Wilson activity coefficient model.

Introduction

Branched ethers have become important in the last few decades as fuel additives by increasing the amount of oxygen in gasoline and substituting for lead tetraethyl.[1] 2-Ethoxy-2-methylpropane (ETBE) has emerged as an alternative to MTBE because ETBE is derived from ethanol, which is a renewable resource produced from abundant biomass. Furthermore, ETBE, when compared to MTBE, has a higher octane rating and a lower volatility and is less hydrophilic with regard to permeating and polluting groundwater supplies as well as being chemically more similar to hydrocarbons. For the production of ETBE, accurate vapor−liquid equilibrium data is an essential part of the process design. In this work, isothermal vapor−liquid equilibrium data for binary systems of 2-propanol + 2-ethoxy-2-methylpropane and ethyl ethanoate + 2-ethoxy-2-methylpropane at 333 K and 2-propanone + 2-ethoxy-2-methylpropane at 323 K were measured. No other VLE measurements of these binary systems have been published.

Experimental Section

Materials. 2-Ethoxy-2-methylpropane (98.6% purity by gas chromatography (GC) peak area) was provided by Oy Tamro Ab, and 2-propanol, (99.8%, GC) was provided by Fluka. 2-Propanone (99.5%, GC) and ethyl ethanoate (99.5%, GC) were supplied by Merck. The materials were used without further purification except for drying over molecular sieves (Merck 3A).

Apparatus for VLE Measurements. The VLE runs were conducted with a circulation still of the Yerazunis-type[2] built at the glass workshop of the Helsinki University of Technology with minor modifications to the original design.[3] Approximately 80 mL of each reagent was needed to run the apparatus.

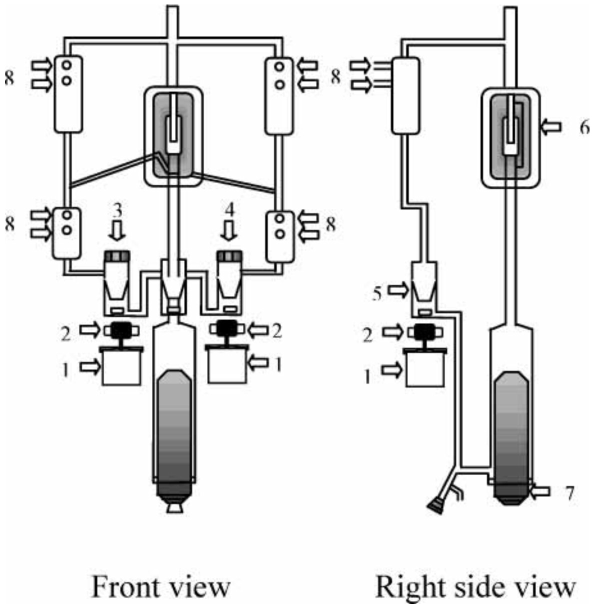

Figure 1. Modification of the existing experimental setup: (1) dc electric motors; (2) magnetic stir bar; (3) liquid-phase chamber; (4) vapor-phase chamber; (5) mixing chamber; (6) VLE cell; (7) immersion heater; and (8) cooling water hole.

Temperature was measured with a Thermolyzer S2541 (Frontec) temperature meter with a Pt-100 probe calibrated at Inspecta Oy. The Pt-100 probe was located at the bottom of the packed section of the equilibrium chamber. The resolution of the temperature measurement system was 0.005 K, and the calibration uncertainty was ±0.015 K. The uncertainty of the whole temperature measurement system was estimated to be ±0.05 K. Pressure was measured with a Druck pressure transducer (0 to 100 kPa) and a Red Lion panel meter. The inaccuracy of the instruments was reported to be ±0.07 kPa by the manufacturer. The pressure measurement system was calibrated against a DH-PPC-2 pressure calibrator. The inaccuracy of the whole pressure measurement system including the calibration uncertainty was expected to be less than ±0.15 kPa. The

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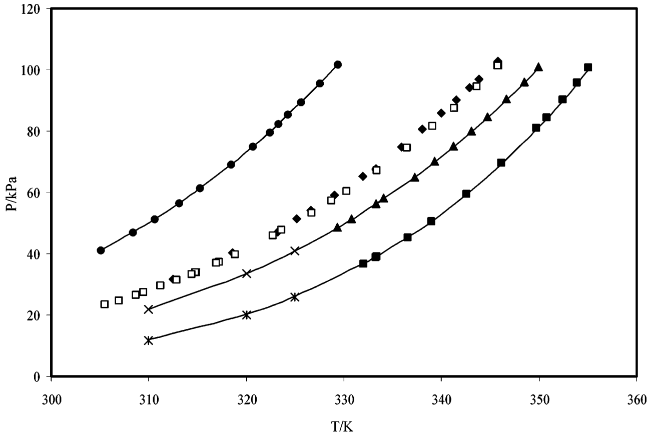

Figure 2. Vapor pressure of pure substances: ♦, 2-ethoxy-2-methylpropane, measured in this work; □, 2-ethoxy-2-methylpropane, Krähenbühl and Gmehling;[14] ■, 2-propanol, measured in this work; *, extrapolated data with Antoine parameters optimized in this work; ●, 2-propanone, measured in this work; ▲, ethyl ethanoate, measured in this work; × extrapolated data with Antoine parameters optimized in this work; −, calculated from Antoine constants in the literature.[15]

Table 1. Experimental Vapor Pressure of 2-Ethoxy-2-methylpropane

T/K	P/kPa
345.77	102.8
343.86	97.0
342.88	94.3
341.49	90.1
340.01	85.8
338.08	80.5
335.92	74.8
333.28	67.4
331.96	65.3
329.02	59.0
326.60	54.1
325.18	51.4
323.25	47.2
318.55	40.2
312.49	31.7

existing experimental setup was described previously.[4] To improve mixing in the sampling chambers and the mixing chamber of the condensed vapor phase and liquid phase, the DC electric motors (Graupner speed 400 motor) were equipped with magnetic stir bars, which deliver smooth and consecutive stirring action in the chambers. This modification of the apparatus is illustrated in Figure 1.

Analysis of VLE and GC Calibration. The equilibrated liquid phase was cooled and withdrawn from the sample chamber. The equilibrated vapor phase was first condensed and then sampled in the liquid phase from the sample chamber. The liquid and vapor samples were analyzed with an HP 6850A gas chromatograph with an autosampler and a flame ionization detector (FID). The GC column used was an HP-1 (methyl siloxane, length 60 m, nominal diameter 250 μm, nominal film thickness 1.0 μm). The oven temperature was 100 °C, run time 11 min, inlet split ratio 50:1, carrier gas He (1.0 mL min^{-1}), and FID temperature 250 °C. Toluene was used as a solvent for the samples to reduce the volume of the sample.

The response factors[5] were calculated from

$$\frac{A_1}{A_2}\frac{F_1}{F_2} = \frac{x_1}{x_2} \tag{1}$$

Table 2. Isothermal 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-Propanol (1) + 2-Ethoxy-2-methylpropane (2) System at 333 K

x_1	y_1	T/K	P/kPa	$\gamma_{1,\mathrm{meas}}$	$\gamma_{2,\mathrm{meas}}$	$\Delta\gamma_1{}^a$	$\Delta\gamma_2{}^b$
0.0000	0.0000	333.28	67.4		1.00		0.00
0.0930	0.1305	333.31	72.3	2.59	1.02	−0.06	−0.01
0.1472	0.1781	333.34	73.2	2.25	1.04	−0.03	−0.01
0.2025	0.2144	333.28	73.3	1.98	1.07	0.00	−0.01
0.2594	0.2454	333.30	73.2	1.76	1.10	0.01	−0.01
0.3209	0.2762	333.35	72.8	1.59	1.14	0.01	−0.01
0.3776	0.3019	333.31	72.0	1.47	1.19	0.01	−0.01
0.4422	0.3315	333.29	71.1	1.36	1.26	0.01	0.00
0.4979	0.3557	333.34	70.1	1.27	1.33	0.01	0.00
0.5597	0.3849	333.28	68.5	1.20	1.42	0.01	0.00
0.6145	0.4121	333.28	66.9	1.15	1.51	0.01	0.00
0.6627	0.4404	333.31	65.4	1.11	1.61	0.01	0.00
0.7102	0.4700	333.31	63.5	1.07	1.72	0.01	−0.01
0.7826	0.5310	333.27	59.7	1.04	1.91	0.01	−0.01
0.8337	0.5872	333.35	56.5	1.02	2.08	0.01	−0.02
0.8700	0.6370	333.28	53.6	1.01	2.23	0.01	−0.04
0.8965	0.6836	333.28	51.2	1.00	2.34	0.01	−0.05
0.9221	0.7439	333.27	48.6	1.01	2.39	0.00	0.01
0.9467	0.8035	333.32	45.9	1.00	2.53	0.00	−0.02
0.9652	0.8639	333.31	43.7	1.01	2.56	−0.01	0.04
0.9800	0.9175	333.26	41.7	1.01	2.58	−0.01	0.10
0.9924	0.9677	333.28	39.9	1.00	2.55	0.00	0.19
1.0000	1.0000	333.28	38.8	1.00		0.00	

[a] $\Delta\gamma_1 = \gamma_{1,\mathrm{model}} - \gamma_{1,\mathrm{meas}}$. [b] $\Delta\gamma_2 = \gamma_{2,\mathrm{model}} - \gamma_{2,\mathrm{meas}}$.

Table 3. Isothermal 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-Propanone (1) + 2-Ethoxy-2-methylpropane (2) System at 323 K

x_1	y_1	T/K	P/kPa	$\gamma_{1,\mathrm{meas}}$	$\gamma_{2,\mathrm{meas}}$	$\Delta\gamma_1{}^a$	$\Delta\gamma_2{}^b$
0.0000	0.0000	323.30	47.2		1.00		0.00
0.0446	0.1476	323.27	53.1	2.17	1.00	−0.08	0.00
0.0775	0.2337	323.23	57.1	2.12	1.00	−0.14	0.01
0.1134	0.2931	323.32	60.3	1.92	1.01	−0.03	0.00
0.1562	0.3556	323.22	63.5	1.78	1.02	0.00	0.00
0.2055	0.4162	323.27	67.1	1.67	1.03	−0.01	0.00
0.2614	0.4690	323.22	70.3	1.55	1.06	0.01	0.00
0.3202	0.5185	323.24	73.3	1.45	1.08	0.00	0.00
0.3799	0.5593	323.30	75.8	1.36	1.12	0.00	0.00
0.5053	0.6320	323.31	79.5	1.21	1.23	0.01	0.00
0.5625	0.6636	323.29	80.8	1.16	1.29	0.01	0.00
0.6150	0.6932	323.30	82.0	1.13	1.36	0.00	0.00
0.6674	0.7236	323.31	83.0	1.10	1.43	0.00	0.00
0.7127	0.7491	323.28	83.6	1.07	1.51	0.00	−0.01
0.7518	0.7732	323.29	84.0	1.05	1.59	0.00	−0.01
0.7909	0.7989	323.29	84.2	1.04	1.68	0.00	−0.02
0.8422	0.8372	323.30	84.4	1.02	1.80	0.00	−0.02
0.8854	0.8718	323.29	84.1	1.01	1.95	0.00	−0.05
0.9088	0.8934	323.29	83.9	1.01	2.04	0.00	−0.06
0.9339	0.9186	323.31	83.6	1.00	2.13	0.00	−0.08
0.9591	0.9469	323.32	83.1	1.00	2.24	0.00	−0.09
0.9702	0.9603	323.30	82.9	1.00	2.30	0.00	−0.11
0.9834	0.9771	323.35	82.7	1.00	2.36	0.00	−0.12
0.9945	0.9923	323.35	82.3	1.00	2.38	0.00	−0.10
1.0000	1.0000	323.35	82.1	1.00		0.00	

[a] $\Delta\gamma_1 = \gamma_{1,\mathrm{model}} - \gamma_{1,\mathrm{meas}}$. [b] $\Delta\gamma_2 = \gamma_{2,\mathrm{model}} - \gamma_{2,\mathrm{meas}}$.

where A_1 and A_2 are the GC peak areas, F_1 and F_2 are response factors, and x_1 and x_2 are mole fractions of components 1 and 2, respectively. The nine gravimetrically prepared samples per binary system were analyzed, and then ratio of A_1/A_2 was plotted as a function of x_1/x_2. The slope of the regressed linear trend is F_2/F_1, and the deviation from the origin is called the bias. The bias was very small and ignored. The composition of component 1 was solved from

Table 4. Isothermal VLE Data, Liquid-Phase (x_1) and Vapor-Phase (y_1) Mole Fractions, Pressure (P), Temperature (T), and Activity Coefficient (γ_i) for the Ethyl Ethanoate (1) + 2-Ethoxy-2-methylpropane (2) System at 333 K

x_1	y_1	T/K	P/kPa	$\gamma_{1,\mathrm{meas}}$	$\gamma_{2,\mathrm{mea}}$	$\Delta\gamma_1$[a]	$\Delta\gamma_2$[b]
0.0000	0.0000	333.29	67.6		1.00		0.00
0.0517	0.0599	333.31	68.2	1.40	1.00	−0.03	0.00
0.0967	0.1079	333.31	68.7	1.35	1.00	−0.02	0.00
0.1377	0.1497	333.30	68.9	1.32	1.00	−0.02	0.00
0.1841	0.1935	333.30	69.1	1.28	1.01	−0.01	0.00
0.2313	0.2364	333.32	69.2	1.25	1.02	−0.01	0.00
0.2787	0.2775	333.31	69.2	1.22	1.02	0.00	0.00
0.3365	0.3261	333.31	69.1	1.18	1.04	0.00	0.00
0.3977	0.3764	333.32	68.8	1.15	1.05	0.00	0.00
0.4539	0.4216	333.29	68.3	1.12	1.07	0.00	0.00
0.5291	0.4826	333.31	67.9	1.09	1.10	0.00	0.00
0.5888	0.5303	333.28	67.0	1.07	1.13	0.00	0.00
0.6383	0.5739	333.29	66.3	1.06	1.16	0.00	0.00
0.6891	0.6191	333.27	65.4	1.04	1.19	0.00	0.00
0.7363	0.6636	333.30	64.6	1.03	1.22	0.00	0.00
0.7845	0.7142	333.27	63.4	1.02	1.25	0.00	0.01
0.8280	0.7601	333.31	62.4	1.01	1.29	0.00	0.01
0.8717	0.8118	333.29	61.0	1.01	1.33	0.00	0.01
0.9065	0.8566	333.28	59.9	1.00	1.36	0.00	0.01
0.9369	0.8995	333.29	58.9	1.00	1.39	0.00	0.02
0.9744	0.9568	333.28	57.3	1.00	1.44	0.00	0.02
1.0000	1.0000	333.29	56.2	1.00		0.00	

[a] $\Delta\gamma_1 = \gamma_{1,\mathrm{model}} - \gamma_{1,\mathrm{meas}}$. [b] $\Delta\gamma_2 = \gamma_{2,\mathrm{model}} - \gamma_{2,\mathrm{meas}}$.

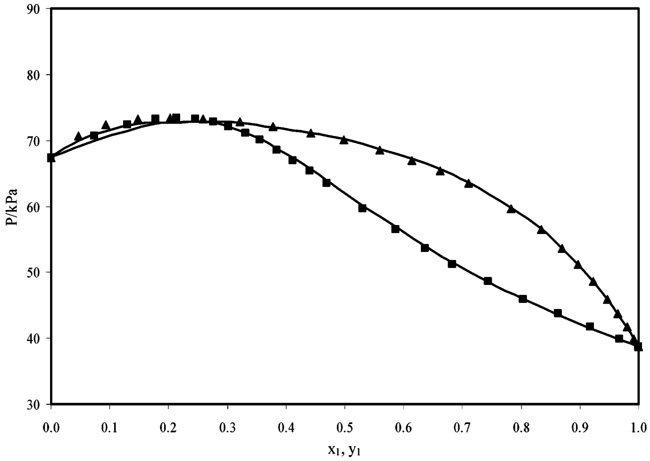

Figure 3. Temperature−composition diagram for the 2-propanol (1) + 2-ethoxy-2-methylpropane (2) system at 333 K: ▲, x_1 from data; ■, y_1 from data; −, x_1, y_1 from the Wilson model.

$$x_1 = \frac{\dfrac{A_1F_1}{A_2F_2}}{1 + \dfrac{A_1F_1}{A_2F_2}} \tag{2}$$

Procedure. Pure component 1 was introduced into the circulation still, and its vapor pressure was measured. Then component 2 was introduced into the equilibrium still. It took approximately (15 to 30) min to achieve constant boiling temperature when the differences in the boiling points of the pure components were large. The temperature was held constant for approximately 35 min to guarantee the steady-state condition before sampling. Approximately 1 mL of toluene was added to the 2-mL autosampler vials before sampling was carried out. The samples from the liquid phase and from the vapor condensate were taken with a 1-mL Hamilton sample lock syringe. The syringe was flushed with 0.1 to 0.2 mL of sample before a 0.4- to 0.5-mL sample was taken and injected into the cooled 2-mL autosampler vial.

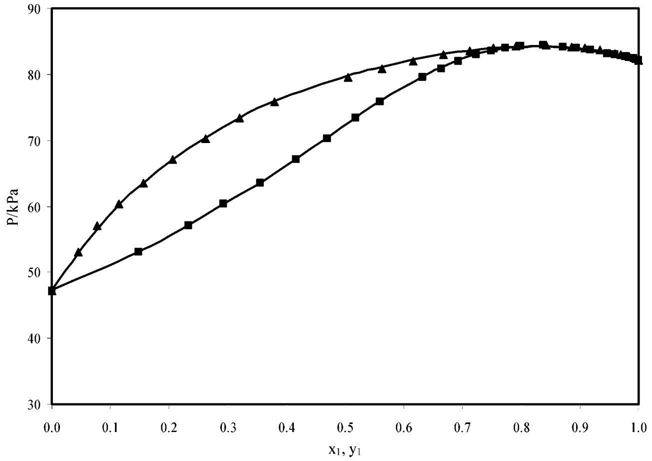

Figure 4. Temperature−composition diagram for the 2-propanone (1) + 2-ethoxy-2-methylpropane (2) system at 323 K: ▲, x_1 from data; ■, y_1 from data; −, x_1, y_1 from the Wilson model.

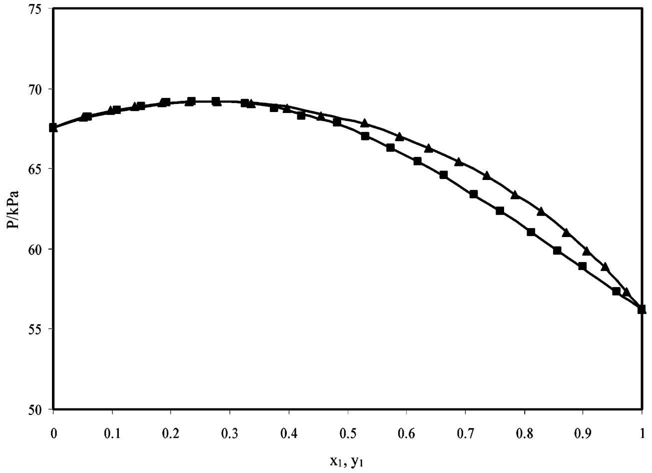

Figure 5. Temperature−composition diagram for the ethyl ethanoate (1) + 2-ethoxy-2-methylpropane (2) system at 333 K: ▲, x_1 from data; ■, y_1 from data; −, x_1, y_1 from the Wilson model.

Results and Discussion

The temperature and vapor pressure of pure components are presented in Figure 2, and 2-ethoxy-2-methylpropane vapor pressure data measured in this work are presented in Table 1. The measured isothermal equilibrium data and calculated activity coefficients are reported in Tables 2 to 4 and shown in Figures 3 to 6. Three systems exhibit positive deviations from Raoult's law. Azeotropic data were determined graphically from the measured value. Azeotropic behavior with a minimum boiling temperature was observed for the 2-propanol (1) + 2-ethoxy-2-methylpropane (2) ($T = 333$ K, $P = 73.3$ kPa, $x_1 = 0.230$), 2-propanone (1) + 2-ethoxy-2-methylpropane (2) ($T = 323$ K, $P = 84.35$ kPa, $x_1 = 0.821$), and ethyl ethanoate (1) + 2-ethoxy-2-methylpropane (2) ($T = 333$ K, $P = 69.20$ kPa, $x_1 = 0.271$) systems, respectively. The activity coefficients γ_i were calculated from the equation

$$y_iP\phi_i = \gamma_i x_i P_{\mathrm{vp}i}\phi_i^{\mathrm{s}} \exp\int_{P_{\mathrm{vp}i}}^{P} \frac{V_{\mathrm{L},i}}{RT}\,\mathrm{d}P \tag{3}$$

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

Table 5. Physical Properties of the Pure Components[a]

component	2-propanol	2-propanoney	ethyl ethanoate	2-ethoxy-2-methylpropane
T_c/K	508.31 ± 5^b	508.20 ± 5^b	523.30 ± 5^b	509.4^d
P_c/MPa	4.764 ± 0.14^b	4.7015 ± 0.1^{b}4	3.8800 ± 0.12^b	2.934^d
ω	0.6689^b	0.3064^b	0.3664^b	0.3222^d
v_i/cm^3 × mol^{-1}	76.784 ± 0.15^b	73.931 ± 0.15^b	98.594 ± 0.9^b	138.967^e
A	9.81865^c	7.74439^c	7.53946^c	6.47833^c
B	3635.460^c	2940.012^c	2930.248^c	2455.647^c
C	−55.0971^c	−36.3209^c	−52.0051^c	−65.5778^c
T_{min}/K	332.04^c	318.55^c	329.32^c	312.49^c
T_{max}/K	355.11^c	345.77^c	349.95^c	345.77^c

[a] Critical temperature (T_c), critical pressure (P_c), acentric factor (ω), Liquid molar volume (v_i), pure-component vapor pressure equation parameters (A, B, C) for the Antoine equation. See eq 4 for dimensions and details. Vapor pressure data measured; recommended temperature range of the vapor pressure correlation (T_{min}), (T_{max}). [b] Daubert and Danner.[11] [c] Measured data. [d] Wilson et al.[12] [e] Domańska.[13]

Table 6. Results of the Consistency Tests and Wilson Interaction Parameters for 2-Propanol + 2-Ethoxy-2-methylpropane (System 1) at 333 K; 2-Propanone + 2-Ethoxy-2-methylpropane (System 2) at 323 K; and Ethyl Ethanoate + 2-Ethoxy-2-methylpropane (System 3) at 333 K

binary pair	integral test	infinite dilution test	point test	$\lambda_{12}-\lambda_{11}$[a]	$\lambda_{21}-\lambda_{22}$[a]
system 1	D = 1.3%	16.1% (x(1) = 0)	$\lvert\Delta y_{ave}\rvert$ = 0.002	3904.3 ± 141.09	−352.9 ± 111.60
		−8.1% (x(1) = 1)	$\lvert\Delta P_{ave}\rvert$ = 0.26 kPa		
system 2	D = 0.7%	−5.1% (x(1) = 0)	$\lvert\Delta y_{ave}\rvert$ = 0.002	2826.9 ± 96.96	−368.0 ± 99.25
		−4.9% (x(1) = 1)	$\lvert\Delta P_{ave}\rvert$ = 0.13 kPa		
system 3	D = 3.5%	−4.6% (x(1) = 0)	$\lvert\Delta y_{ave}\rvert$ = 0.001	1093.6 ± 44.42	19.1 ± 51.98
		5.4% (x(1) = 1)	$\lvert\Delta P_{ave}\rvert$ = 0.03 kPa		

[a] In units of J·mol^{-1}; uncertainty at the 95% confidence limit.

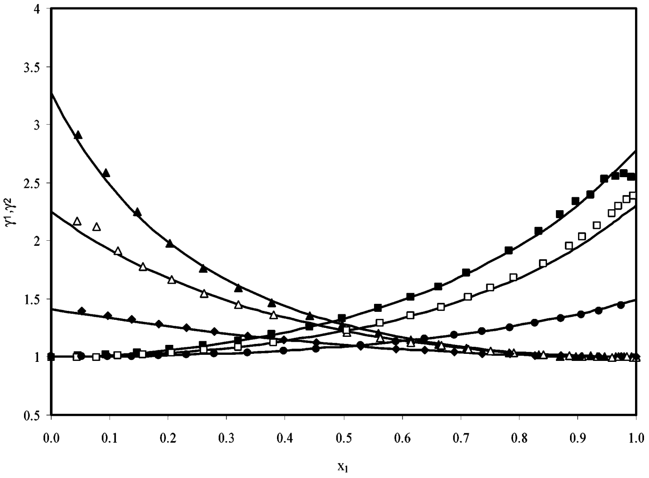

Figure 6. Activity coefficient−composition diagram for the 2-propanol (1) + 2-ethoxy-2-methylpropane (2) system at 333 K: ▲, γ_1 from data; ■, γ_2 from data; −, γ_1, γ_2 from the Wilson model. activity coefficient−composition diagram for the 2-propanone (1) + 2-ethoxy-2-methylpropane (2) system at 323 K: △, γ_1 from data; □, γ_2 from data; −, γ_1, γ_2 from the Wilson model. activity coefficient−composition diagram for the ethyl ethanoate (1) + 2-ethoxy-2-methylpropane (2) system at 333 K: ◆, γ_1 from data; ●, γ_2 from data; −, γ_1, γ_2 from the Wilson model.

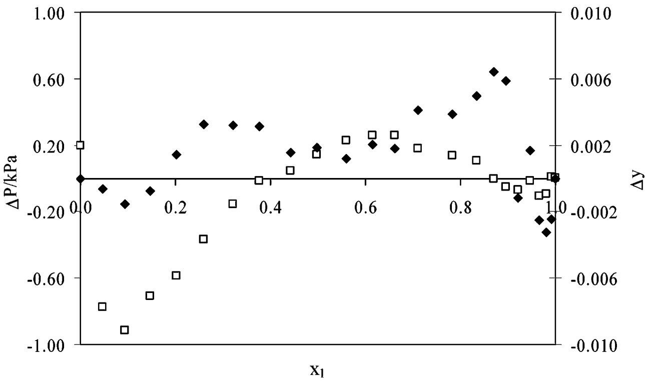

Figure 7. Point test for the 2-propanol (1) + 2-ethoxy-2-methylpropane (2) system at 333 K: ◆, Δy; □, ΔP.

fugacity coefficient of component i in the vapor phase, x_i is the mole 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, $v_{L,i}$ is the molar volume of component i in the liquid phase at the system temperature, T is temperature in Kelvin, and R is the universal gas constant (8.31441 J·K^{-1}·mol^{-1}).

The Soave−Redlich−Kwong equation of state with quadratic mixing rules in the attractive parameter and linear in covolume was used for the vapor-phase calculation.[6] The liquid phase was modeled with the Wilson equation.[7] The critical temperature, critical pressure, acentric factor, and liquid molar volume for each component needed in the calculation are presented in Table 5. The vapor pressures of the pure substances were calculated from an Antoine-type equation,

$$P/\mathrm{MPa} = \exp\left(A - \frac{B}{(T/\mathrm{K} + C)}\right) \qquad (4)$$

In this work, VLE measurements of 2-propanol + 2-ethoxy-2-methylpropane and ethyl ethanoate + 2-ethoxy-2-methylpropane were made near the lower limit of the measured pure-component vapor pressure of 2-propanol and ethyl ethanoate. The extrapolation of VLE to lower temperature required the extrapolation of the vapor pressure of the pure component . The extrapolation capability of the Antoine parameters optimized in this work was checked against the Antoine parameters reported in the literature. The ex-

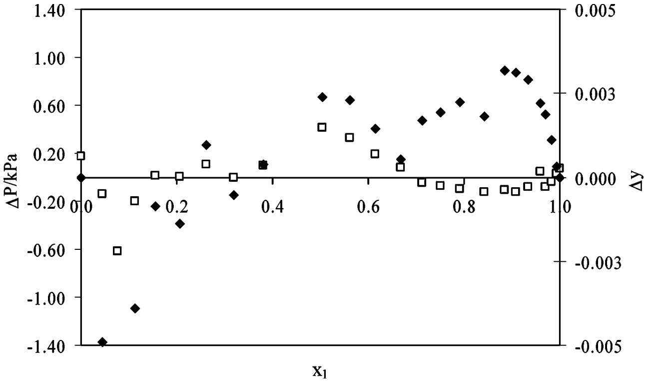

Figure 8. Point test for the 2-propanone (1) + 2-ethoxy-2-methylpropane (2) system at 323 K: ◆, Δy; □, ΔP.

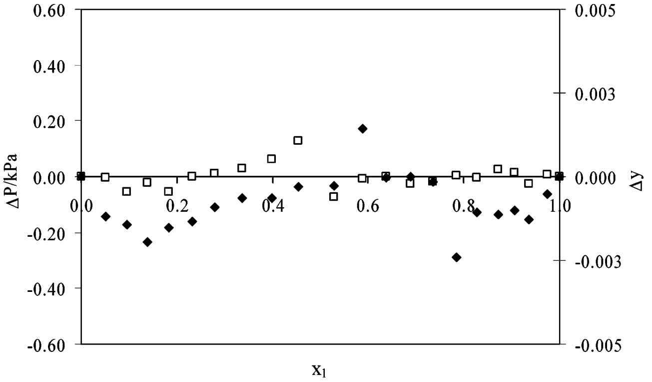

Figure 9. Point test for the ethyl ethanoate (1) + 2-ethoxy-2-methylpropane (2) system at 333 K: ◆, Δy; □, ΔP.

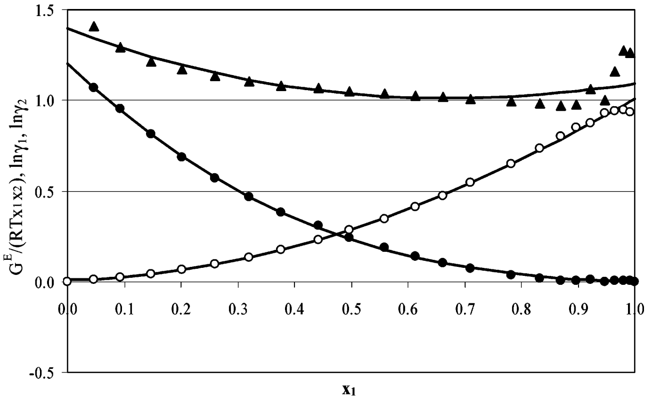

Figure 10. Infinite dilution test for the 2-propanol (1) + 2-ethoxy-2-methylpropane (2) system at 333 K: ▲, $G^E/(RTx_1x_2)$; ●, ln γ_1; ○, ln γ_2.

trapolation did not show a significant difference as presented in Figure 2. The parameters optimized in this work with the recommended temperature range of the vapor pressure equations are also presented in Table 5.

The objective function,[8] OF, used to fit the Wilson equation parameters is given by eq 3, where N is the number of points used in the fit.

$$\mathrm{OF} = \frac{1}{N}\sum_{i=1}^{N}\frac{|P_{\mathrm{model}} - P_{\mathrm{meas}}|}{P_{\mathrm{meas}}} \tag{5}$$

The parameters of the Wilson model[7] are presented in Table 6 together with their uncertainties at the 95% confidence limit. Comparisons of the experimental points and the fitted Wilson model are given in Figures 3 to 6. Good agreement between experiment and the model is achieved.

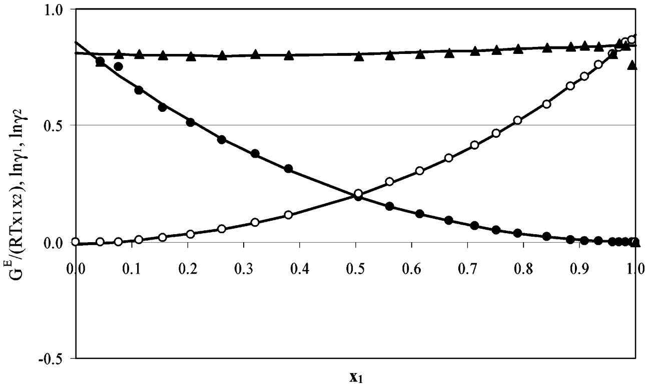

Figure 11. Infinite dilution test for the 2-propanone (1) + 2-ethoxy-2-methylpropane (2) system at 323 K: ▲, $G^E/(RTx_1x_2)$; ●, ln γ_1; ○, ln γ_2.

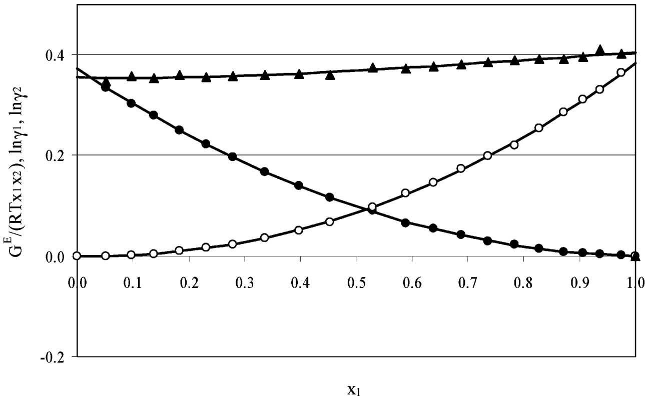

Figure 12. Infinite dilution test for the ethyl ethanoate (1) + 2-ethoxy-2-methylpropane (2) system at 333 K: ▲, $G^E/(RTx_1x_2)$; ●, ln γ_1; ○, ln γ_2.

The results of the integral test,[9] the point test[9] (Figures 7−9), and the infinite dilution test[10] (Figures 10−12) are presented in Table 5. These data sets satisfy the consistency criteria of all three tests. In the point test, the data set is considered to be consistent if the average deviations between the measured and calculated mole fractions of the vapor phase are smaller than 0.01. This is shown in Table 6 and Figures 7−9.

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