Vapor−Liquid Equilibria in the Binary and Ternary Systems Composed of 2-Methylpentane, 3-Methyl-2-butanone and 3-Methyl-2-butanol

Stepan Psutka and Ivan Wichterle*

Institute of Chemical Process Fundamentals, Academy of Sciences of the Czech Republic, Rozvojová 135,
165 02 Praha 6, Czech Republic

Vapor−liquid equilibrium data in the three binary 2-methylpentane + 3-methyl-2-butanone, 2-methylpentane + 3-methyl-2-butanol, and 3-methyl-2-butanone + 3-methyl-2-butanol systems and in the ternary 2-methylpentane + 3-methyl-2-butanone + 3-methyl-2-butanol system are reported. The data were measured isothermally at (330.00 and 340.00) K covering the pressure range (9 to 100) kPa. The binary vapor−liquid equilibrium data were correlated using the Wilson, NRTL, and Redlich−Kister equations; resulting parameters were then used for calculation of phase behavior in the ternary system and for subsequent comparison with experimental data.

Introduction

The paper reports phase equilibria data for mixtures of a distinct group of organic compounds as part of an ongoing project. Vapor−liquid equilibria are determined in systems containing compounds with a common structural group to collect data for possible upgrading of the UNIFAC prediction method. Within the series of papers, the systems of components having a common alkyl group (isopropyl), namely, 2-propanol + diisopropyl ether + 2,2,4-trimethylpentane,[1] 2-propanol + diisopropyl ether + 1-methoxy-2-propanol,[2] and propanol + diisopropyl ether + 4-methyl-2-pentanone,[3] have already been investigated. Every compound studied in this paper contains an isopropyl group on one end of molecule while on the other end is a different group, namely, an alkyl, hydroxyl, or ketonic group. The new data were measured at the two constant temperatures, (330.00 and 340.00) K, to be consistent with the three previous papers.

Experimental Section

Apparatus and Procedure. Experimental vapor−liquid equilibrium data were measured in an all glass circulation still chargeable with 150 mL of liquid phase; essentially it was the Dvorak−Boublik type with modifications described in detail elsewhere.[4] The pressure was measured indirectly via the boiling point of water in an ebulliometer connected in parallel to the still; the relative accuracy is ±0.1 % of the measured value. The equilibrium temperature was determined with the digital thermometer S1220 (Systemteknik, Sweden) calibrated against a Pt-resistance thermometer traceable to the NBS (Washington, DC); the absolute accuracy of temperature measurement (on ITS-90 scale) is estimated as ±0.02 K. Liquid-phase and vapor-phase compositions in all systems were analyzed using a gas chromatograph HP5890 (Hewlett-Packard) with HP-5 capillary column and flame ionization detection. Calibration was based on 10 mixtures covering the whole concentration range, prepared synthetically by weighing. Estimated accuracy of composition measurement is better than ±0.001 mol fraction. Densities were measured with a vibrating tube densimeter DMA 58 (A. Paar, Austria).

Materials. 2-Methylpentane ≥99 % (Sigma-Aldrich) was used as received; however, it was stored over a 4A molecular sieve to remove traces of water. Purity determined by GC was 99.83 %. Density at 298.15 K is 0.64846 $g\cdot cm^{-3}$ (literature:[5] 0.64852 $g\cdot cm^{-3}$); Refractive index n_D^{25} is 1.36877 (literature:[5] 1.36873).

3-Methyl-2-butanone (Fluka), puriss. grade, material of stated purity ≥98.5 %, was used without further purification. Molecular sieve 4A was used to remove water content. Purity was tested by GC: 99.68 %. Density at 298.15 K is 0.79955 $g\cdot cm^{-3}$ (literature:[5,6] 0.7982, 0.8061 $g\cdot cm^{-3}$, respectively); refractive index n_D^{25} is 1.38620 (literature:[6] 1.38599).

3-Methyl-2-butanol (Fluka) purum grade, declared purity ≥98.0 %, was once fractionally distilled and then stored over a 4A molecular sieve. The purity determined by GC was 99.14 %. Density at 298.15 K is 0.81342 $g\cdot cm^{-3}$ (literature: 0.8137[5] $g\cdot cm^{-3}$); refractive index n_D^{25} is 1.40700 (literature:[5] 1.4075).

Results

At first, vapor pressures of pure 3-methyl-2-butanone and 3-methyl-2-butanol were measured in the same experimental setup. The experimental data are summarized in Table 1; they were correlated by the Antoine equation with use of the maximum likelihood method. The standard deviations necessary for calculation were estimated as 0.01 K for temperature and 0.05 % of the value for pressure. The resulting equation with evaluated parameters is $\log(P/\mathrm{kPa}) = 6.114485 - 1279.340/(T/\mathrm{K} - 56.178)$ for 3-methyl-2-butanone, and $\log(P/\mathrm{kPa}) = 6.059153 - 1099.366/(T/\mathrm{K} - 113.938)$ for 3-methyl-2-butanol. The deviations between correlated and measured data are provided in Table 1.

The direct experimental $x-y-P$ values for the three binary systems are given in Table 2. The data were correlated using the Wilson, NRTL, and fourth-order Redlich−Kister equation. Vapor-phase imperfection and

---

* Corresponding author. E-mail: wi@icpf.cas.cz.

10.1021/je050062a CCC: $30.25 © 2005 American Chemical Society
Published on Web 06/18/2005

Table 1. Vapor Pressure of 3-Methyl-2-butanone and 3-Methyl-2-butanol[a]

3-methyl-2-butanone				3-methyl-2-butanol			
T/K	P/kPa	ΔT/K	ΔP/kPa	T/K	P/kPa	ΔT/K	ΔP/kPa
310.446	12.099	−0.006	0.004	323.609	6.527	−0.026	0.008
318.084	16.984	0.006	−0.006	329.800	9.280	0.030	−0.013
324.323	22.058	0.004	−0.005	333.309	11.164	0.003	−0.001
328.847	26.459	0.000	0.000	336.517	13.194	0.010	−0.007
333.485	31.699	0.000	0.000	340.668	16.230	−0.001	0.001
337.184	36.453	−0.001	0.002	346.128	21.094	−0.005	0.006
340.264	40.837	−0.002	0.005	354.076	30.238	−0.012	0.021
346.230	50.544	−0.002	0.007	360.745	40.248	−0.001	0.003
348.872	55.399	−0.002	0.006	365.975	49.794	−0.001	0.004
353.570	64.947	−0.001	0.006	370.472	59.385	0.000	0.001
357.905	74.899	0.001	−0.006	374.441	69.016	−0.001	0.003
361.862	84.971	−0.001	0.006	380.988	87.649	0.007	−0.041
365.360	94.785	0.002	−0.013	382.587	92.609	−0.007	0.041
mean deviation		0.002	0.005			0.008	0.013
root-mean-square deviation		0.003	0.006			0.012	0.020
standard deviation		0.003	0.007			0.014	0.022

[a] Δ = calculated − experimental.

Table 2. Vapor−Liquid Equilibrium Experimental Data in Binary Systems

T = 330.00 K						T = 340.00 K					
x_1[a]	y_1[a]	P/kPa[a]	x_1[a]	y_1[a]	P/kPa[a]	x_1[b]	y_1[b]	P/kPa[b]	x_1[b]	y_1[b]	P/kPa[b]
2-Methylpentane (1) + 3-Methyl-2-butanone (2)											
0.0000	0.0000	27.69	0.2603	0.6395	61.79	0.0000	0.0000	40.45	0.2896	0.6247	86.05
0.0041	0.0313	28.60	0.3541	0.6885	67.29	0.0047	0.0322	41.80	0.3575	0.6764	93.40
0.0132	0.0665	30.24	0.4331	0.7322	72.56	0.0145	0.0938	44.26	0.4294	0.7175	100.09
0.0268	0.1678	32.83	0.4898	0.7559	75.20	0.0297	0.1687	47.88	0.4788	0.7453	103.71
0.0476	0.2651	36.44	0.5672	0.7861	78.65	0.0541	0.2647	52.97	0.5556	0.7759	108.33
0.0758	0.3578	40.73	0.6072	0.8104	81.94	0.0827	0.3536	58.64	0.6169	0.7860	111.65
0.1020	0.4433	45.59	0.6984	0.8394	85.28	0.1186	0.4287	65.16	0.6764	0.8157	114.92
0.1505	0.5215	50.63	1.0000	1.0000	90.76	0.1581	0.5041	71.44	1.0000	1.0000	124.32[c]
0.1977	0.5753	55.91				0.2212	0.5641	78.32			
2-Methylpentane (1) + 3-Methyl-2-butanol (2)											
0.0000	0.0000	9.35	0.6976	0.9339	81.32	0.0000	0.0000	15.70	0.4562	0.8827	95.23
0.0675	0.6607	25.86	0.7945	0.9454	84.99	0.0345	0.4463	27.31	0.5664	0.9055	104.78
0.1504	0.7954	41.15	0.8767	0.9567	87.53	0.0863	0.6564	42.12	0.6631	0.9206	111.62
0.2756	0.8698	57.91	0.9370	0.9694	89.38	0.1673	0.7744	61.08	1.0000	1.0000	124.32[c]
0.4325	0.9032	68.93	0.9791	0.9855	90.52	0.3177	0.8476	81.46			
0.5710	0.9209	76.25	1.0000	1.0000	90.76						
3-Methyl-2-butanone (1) + 3-Methyl-2-butanol (2)											
0.0000	0.0000	9.35	0.5080	0.7511	20.00	0.0000	0.0000	15.70	0.5198	0.7325	30.23
0.0107	0.0387	9.67	0.5826	0.7965	21.28	0.0117	0.0367	16.16	0.5935	0.7804	31.87
0.0283	0.0983	10.11	0.6507	0.8334	22.36	0.0315	0.0930	16.81	0.6580	0.8191	33.29
0.0538	0.1760	10.76	0.7112	0.8636	23.28	0.0603	0.1668	17.74	0.7158	0.8532	34.52
0.0881	0.2622	11.59	0.7616	0.8892	24.06	0.0974	0.2496	18.96	0.7666	0.8802	35.58
0.1307	0.3525	12.61	0.8085	0.9117	24.79	0.1424	0.3325	20.35	0.8119	0.9043	36.53
0.1818	0.4381	13.77	0.8482	0.9299	25.34	0.1921	0.4163	21.87	0.8508	0.9240	37.30
0.2366	0.5159	14.96	0.8828	0.9459	25.87	0.2514	0.4924	23.49	0.8840	0.9418	38.00
0.2953	0.5833	16.17	0.9111	0.9591	26.31	0.3112	0.5584	25.11	0.9128	0.9561	38.58
0.3716	0.6521	17.66	0.9498	0.9769	26.92	0.3852	0.6249	26.99	0.9506	0.9752	39.44
0.4287	0.6956	18.61	1.0000	1.0000	27.69	0.4381	0.6754	28.35	1.0000	1.0000	40.45

[a] T = 330.00 K. [b] T = 340.00 K. [c] Calculated from the Antoine equation.

variation of the Gibbs energy of the pure liquid components with pressure were accounted for in terms of the second virial coefficients and the molar volumes under saturation pressure estimated by the Hayden and O'Connell method[7] and the Hougen and Watson method,[8] respectively. The experimental vapor pressures of pure components were calculated using the Antoine equation (for 3-methyl-2-butanone and 3-methyl-2-butanol, see above) and for 2-methylpentane from the equation[9] $\log (P/\text{kPa}) = 5.99329 - 1151.401/(T/\text{K} - 44.67)$ due to the fact that its vapor pressure is beyond the experimental conditions. The adjustable parameters for binary systems were evaluated with use of the program based on the maximum likelihood procedure[10] and are presented in Tables 3 to 5 together with resulting average absolute deviations for all variables (x, y, P, T). The standard deviations necessary for computation input were estimated as 0.003 for composition of phases, 0.02 K for temperature, and 0.1 % of measured value for pressure. The experimental data are illustrated in Figures 1 to 3 as $x-y-P$ plots. Solid lines represent the smoothed values based on optimized Wilson equation parameters.

Table 3. Parameters of the Wilson Equation and Evaluated Average Absolute Deviations

T	$(\lambda_{12} - \lambda_{11})$	$(\lambda_{21} - \lambda_{22})$			ΔP	ΔT
K	J·mol^{-1}	J·mol^{-1}	Δx	Δy	kPa	K
2-Methylpentane (1) + 3-Methyl-2-butanone (2)						
330.00	343.022	2904.16	0.0069	0.0055	0.040	0.05
340.00	211.547	2931.22	0.0040	0.0058	0.020	0.02
2-Methylpentane (1) + 3-Methyl-2-butanol (2)						
330.00	383.480	5003.26	0.0073	0.0021	0.052	0.05
340.00	252.147	4919.29	0.0104	0.0022	0.049	0.04
3-Methyl-2-butanone (1) + 3-Methyl-2-butanol (2)						
330.00	177.033	688.301	0.0007	0.0009	0.001	0.01
340.00	253.686	493.823	0.0007	0.0009	0.002	0.01

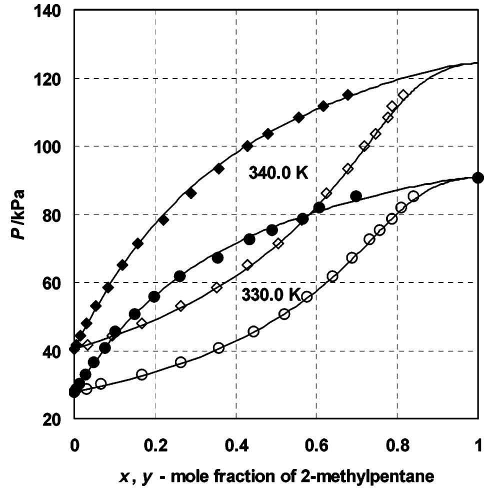

Figure 1. Isothermal vapor−liquid equilibrium in the 2-methylpentane + 3-methyl-2-butanone system; $P-x-y$ diagram: (○, ◇), experimental data for vapor phase, y; (●, ◆), experimental data for liquid phase, x; (—), Wilson correlation.

Table 4. Parameters of the NRTL Equation and Evaluated Average Absolute Deviations

T	$(g_{12} - g_{22})$	$(g_{21} - g_{11})$				ΔP	ΔT
K	J·mol^{-1}	J·mol^{-1}	α_{ij}	Δx	Δy	kPa	K
2-Methylpentane (1) + 3-Methyl-2-butanone (2)							
330.00	825.330	1021.57	−2.7716	0.0050	0.0048	0.020	0.03
340.00	827.939	1080.00	−2.2327	0.0032	0.0047	0.012	0.01
2-Methylpentane (1) + 3-Methyl-2-butanol (2)							
330.00	1006.32	1614.93	−1.6889	0.0056	0.0019	0.037	0.04
340.00	957.171	1489.55	−2.1563	0.0039	0.0028	0.015	0.02
3-Methyl-2-butanone (1) + 3-Methyl-2-butanol (2)							
330.00	859.947	−1.7205	0.2833	0.0007	0.0009	0.001	0.01
340.00	637.661	98.5838	0.2146	0.0007	0.0009	0.002	0.01

Table 5. Parameters of the Redlich−Kister Equation and Evaluated Average Absolute Deviations

T/K	b	c	d	Δx	Δy	ΔP/kPa	ΔT/K
2-Methylpentane (1) + 3-Methyl-2-butanone (2)							
330.00	0.9691	0.0986	0.1931	0.0052	0.0047	0.021	0.03
340.00	0.9208	0.0989	0.1262	0.0031	0.0047	0.011	0.01
2-Methylpentane (1) + 3-Methyl-2-butanol (2)							
330.00	1.3389	0.2738	0.2349	0.0085	0.0022	0.058	0.06
340.00	1.2556	0.2680	0.2639	0.0058	0.0029	0.025	0.02
3-Methyl-2-butanone (1) + 3-Methyl-2-butanol (2)							
330.00	0.3001	0.0143	−0.0079	0.0007	0.0008	0.001	0.01
340.00	0.2559	0.0068	−0.0096	0.0007	0.0008	0.001	0.01

The experimental data for the ternary system were determined at the same isothermal conditions as the binary systems and are presented in Table 6. Overall compositions of mixtures in the equilibrium still were formed approximately by subsequent addition of 3-methyl-2-butanol to several initial 2-methylpentane + 3-methyl-2-butanone mixtures; then, the region of ternary compositions was regularly covered; in total 64 experimental points were measured. No azeotropes were found in the binary systems or in the ternary system.

The parameters obtained from the correlation of the three binary VLE data were exploited for prediction of ternary data using both the Wilson and NRTL equations expressing the activity coefficient, γ_i (i = 1, 2, 3) as

$$\ln \gamma_i = -\ln \left(\sum_{s=1}^{3} x_s A_{is}\right) + 1 - \sum_{r=1}^{3} \frac{x_r A_{ri}}{\sum_{s=1}^{3} x_s A_{rs}} \tag{1}$$

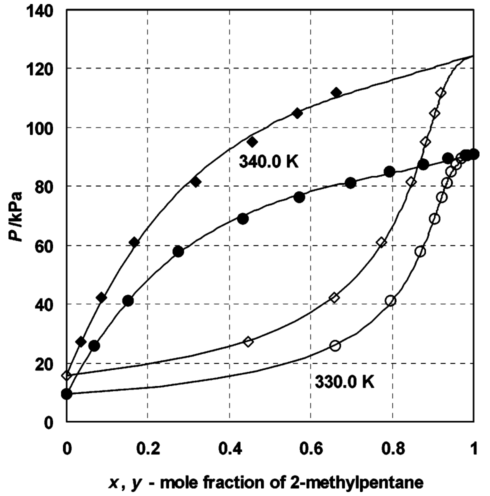

Figure 2. Isothermal vapor−liquid equilibrium in the 2-methylpentane + 3-methyl-2-butanol; $P-x-y$ diagram: (○, ◇), experimental data for vapor phase, y; (●, ◆), experimental data for liquid phase, x; (—), Wilson correlation.

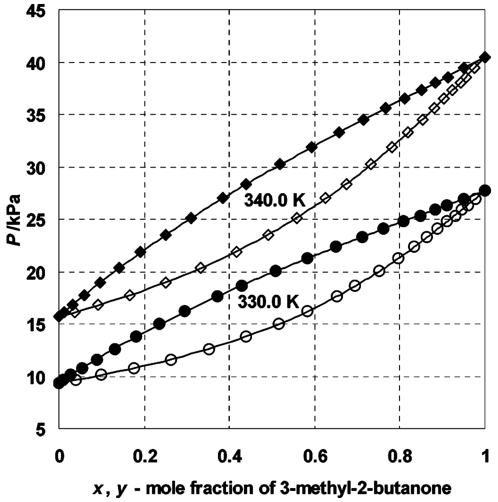

Figure 3. Isothermal vapor−liquid equilibrium in the 3-methyl-2-butanone + 3-methyl-2-butanol system; $P-x-y$ diagram: (○, ◇), experimental data for vapor phase, y; (●, ◆), experimental data for liquid phase, x; (—), Wilson correlation.

where $A_{ij} = (V_j/V_i) \exp[-(\lambda_{ij} - \lambda_{ii})/RT]$ and

$$\ln \gamma_i = \frac{\sum_{r=1}^{3} \tau_{ri} G_{ri} x_r}{\sum_{s=1}^{3} G_{si} x_s} + \sum_{r=1}^{3} \frac{x_r G_{ir}}{\sum_{s=1}^{3} G_{sr} x_s} \left(\tau_{ir} - \frac{\sum_{t=1}^{3} \tau_{tr} G_{tr} x_t}{\sum_{s=1}^{3} G_{sr} x_s} \right) \tag{2}$$

where $G_{ij} = \exp[-\alpha_{ij}\tau_{ij}]$; $\tau_{ij} = (g_{ij} - g_{jj})/RT$; $\tau_{ii} = 0$; $\alpha_{ij} = \alpha_{ji}$; and $G_{ii} = 1$, respectively. The necessary molar volumes were estimated with use of the method.[8] The parameters $\lambda_{ij} - \lambda_{ii}$ are listed in Table 3 while $g_{ij} - g_{jj}$ and α_{ij} can be found in Table 4.

The computation was carried out by means of the method published in ref 10 enabling the calculation of the "closest" solution by minimization of standard deviations of all involved variables (temperature, pressure, vapor, and liquid compositions). Resulting absolute deviations are averaged and summarized in Table 7.

Discussion and Conclusions

No published vapor−liquid equilibrium data for the systems under study were found in the bibliography

Table 6. Vapor−Liquid Equilibrium Experimental Data in the Ternary 2-Methylpentane (1) + 3-Methyl-2-Butanone (2) + 3-Methyl-2-Butanol (3) System

x_1	x_2	y_1	y_2	P/kPa	x_1	x_2	y_1	y_2	P/kPa	x_1	x_2	y_1	y_2	P/kPa
T = 330.00 K														
0.3533	0.5866	0.7077	0.2788	67.36	0.4792	0.3194	0.8075	0.1514	73.70	0.0660	0.7300	0.3693	0.5664	36.27
0.2748	0.5981	0.6970	0.2771	64.05	0.4028	0.3011	0.7906	0.1505	68.92	0.0417	0.6501	0.2962	0.5966	30.90
0.2574	0.5470	0.6776	0.2800	59.36	0.3098	0.2802	0.7748	0.1480	62.05	0.0225	0.5542	0.2087	0.6232	25.84
0.1865	0.5186	0.6505	0.2868	53.01	0.1898	0.2573	0.7363	0.1566	52.20	0.0125	0.4492	0.1351	0.6197	21.78
0.1347	0.4678	0.5956	0.3102	44.68	0.1210	0.2175	0.6621	0.1760	40.08	0.0056	0.3432	0.0712	0.5852	18.29
0.0800	0.4079	0.4900	0.3591	35.15	0.0534	0.1717	0.4671	0.2301	26.22	0.0030	0.2585	0.0460	0.5174	16.01
0.0369	0.3321	0.3441	0.4119	25.44	0.0043	0.1132	0.0798	0.2933	13.29	0.0012	0.1846	0.0245	0.4394	14.18
0.0118	0.2495	0.2105	0.4280	19.40	0.1242	0.8551	0.4970	0.4975	47.85	0.2183	0.0972	0.7895	0.0676	49.57
0.0047	0.1832	0.0752	0.4096	14.91	0.1156	0.8268	0.4714	0.5119	45.34	0.1062	0.0799	0.6844	0.0815	32.10
0.0011	0.1267	0.0179	0.3362	12.79	0.0897	0.7956	0.4463	0.5217	42.37	0.0477	0.0587	0.4682	0.0967	21.84
0.5997	0.3390	0.8161	0.1684	79.74	0.0914	0.7944	0.4301	0.5366	41.29	0.0025	0.0330	0.0435	0.1043	10.46
0.5508	0.3291	0.8108	0.1610	77.18										
T = 340.00 K														
0.3643	0.5771	0.6938	0.2907	93.33	0.5400	0.3359	0.8009	0.1669	106.27	0.1038	0.7848	0.4339	0.5303	61.04
0.3299	0.5553	0.6841	0.2865	88.95	0.4831	0.3177	0.7949	0.1572	101.50	0.0983	0.7895	0.4195	0.5437	59.28
0.2699	0.5392	0.6636	0.2880	82.89	0.4124	0.2973	0.7802	0.1525	94.96	0.0721	0.7278	0.3654	0.5642	52.62
0.2089	0.5074	0.6331	0.2942	74.78	0.3397	0.2720	0.7590	0.1505	86.08	0.0475	0.6508	0.2972	0.5865	45.49
0.1475	0.4641	0.5865	0.3079	64.33	0.2218	0.2515	0.7225	0.1550	73.85	0.0278	0.5594	0.2165	0.6038	38.74
0.0906	0.4080	0.4982	0.3404	51.85	0.1351	0.2186	0.6475	0.1710	58.40	0.0152	0.4579	0.1430	0.5950	33.07
0.0438	0.3380	0.3625	0.3825	39.51	0.0632	0.1761	0.4965	0.2042	40.51	0.0070	0.3564	0.0779	0.5579	28.09
0.0233	0.2666	0.2416	0.3933	31.06	0.0321	0.1343	0.3548	0.2119	30.17	0.0038	0.2711	0.0501	0.4915	25.02
0.0109	0.1990	0.1380	0.3696	25.32	0.1369	0.8429	0.4795	0.5131	67.75	0.0020	0.1991	0.0297	0.4130	22.49
0.0027	0.1407	0.0429	0.3175	21.08	0.1218	0.8209	0.4695	0.5130	64.62	0.2245	0.0971	0.7768	0.0658	71.86

Table 7. Prediction of Vapor−Liquid Equilibrium in the 2-Methylpentane (1) + 3-Methyl-2-butanone (2) + 3-Methyl-2-butanol (3) System Using the Binary Parameters of the Wilson and NRTL Equations[a]

T/K	Δx_1	Δx_2	Δx_3	Δx	Δy_1	Δy_2	Δy_3	Δy	ΔP/kPa	ΔT/K
Wilson Equation										
330.00	0.0050	0.0034	0.0039	0.0041	0.0054	0.0027	0.0040	0.0040	0.004	0.04
340.00	0.0036	0.0024	0.0025	0.0029	0.0038	0.0020	0.0026	0.0028	0.004	0.02
NRTL Equation										
330.00	0.0083	0.0044	0.0064	0.0064	0.0068	0.0039	0.0044	0.0051	0.006	0.05
340.00	0.0047	0.0026	0.0040	0.0038	0.0046	0.0029	0.0033	0.0036	0.005	0.03

[a] Δ is an absolute average deviation of calculated and experimental data.

covering the period 1888 to 2003;[11] therefore, no comparison with literature data was possible. However, the reliability of both the data and the correlation procedure is verified by the fact that the resulting standard deviations are approximately proportional to the magnitudes of uncertainties input. Generally, the inspection of deviation distribution from smoothed data confirms that there are only expectable, random and nonsystematic errors. A thermodynamic test of consistency has been carried out with use of the procedure proposed by Van Ness.[12] According to it, the consistency index was determined as equal to 1, 3, and 3 for the systems 3-methyl-2-butanone + 3-methyl-2-butanol, 2-methylpentane + 3-methyl-2-butanone, and 2-methylpentane + 3-methyl-2-butanol, respectively, on the ten-degree scale (1, excellent; 10, nonacceptable). The worse results found for the systems containing 2-methylpentane are due to the large difference in relative volatilities and, subsequently, more difficult measurement.

The experimental ternary data were compared with the data predicted using binary parameters. The absolute average deviations presented in Table 7 indicate that predicted results are better with use of the Wilson equation in comparison with the NRTL equation; generally, both results are very good. It should be pointed out that these results need not necessarily reflect the quality of data. The experimental data are most likely better because the imperfections of models also contribute to certain “worsening” of calculated values.

The parameters of the classical Redlich−Kister equation of the fourth order were also evaluated (see Table 5) since they enable more reliable extrapolation of activity coefficients to the limiting values. Nevertheless, these parameters cannot be used directly for prediction of vapor−liquid equilibrium in a multicomponent system because additional ternary parameters would be needed and had to be evaluated from ternary data beforehand.

Literature Cited

(1) Wichterle, I. Isothermal vapor−liquid equilibria in the ternary system propan-2-ol + diisopropyl ether + 2,2,4-trimethylpentane and the three binary subsystems at 330 K and 340 K. *ELDATA: Int. Electron. J. Phys.-Chem. Data* **1999**, *5*, 179−189.

(2) Psutka, S.; Wichterle, I. Isothermal vapour−liquid equilibria in the binary and ternary systems composed of 2-propanol, diisopropyl ether and 1-methoxy-2-propanol. *Fluid Phase Equilib.* **2004**, *220*, 161−165.

(3) Psutka, S.; Wichterle, I. Isothermal vapour−liquid equilibria in the binary and ternary systems composed of 2-propanol, diisopropyl ether and 4-methyl-2-pentanone. *Fluid Phase Equilib.* (MS Ref. No.: FPE-D-05-00007R1) in press.

(4) Teodorescu, M.; Aim, K.; Wichterle, I. Isothermal Vapour−Liquid Equilibria for Pentan-3-one + 1,4-Dichlorobutane, + Trichloromethane, + 1,1,1-Trichloroethane, + 1,1,2,2-Tetrachloroethane Binary Mixtures. *Fluid Phase Equilib.* **1998**, *147*, 215−228.

(5) *TRC Thermodynamic Tables—Hydrocarbons*; *TRC Thermodynamic Tables—Non-Hydrocarbons*; Thermodynamic Research Center: College Station, TX, 1999.

(6) *Beilstein Handbuch der Organischen Chemie*; Springer: Berlin, 1974; Vol. I, Suppl. V.; p 3288.

(7) Hayden, J. G.; O'Connell, J. P. A generalized method for predicting second virial coefficients. *Ind. Eng. Chem., Proc. Des. Dev.* **1975**, *14*, 209−216.

(8) Hougen, O. A.; Watson, K. M. *Chemical Process Principles*; John Wiley: New York, 1947; Part II.

(9) Boublík, T.; Fried, V.; Hála, E. *The Vapor Pressure of Pure Substances: Selected Values of the Temperature Dependence of the Vapor Pressures of Some Pure Substances in the Normal and Low-Pressure Region*; Elsevier: Amsterdam, 1984.

(10) Hála, E.; Aim, K.; Boublík, T.; Linek J.; Wichterle, I. *Vapor−Liquid Equilibrium at Normal and Reduced Pressures*; Academia: Prague, 1982 (in Czech).

(11) Wichterle, I.; Linek, J.; Wagner Z.; Kehiaian, H. V. Vapor−liquid equilibrium in mixtures and solutions. Bibliographic Database EVLM 2003; ELDATA: Paris, 2004 (CD-ROM).

(12) Van Ness, H. C. Thermodynamics in the treatment of vapor/liquid equilibrium (VLE) data. *Pure Appl. Chem.* **1995**, *67*, 859−872.

Received for review February 10, 2005. Accepted May 24, 2005. The authors acknowledge the partial support of the Grant Agency of the Czech Republic (Grant No. 104/03/1555) and of the Academy of Sciences of the Czech Republic (Project No. K4040110).

JE050062A