Liquid−Liquid Equilibria for Mixtures of Diisobutyl Ketone + an Alkanol + Water at 298.15 K

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Liquid−liquid equilibrium data are presented for mixtures of 2,6-dimethyl-4-heptanone (diisobutyl ketone) + an alkanol + water at 298.15 K. The alkanols are methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. The addition of ethanol, 2-propanol, or 2-methyl-2-propanol is found to increase the solubility of water in the diisobutyl ketone more than the other alkanols. The relative mutual solubility of methanol and ethanol is higher in the water layer than in the diisobutyl ketone layer. The converse is true for the other alkanols. Three three-parameter equations have been fitted to points on the binodal curve. The results are compared and discussed in terms of statistical consistency. The NRTL and UNIQUAC models were used to correlate the experimental results and to calculate the phase compositions of the ternary systems. The NRTL equation fitted the experimental data better than did the UNIQUAC equation, and the average root mean square deviation phase composition error was 0.013 for the NRTL model and 0.046 for the UNIQUAC model.

Introduction

A great number of industrial separation processes are concerned with liquid mixtures containing an organic phase and a water phase. In previous studies by Letcher and Sizwana (1992) and Letcher and co-workers (1986, 1989, 1990, 1992, 1993, 1994) LLE measurements were made on tertiary mixtures: heptane, *p*-xylene, benzene, toluene, *o*-*m*-xylene, mesitylene, 1-heptene, or 1-heptyne + an alkanol + water mixtures. The latest results of Wagner and Sandler (1995) also discuss toluene + ethanol + water mixtures as well as toluene or other hydrocarbons + *tert*-amyl alcohol + water mixtures at different temperatures. The alkanols in all the cited publications by Letcher refer to methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol.

In this work the LLE for 2,6-dimethyl-4-heptanone (diisobutyl ketone) + an alkanol + water mixtures has been determined for each of the C_1, C_2, C_3, and C_4 alkanols. The data have been compared with mixtures of diisopropyl ether + an alkanol + water of Letcher *et al.* (1992). The results are analyzed to establish the ability of the diisobutyl ketone to extract an alkanol from binary alkanol + water mixtures.

The binodal curve data have been summarized using a modified Hlavatý equation (Hlavatý, 1972), a β function, and a log γ function using methods previously described by Letcher *et al.* (1990). The tie lines were correlated using the NRTL model of Renon and Prausnitz (1968) and UNIQUAC model of Abrams and Prausnitz (1975).

Experimental Section

Chemicals. The alkanols were prepared according to the methods given by Furniss *et al.* (1978) and previously discussed by Letcher *et al.* (1992). The methanol, ethanol, and two propanols were purified and dried by refluxing with magnesium and iodine, followed by distillation. The four butanols were dried by addition of anhydrous potassium carbonate and purified by distillation. The diisobutyl ketone, supplied by Aldrich 99 mass % reagent, was used without further purification. The purity of each of the components was determined by GLC and was always better than 99.8 mol %. The physical properties of the reagents used in this work are listed in Table 1 together with literature values.

Procedure. The binodal curves were carried out by the titration method described by Letcher and Sizwana (1992). The tie lines were analyzed by two methods which proved to be consistent to within 5×10^{-3} mole fraction. The refractive index method of Briggs and Comings (1943) described by Letcher and Sizwana (1992) was used and supported in one case by a similar technique which involved density measurements. The densities were determined using a high-precision Anton Paar DMA (601) vibrating-tube density meter. The estimated precision of the composition of mixtures on the binodal curve was within 5×10^{-3} mole fraction and that of the tie lines was within 1×10^{-3} mole fraction. Temperature was measured with the accuracy of 0.05 K. The exact experimental data, obtained for refractive indices and densities of the studied mixtures, are reported by Redhi (1996).

Results

The composition of mixtures on the binodal curve at 298.15 K are given in Table 2, and tie-line compositions are given in Table 3 and are plotted in Figure 1.

Three equations have been fitted to the data following the work of Hlavatý (1972). The coefficients A_i relate to a modified Hlavatý equation

$$x_2 = A_1 x_A \ln x_A + A_2 x_B \ln x_B + A_3 x_A x_B \qquad (1)$$

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Table 1. Physical Properties of the Pure Components at 298.15 K; Molar Volumes, V_{mi}, Refractive Indexes, n_D, Volume and Surface Parameters, R and Q

component	V_{mi}/cm^3·mol^{-1} [a]	n_D		R[b]	Q[b]
		exp	lit.[a]		
diisobutyl ketone	177.10	1.410 80	1.410 6	6.1323	7.2163
methanol	40.70	1.326 58	1.326 52	1.8627	1.9535
ethanol	58.50	1.359 46	1.359 41	2.4952	2.6616
1-propanol	75.20	1.383 68	1.383 70	3.1277	3.3697
2-propanol	76.80	1.374 92	1.375 2	2.9605	3.3433
1-butanol	91.50	1.397 46	1.397 41	3.7602	4.0778
2-butanol	92.00	1.395 32	1.395 30	3.5930	4.0514
2-methyl-1-propanol	92.90	1.393 86	1.393 89	3.7602	4.0922
2-methyl-2-propanol	94.88	1.385 82	1.385 2	3.2195	4.0169
water	18.07	1.332 50	1.332 502 9	1.7334	2.4561

[a] Riddick *et al.* (1986). [b] Gmehling *et al.* (1993).

the coefficients B_i relate to a β function equation

$$x_2 = B_1(1 - x_A)^{B2}x_A^{B3} \tag{2}$$

and the coefficients C_i relate to a log γ equation

$$x_2 = C_1(-\ln x_A)^{C2}x_A^{C3} \tag{3}$$

where

$$x_A = (x_1 + 0.5x_2 - x_1^0)/(x_{11}^0 - x_1^0) \tag{4}$$

$$x_B = (x_{11}^0 - x_1 - 0.5x_2)/(x_{11}^0 - x_1^0) \tag{5}$$

x_1 refers to the mole fraction composition of the diisobutyl ketone, x_2 refers to the mole fraction of an alkanol, and x_{11}^0 and x_1^0 are the values of x_1 on the binodal curve which cuts the $x_2 = 0$ axis and have been used to summarize the binodal curve data. These equations have been discussed by Letcher *et al.* (1992). The coefficients B_i, and C_i are given in Table 4.

Equations 1−3 have been fitted to the binodal curves with the standard deviation σ. This is defined as

$$\sigma = [\sum[x_2(\text{calc}) - x_2(\text{exp})]^2/(n - 3)]^{1/2} \tag{6}$$

where n is the number of data points and 3 is the number of coefficients (Sen and Srivastava, 1990). The standard errors defined by Sen and Srivastava (1990) as the square root of the variance of the estimated coefficients are larger for the modified Hlavatý equation (6% to 413%) than the standard errors for the β function and the log γ equations (1% to 10%).

Discussion

The binodal curves in Figure 1a−h show that the solubility of water in diisobutyl ketone + an alkanol is very much dependent on the type of alkanol. Water is most soluble in the systems containing ethanol or 2-propanol or 2-methyl-2-propanol. Similar results were obtained by Letcher *et al.* (1992) for mixtures of diisopropyl ether with an alkanol + water. For a particular alcohol, water is less soluble in diisobutyl ketone than in diisopropyl ether; i.e. the two-phase region is larger for the ketone mixtures than for the ether mixtures.

The slope of the binodal curves for diisobutyl ketone (1) + 1-butanol, 2-butanol, or 2-methyl-1-propanol (2) + water (3) are similar; showing a skewing toward the water axis. Figure 1 shows that the area of the two-phase region for the C_4 alkanols increases in the order 2-methyl-2-propanol < 2-butanol < 1-butanol < 2-methyl-1-propanol.

The relative solubility of an alkanol in water or in diisobutyl ketone is evident from the tie lines. Methanol and ethanol are the only alkanols which are more soluble in the water than in the ketone. The C_3 alkanols are more soluble in ketone than in water with the order of solubility being 1-propanol > 2-propanol. The slopes of the tie lines presented here (Figure 1c,d) show also the big difference between 1-propanol and 2-propanol.

From the LLE data presented here we see that an increase in the concentration of C_4 alkanols results in an increase in water solubility in the organic phase and a decrease in diisobutyl ketone solubility in the aqueous phase.

The effectiveness of extraction of compound 2 by the diisobutyl ketone is given by its selectivity (ω), which is a measure of the ability of diisobutyl ketone to separate compound 2 from water:

$$\omega = \frac{\text{distribution coefficient of alkanols}}{\text{distribution coefficient of water}} = \frac{\dfrac{\text{\% compound 2 of ketone rich phase}}{\text{\% compound 2 of water rich phase}}}{\dfrac{\text{\% water of ketone rich phase}}{\text{\% water of water rich phase}}}$$

The values of selectivity for the middle of the area of measured tie lines are 3.7, 5.6, 13.3, 4.4, 336, 124, 550, and 32.6 for methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol, respectively. From these values we may conclude that diisobutyl ketone is an especially good component for the extraction of 1-butanol and 2-methyl-1-propanol.

Tie-Line Correlation

Thermodynamic models such as the nonrandom two liquid equation NRTL (Renon and Prausnitz, 1968) and the universal quasichemical equation UNIQUAC (Abrams and Prausnitz, 1975) are used to correlate the experimental data for eight ternary systems discussed here. The equations and algorithms used in the calculation of the compositions of liquid phases follow the method used by Walas (1985). The objective function $F(P)$, used to minimize the difference between the experimental and calculated concentrations is defined as

$$F(P) = \sum_{i=1}^{n} [x'_{1i} - x'_{1i}(\text{calc})(PT)]^2 + [x_{2i} - x_{2i}(\text{calc})(PT)]^2 + [x''_{1i} - x''_{1i}(\text{calc})(PT)]^2 + [x''_{2i} - x''_{2i}(\text{calc})(PT)]^2 \tag{7}$$

where P is the set of parameters vector, n is the number

Table 2. Compositions of Points on the Binodal Curve at 298.15 K for the Systems: Diisobutyl Ketone (1) + an Alkanol (2) + Water (3), Equilibrium Mole Fraction, x_1, x_2, x_3

x_1	x_2	x_3	x_1	x_2	x_3
		Methanol			
1.000	0.000	0.000	0.266	0.503	0.231
0.943	0.053	0.004	0.199	0.536	0.265
0.855	0.125	0.020	0.124	0.562	0.314
0.761	0.197	0.042	0.087	0.568	0.345
0.707	0.238	0.055	0.046	0.552	0.402
0.626	0.291	0.083	0.019	0.502	0.479
0.520	0.360	0.120	0.004	0.374	0.622
0.393	0.435	0.172	0.001	0.204	0.795
0.329	0.471	0.200	0.000	0.000	1.000
		Ethanol			
1.000	0.000	0.000	0.305	0.414	0.281
0.884	0.095	0.021	0.205	0.425	0.370
0.861	0.114	0.025	0.134	0.410	0.456
0.740	0.200	0.060	0.091	0.392	0.517
0.651	0.251	0.098	0.050	0.355	0.595
0.525	0.327	0.148	0.024	0.314	0.662
0.475	0.393	0.132	0.010	0.201	0.789
0.414	0.367	0.219	0.002	0.118	0.880
0.362	0.398	0.240	0.000	0.000	1.000
		1-Propanol			
1.000	0.000	0.000	0.210	0.440	0.350
0.919	0.071	0.010	0.176	0.438	0.386
0.866	0.119	0.015	0.108	0.407	0.485
0.782	0.189	0.029	0.064	0.363	0.573
0.687	0.255	0.058	0.047	0.336	0.617
0.575	0.326	0.099	0.014	0.217	0.769
0.509	0.361	0.130	0.002	0.102	0.896
0.377	0.412	0.211	0.001	0.064	0.935
0.266	0.438	0.296	0.000	0.000	1.000
		2-Propanol			
1.000	0.000	0.000	0.231	0.411	0.358
0.920	0.073	0.007	0.161	0.400	0.439
0.851	0.127	0.022	0.118	0.379	0.503
0.755	0.195	0.050	0.105	0.366	0.529
0.654	0.255	0.091	0.061	0.323	0.616
0.573	0.301	0.126	0.040	0.271	0.689
0.491	0.346	0.163	0.031	0.258	0.711
0.427	0.375	0.198	0.020	0.211	0.769
0.392	0.387	0.221	0.010	0.123	0.867
0.369	0.393	0.238	0.004	0.070	0.926
0.310	0.410	0.280	0.000	0.000	1.000
		1-Butanol			
1.000	0.000	0.000	0.192	0.550	0.258
0.896	0.093	0.011	0.099	0.555	0.346
0.770	0.197	0.033	0.031	0.520	0.449
0.672	0.268	0.060	0.000	0.485	0.515
0.581	0.330	0.089	0.000	0.019	0.981
0.494	0.389	0.117	0.001	0.010	0.989
0.382	0.455	0.163	0.000	0.000	1.000
0.296	0.503	0.201			
		2-Butanol			
1.000	0.000	0.000	0.190	0.504	0.306
0.940	0.055	0.005	0.122	0.495	0.383
0.825	0.155	0.020	0.047	0.441	0.512
0.676	0.270	0.054	0.000	0.322	0.678
0.589	0.330	0.081	0.000	0.054	0.946
0.470	0.402	0.128	0.003	0.035	0.962
0.396	0.438	0.166	0.000	0.000	1.000
		2-Methyl-1-propanol			
1.000	0.000	0.000	0.306	0.527	0.167
0.927	0.070	0.003	0.239	0.571	0.190
0.835	0.155	0.010	0.100	0.599	0.301
0.734	0.235	0.031	0.038	0.586	0.376
0.624	0.316	0.060	0.000	0.548	0.452
0.513	0.395	0.092	0.000	0.021	0.979
0.412	0.465	0.123	0.000	0.000	1.000
		2-Methyl-2-propanol			
1.000	0.000	0.000	0.240	0.398	0.362
0.941	0.050	0.009	0.128	0.360	0.512
0.808	0.152	0.040	0.092	0.327	0.581
0.717	0.215	0.068	0.050	0.259	0.691
0.619	0.271	0.110	0.010	0.172	0.818
0.494	0.341	0.165	0.003	0.102	0.895
0.376	0.382	0.242	0.001	0.050	0.949
0.278	0.400	0.322	0.000	0.000	1.000

Table 3. Compositions of the Conjugate Solutions, x'_1, x'_2 and x''_1, x''_2, at 298.15 K for the Systems Diisobutyl Ketone (1) + an Alkanol (2) + Water (3)

water rich		ketone rich	
x'_1	x'_2	x''_1	x''_2
Methanol			
0.002	0.224	0.886	0.100
0.004	0.376	0.811	0.158
0.021	0.509	0.711	0.232
0.075	0.565	0.583	0.319
0.169	0.549	0.508	0.369
Ethanol			
0.011	0.211	0.879	0.101
0.019	0.298	0.835	0.132
0.085	0.388	0.789	0.170
0.202	0.423	0.716	0.214
0.362	0.398	0.659	0.249
1-Propanol			
0.001	0.041	0.731	0.226
0.002	0.072	0.463	0.384
0.003	0.096	0.250	0.440
0.003	0.112	0.100	0.400
0.005	0.140	0.048	0.339
2-Propanol			
0.016	0.183	0.761	0.190
0.030	0.257	0.640	0.262
0.060	0.320	0.531	0.325
0.110	0.371	0.420	0.376
1-Butanol			
0.001	0.005	0.772	0.199
0.001	0.010	0.507	0.381
0.001	0.015	0.224	0.536
2-Butanol			
0.002	0.015	0.764	0.206
0.003	0.027	0.515	0.377
0.002	0.040	0.248	0.496
2-Methyl-1-propanol			
0.000	0.003	0.771	0.202
0.000	0.009	0.580	0.350
0.000	0.015	0.301	0.528
2-Methyl-2-propanol			
0.001	0.049	0.792	0.165
0.002	0.071	0.601	0.285
0.003	0.100	0.461	0.358
0.007	0.137	0.312	0.397
0.015	0.180	0.154	0.378

of experimental points, x'_{1i}, x'_{2i} and x'_{1i} (calc)*(PT)*, x'_{2i}(calc)*(PT)* are the experimental and calculated mole fractions of one phase and x''_{1i}, x''_{2i} and x''_{1i}(calc)*(PT)*, x''_{2i}(calc)*(PT)* are the experimental and calculated mole fractions of the respective phases.

The pure component structural parameters *R* (volume parameter) and *Q* (surface parameter) in the UNIQUAC equation were obtained from the tables of modified UNIFAC, published by Gmehling *et al.* (1993) (see Table 1).

For the NRTL model, the third nonrandomness parameter, α_{ij}, was set at a value of 0.2 or 0.3. The values of the starting parameters for binary systems with diisobutyl ketone were taken from LLE data published by Wagner and Sandler (1995) for related systems. The parameters calculated in this way are shown in Table 5. A comparison of the experimental and calculated tie lines by NRTL is shown for each system in Figure 1. Good results obtained for the systems containing 1-butanol, 2-butanol, and 2-methyl-1-propanol may be a result of statistical inconsistency since the number of experimental tie lines (only three tie lines each) is very close to the total number of fitted parameters for each system. The plaint points of the systems, when defining the composition at which the three components are completely miscible, both those experi-

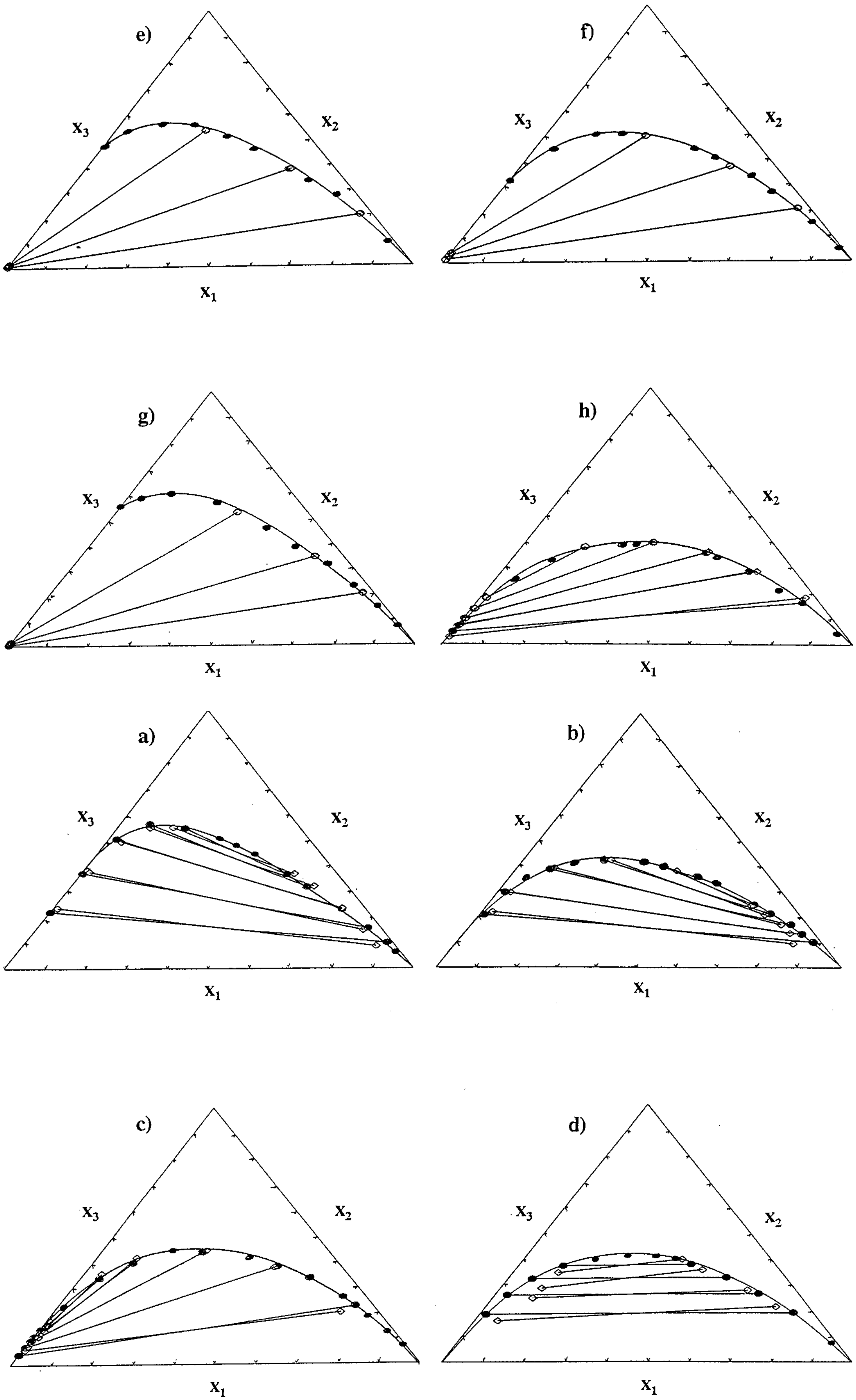

Figure 1. NRTL correlations for the liquid−liquid equilibrium data for the following systems: (a) diisobutyl ketone (1) + methanol (2) + water (3); (b) diisobutyl ketone (1) + ethanol (2) + water (3); (c) diisobutyl ketone (1) + 1-propanol (2) + water (3); (d) diisobutyl ketone (1) + 2-propanol (2) + water (3); (e) diisobutyl ketone (1) + 1-butanol (2) + water (3); (f) diisobutyl ketone (1) + 2-butanol (2) + water (3); (g) diisobutyl ketone (1) + 2-methyl-1-propanol (2) + water (3); (h) diisobutyl ketone (1) + 2-methyl-2-propanol (2) + water (3). Key: (●) experimental points, (◇) predicted points. The solid line was calculated by the log γ equation.

Table 4. Coefficients A_i, B_i, and C_i in Eqs 1−3, Respectively, for the Systems Diisobutyl Ketone (1) + an Alkanol (2) + Water (3) at 298.15 K[a]

Hlavatý	β	$\log \gamma$
	Methanol	
$A_1 = -0.51(0.25)$	$B_1 = 1.93(0.19)$	$C_1 = 1.80(0.16)$
$A_2 = 0.48(0.22)$	$B_2 = 1.06(0.05)$	$C_2 = 1.04(0.04)$
$A_3 = 2.07(0.64)$	$B_3 = 0.86(0.07)$	$C_3 = 1.26(0.08)$
$\sigma = 0.032$	$\sigma = 0.047$	$\sigma = 0.043$
	Ethanol	
$A_1 = -0.47(0.08)$	$B_1 = 1.58(0.08)$	$C_1 = 1.43(0.05)$
$A_2 = 0.11(0.08)$	$B_2 = 1.04(0.03)$	$C_2 = 1.00(0.02)$
$A_3 = 1.16(0.21)$	$B_3 = 0.88(0.03)$	$C_3 = 1.24(0.03)$
$\sigma = 0.025$	$\sigma = 0.026$	$\sigma = 0.022$
	1-Propanol	
$A_1 = -0.29(0.05)$	$B_1 = 1.76(0.05)$	$C_1 = 1.55(0.03)$
$A_2 = 0.01(0.05)$	$B_2 = 1.02(0.01)$	$C_2 = 0.97(0.01)$
$A_3 = 1.38(0.15)$	$B_3 = 0.95(0.01)$	$C_3 = 1.28(0.01)$
$\sigma = 0.013$	$\sigma = 0.017$	$\sigma = 0.009$
	2-Propanol	
$A_1 = -0.30(0.05)$	$B_1 = 1.53(0.06)$	$C_1 = 1.37(0.03)$
$A_2 = 0.04(0.06)$	$B_2 = 0.98(0.02)$	$C_2 = 0.94(0.01)$
$= 1.29(0.14)$	$B_3 = 0.91(0.02)$	$C_3 = 1.25(0.02)$
$= 0.015$	$\sigma = 0.020$	$\sigma = 0.014$
	1-Butanol	
$= -0.99(0.18)$	$B_1 = 2.52(0.18)$	$C_1 = 2.04(0.10)$
$= 0.18(0.14)$	$B_2 = 1.18(0.04)$	$C_2 = 1.10(0.03)$
$= 0.98(0.45)$	$B_3 = 1.04(0.02)$	$C_3 = 1.35(0.02)$
$= 0.009$	$\sigma = 0.040$	$\sigma = 0.024$
	2-Butanol	
$= -0.33(0.13)$	$B_1 = 2.20(0.16)$	$C_1 = 1.91(0.08)$
$= 0.23(0.12)$	$B_2 = 1.09(0.04)$	$C_2 = 1.04(0.02)$
$= 1.85(0.35)$	$B_3 = 1.03(0.03)$	$C_3 = 1.37(0.02)$
$= 0.073$	$\sigma = 0.036$	$\sigma = 0.051$
	2-Methyl-1-propanol	
$= -1.16(0.23)$	$B_1 = 2.56(0.21)$	$C_1 = 2.18(0.12)$
$= 0.12(0.16)$	$B_2 = 1.13(0.05)$	$C_2 = 1.07(0.03)$
$= 0.83(0.53)$	$B_3 = 1.04(0.04)$	$C_3 = 1.36(0.03)$
$= 0.011$	$\sigma = 0.047$	$\sigma = 0.031$
	2-Methyl-2-propanol	
$= -0.26(0.03)$	$B_1 = 1.50(0.04)$	$C_1 = 1.32(0.02)$
$= 0.05(0.03)$	$B_2 = 1.01(0.01)$	$C_2 = 0.96(0.01)$
$= 1.29(0.08)$	$B_3 = 0.91(0.01)$	$C_3 = 1.23(0.01)$
$= 0.005$	$\sigma = 0.014$	$\sigma = 0.009$

The corresponding standard errors are given in parentheses.

mentally derived and calculated with the two models, are published as well by Redhi (1996).

Six parameters of two models are fitted to a ternary data set in such a way that the solute distribution ratio at infinite dilution is reproduced as correctly as possible. In type 2 systems either of the two totally miscible components may be chosen as the solute. Imposing this constraint on both miscible components worsened the fit to the experimental data very much. It was decided to use this constraint only for that solute whose distribution ratio in infinite dilution is closest to unity. Fitting four (type one) or two (type two) parameters to ternary data sets results in only a slightly increased deviation between experimental and calculated mole fractions as compared with fitting six parameters (Sørensen *et al.*, 1979).

The model correlation parameters are included in Table 5, together with the rms values, defined below, which can be taken as a measure of the precision of the correlations:

$$\mathrm{rms} = \Big(\sum_i \sum_l \sum_m [x_{ilm} - x_{ilm}(\mathrm{calc})]^2/6k\Big)^{1/2} \qquad (8)$$

where x is the mole fraction and the subscripts i, l, and m designate the component, phase, and tie line, respectively. As can be seen from the tables, the correlation obtained

Table 5. Values of the Parameters for the NRTL and UNIQUAC Equations, Determined from Ternary Liquid−Liquid Equilibria for the Systems Diisobutyl Ketone (1) + an Alkanol (2) + Water (3), as Well as the Calculated Root Mean Square Deviation, rms

component	parameters			
	NRTL[a]		UNIQUAC	
$i-j$	$g_{ij} - g_{jj}$	$g_{ji} - g_{ii}$	Δu_{ij}	Δu_{ji}
	Methanol			
	(0.016)[b]		(0.024)	
1−2 2−1	−1090.49	6407.01	−683.37	5756.78
1−3 3−1	3901.07	11060.29	1745.20	1984.13
2−3 3−2	−2442.38	2188.14	−215.17	739.54
	Ethanol			
	(0.021)*		(0.043)	
1−2 2−1	4020.83	1232.28	−947.6	4836.41
1−3 3−1	5537.83	13881.37	1824.53	2658.44
2−3 3−2	3621.45	−481.14	614.24	479.43
	1-Propanol			
	(0.018)		(0.071)	
1−2 2−1	762.69	5408.80	−2248.58	5252.88
1−3 3−1	3527.41	11121.07	3243.80	11065.82
2−3 3−2	−1093.26	8475.31	−1044.01	8518.05
	2-Propanol			
	(0.036)		(0.046)	
1−2 2−1	−211.16	3386.59	−720.95	2970.93
1−3 3−1	4755.67	4815.55	4191.66	3589.98
2−3 3−2	−206.32	3881.67	−1505.20	8359.56
	1-Butanol			
	(0.002)[b]		(0.025)	
1−2 2−1	−3047.40	4500.87	−2388.53	5489.67
1−3 3−1	8336.31	15467.14	7255.36	41465.40
2−3 3−2	−1965.47	11888.04	−2001.97	11554.83
	2-Butanol			
	(0.002)		(0.064)	
1−2 2−1	−2478.45	5666.07	−2478.09	5666.22
1−3 3−1	11948.41	22518.62	11948.26	22518.21
2−3 3−2	−2406.28	10667.76	−2405.45	10667.09
	2-Methyl-1-propanol			
	(0.001)		(0.054)	
1−2 2−1	−4807.86	10966.16	−727.96	12427.00
1−3 3−1	10310.84	23341.05	13574.56	12275.72
2−3 3−2	−1723.35	11767.51	724.98	10203.45
	2-Methyl-2-propanol			
	(0.009)		(0.044)	
1−2 2−1	−3921.14	8821.02	−2334.62	6980.96
1−3 3−1	12147.42	12243.37	3450.00	4132.33
2−3 3−2	−3601.04	10864.45	−145.37	3545.13

[a] Calculated with $\alpha_{ij} = 0.2$ and(for the value with an asterisk) $\alpha_{ij} = 0.3$. [b] The rmsdeviations are given in parentheses.

with the NRTL model is significantly better than that obtained with the UNIQUAC model.

Conclusions

Liquid−liquid equilibrium data for the eight ternary mixtures: diisobutyl ketone (1) + methanol, ethanol, 1-propanol, 2-propanol, 1-butanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol (2) + water (3) were determined at 298.15 K.

The separation of an alkanol from water by extraction with diisobutyl ketone is feasible, as can be concluded from the distribution and selectivity data.

Three equations have been fitted to the binodal curve data. An equation relating to the NRTL and UNIQUAC models has been fitted to the experimental tie lines. The better results were obtained with the NRTL model.

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