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Influence of the Temperature on the Liquid−Liquid Equilibria of Tridecane + Butylbenzene + Sulfolane and Tridecane + 1,4-Diisopropylbenzene + Sulfolane

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Equilibrium tie line data have been determined at 323.15 K, 335.65 K, 348.15 K, 360.65 K, and 373.15 K for the ternary liquid−liquid equilibria (LLE) of tridecane + (butylbenzene or 1,4-diisopropylbenzene) + sulfolane systems. The relative mutual solubility of butylbenzene is higher than that of 1,4-diisopropylbenzene in tridecane + sulfolane mixtures. The tie line data were correlated with the well-known UNIQUAC and NRTL models. The calculated values based on the UNIQUAC model were found to be better than those based on the NRTL model, and showed that the higher accuracy of predictions existed at lower temperature. The values of selectivity and the distribution coefficient were derived from the equilibrium data at different temperatures.

Introduction

Ternary phase equilibrium data are essential for a proper understanding of the solvent extraction process. Sulfolane is used widely in the chemical industry for the extraction of aromatic hydrocarbons,[1−4] and many investigators[5−12] have studied liquid−liquid equilibria (LLE) for the ternary systems containing sulfolane + alkanes (C5−C8) + (benzene, toluene, or xylene), but quantitative phase equilibrium data for the systems containing sulfolane and hydrocarbons where the carbon number is larger than nine[13,14] are scarce.

The purpose of this study is to obtain LLE data for the ternary mixtures of tridecane + butylbenzene + sulfolane and tridecane + 1,4-diisopropylbenzene + sulfolane. The LLE data for these ternary systems were measured at 323.15 K, 335.65 K, 348.15 K, 360.65 K, and 373.15 K, and correlated by the UNIQUAC model of Abrams and Prausnitz[15] and the NRTL model of Renon and Prausnitz.[16] The effects of temperature on the selectivity and the distribution coefficient were also discussed.

Experimental Section

Chemicals. The source, grade, density, boiling point, and purity of each substance used are given in Table 1. All compounds were stored in a desiccator with a drying agent before use. They were used without further purification.

Apparatus and Procedure. The experimental points that define the binodal curves were determined by using a 5.0×10^{-5} m^3 jacketed glass cell controlled at a given temperature. Temperatures were controlled to ±0.03 K. Mixtures, composed of 11 g to 27 g of sulfolane, 7 g to 16 g of tridecane, and up to 23 g of butylbenzene or 1,4-diisopropylbenzene, were introduced into the cell and agitated while the cell was maintained at a constant temperature by circulation of silicon oil through the external jacket from a thermostatic bath. The sample was stirred for 1 h with a stirrer at a speed of 1300 rpm, and then it was left to settle for at least 6 h. After equilibrium was attained, the phases were allowed to separate and small samples of approximately 1 g were taken from each phase. A fixed amount of anisole was added as internal standard and diluted with 50 g of carbon disulfide[5] to prepare them for analysis. The accuracy of weighing was ±0.0001 g. The sample analysis was performed using a Hewlett-Packard model 5890 gas chromatograph equipped with a flame ionization detector and a HP Ultra 1 column (cross-linked methyl silicone gum, 25 m × 3.2×10^{-4} m × 5.2×10^{-7} m film thickness). The injector and detector temperatures were maintained at 573.15 K. The column temperature was programmed for an initial temperature of 353.15 K, maintained for 1 min, and a final temperature of 393.15 K, maintained for 1 min. The heating rate was 5 K/min, and the flow rate of the nitrogen carrier gas was 2.5×10^{-5} m^3/min. Mass fraction measurements were reproducible to within ±0.005. The greatest error in the material balance in these experiments was found to be less than 2%.

Table 1. Source, Grade, Density, ρ, Boiling Point, T_b, and Purity of Materials Used

substance	source	grade	ρ/g·cm^{-3}	T_b/K	purity
sulfolane	Merck	synthesis	1.2610[17]	560.45	>99.0%
tridecane	Merck	synthesis	0.7567[18]	516.15	>99.0%
butylbenzene	Acros Organics	synthesis	0.8601[18]	456.46	99.0%
1,4-diisopropylbenzene	Acros Organics	synthesis	0.8568[18]	483.65	99.0%
anisole	Merck	synthesis	0.9940[18]	426.85	>99.0%
carbon disulfide	Merck	E.P.	1.2632[18]	319.15	>99.5%

Results and Discussion

The experimental tie line data are given in Tables 2 and 3 for the ternary systems formed by tridecane (1) +

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Table 2. Experimental LLE Data for the System Tridecane (1) + Butylbenzene (2) + Sulfolane (3)

		tridecane-rich phase			sulfolane-rich phase		
T/K	sample no.	x_{11}	x_{21}	x_{31}	x_{13}	x_{23}	x_{33}
323.15	1	0.9940	0.0000	0.0060	0.0015	0.0000	0.9985
	2	0.8435	0.1493	0.0072	0.0016	0.0149	0.9835
	3	0.7203	0.2672	0.0125	0.0017	0.0287	0.9696
	4	0.5260	0.4514	0.0226	0.0021	0.0574	0.9405
	5	0.3805	0.5824	0.0371	0.0024	0.0861	0.9115
	6	0.2690	0.6717	0.0593	0.0027	0.1173	0.8800
	7	0.1848	0.7096	0.1056	0.0029	0.1493	0.8478
335.65	8	0.9918	0.0000	0.0082	0.0020	0.0000	0.9980
	9	0.8488	0.1393	0.0119	0.0021	0.0165	0.9814
	10	0.7180	0.2656	0.0165	0.0023	0.0332	0.9645
	11	0.5146	0.4560	0.0294	0.0028	0.0668	0.9304
	12	0.3779	0.5755	0.0466	0.0033	0.0968	0.8999
	13	0.2628	0.6643	0.0729	0.0038	0.1303	0.8659
	14	0.1765	0.7131	0.1104	0.0044	0.1681	0.8275
348.15	15	0.9883	0.0000	0.0117	0.0028	0.0000	0.9972
	16	0.8486	0.1390	0.0124	0.0029	0.0167	0.9804
	17	0.7166	0.2620	0.0214	0.0032	0.0354	0.9614
	18	0.5160	0.4470	0.0370	0.0038	0.0703	0.9259
	19	0.3751	0.5661	0.0588	0.0046	0.1044	0.8910
	20	0.2639	0.6459	0.0902	0.0057	0.1434	0.8509
	21	0.1719	0.6860	0.1421	0.0070	0.1901	0.8029
360.65	22	0.9847	0.0000	0.0153	0.0037	0.0000	0.9963
	23	0.8469	0.1340	0.0191	0.0041	0.0175	0.9784
	24	0.7146	0.2576	0.0278	0.0049	0.0363	0.9588
	25	0.5195	0.4342	0.0464	0.0055	0.0723	0.9222
	26	0.3649	0.5600	0.0751	0.0070	0.1186	0.8744
	27	0.2561	0.6312	0.1127	0.0074	0.1596	0.8330
	28	0.1596	0.6510	0.1894	0.0083	0.2083	0.7834
373.15	29	0.9786	0.0000	0.0214	0.0048	0.0000	0.9952
	30	0.8583	0.1184	0.0233	0.0052	0.0178	0.9770
	31	0.7093	0.2549	0.0358	0.0061	0.0404	0.9536
	32	0.5183	0.4234	0.0583	0.0071	0.0802	0.9127
	33	0.3627	0.5371	0.1002	0.0080	0.1223	0.8697
	34	0.2425	0.5926	0.1649	0.0082	0.1671	0.8247
	35	0.1473	0.6009	0.2518	0.0117	0.2244	0.7639

Table 3. Experimental LLE Data for the System Tridecane (1) + 1,4-Diisopropylbenzene (2) + Sulfolane (3)

		tridecane-rich phase			sulfolane-rich phase		
T/K	sample no.	x_{11}	x_{21}	x_{31}	x_{13}	x_{23}	x_{33}
323.15	36	0.9940	0.0000	0.0060	0.0015	0.0000	0.9985
	37	0.8504	0.1409	0.0087	0.0014	0.0083	0.9903
	38	0.7433	0.2428	0.0139	0.0014	0.0164	0.9822
	39	0.5466	0.4365	0.0169	0.0014	0.0307	0.9679
	40	0.4102	0.5590	0.0308	0.0013	0.0421	0.9566
	41	0.3019	0.6559	0.0422	0.0000	0.0529	0.9471
	42	0.2141	0.7305	0.0554	0.0000	0.0623	0.9377
	43	0.0000	0.8755	0.1245	0.0000	0.1018	0.8982
335.65	44	0.9918	0.0000	0.0082	0.0020	0.0000	0.9980
	45	0.8478	0.1401	0.0121	0.0019	0.0097	0.9884
	46	0.7391	0.2473	0.0136	0.0019	0.0177	0.9804
	47	0.5539	0.4249	0.0212	0.0019	0.0330	0.9651
	48	0.4112	0.5501	0.0387	0.0018	0.0464	0.9518
	49	0.2985	0.6490	0.0526	0.0017	0.0594	0.9388
	50	0.2107	0.7197	0.0696	0.0016	0.0716	0.9269
	51	0.0000	0.8479	0.1521	0.0000	0.1119	0.8881
348.15	52	0.9883	0.0000	0.0117	0.0028	0.0000	0.9972
	53	0.8392	0.1438	0.0170	0.0028	0.0106	0.9866
	54	0.7339	0.2442	0.0218	0.0027	0.0195	0.9778
	55	0.5470	0.4248	0.0282	0.0027	0.0367	0.9606
	56	0.3393	0.6026	0.0582	0.0027	0.0616	0.9357
	57	0.2947	0.6390	0.0663	0.0026	0.0679	0.9295
	58	0.2095	0.7050	0.0854	0.0024	0.0816	0.9159
	59	0.0000	0.7935	0.2065	0.0000	0.1216	0.8784
360.65	60	0.9847	0.0000	0.0153	0.0037	0.0000	0.9963
	61	0.8375	0.1447	0.0178	0.0035	0.0119	0.9846
	62	0.7330	0.2440	0.0230	0.0035	0.0206	0.9759
	63	0.5475	0.4142	0.0382	0.0034	0.0400	0.9566
	64	0.4122	0.5298	0.0580	0.0032	0.0547	0.9421
	65	0.2885	0.6302	0.0813	0.0030	0.0727	0.9243
	66	0.2032	0.6880	0.1088	0.0025	0.0877	0.9098
	67	0.0000	0.7040	0.2960	0.0000	0.1348	0.8652
373.15	68	0.9786	0.0000	0.0214	0.0048	0.0000	0.9952
	69	0.8286	0.1453	0.0261	0.0048	0.0128	0.9824
	70	0.7325	0.2315	0.0360	0.0048	0.0220	0.9731
	71	0.5442	0.4076	0.0482	0.0046	0.0424	0.9530
	72	0.3968	0.5260	0.0772	0.0044	0.0625	0.9331
	73	0.2851	0.6054	0.1095	0.0039	0.0810	0.9151
	74	0.1930	0.6585	0.1485	0.0030	0.0936	0.9034
	75	0.0000	0.5841	0.4159	0.0000	0.1483	0.8517

sulfolane (3) with butylbenzene or 1,4-diisopropylbenzene (2), respectively. Concentrations of components i (i = 1, 2, 3) in phase L (L = 1, raffinate phase; L = 2, extract phase) are given in mole fraction, x_{iL}. The effect of temperature on the equilibrium for the system tridecane (1) + 1,4-diisopropylbenzene (2) + sulfolane (3) is shown in Figure 1. As seen, the size of the two-phase region decreases with an increase in temperature. A similar trend was observed for the other system containing butylbenzene. These systems studied present a wide two-phase region which is important, together with the slope of the tie lines, when establishing the selectivity of sulfolane.

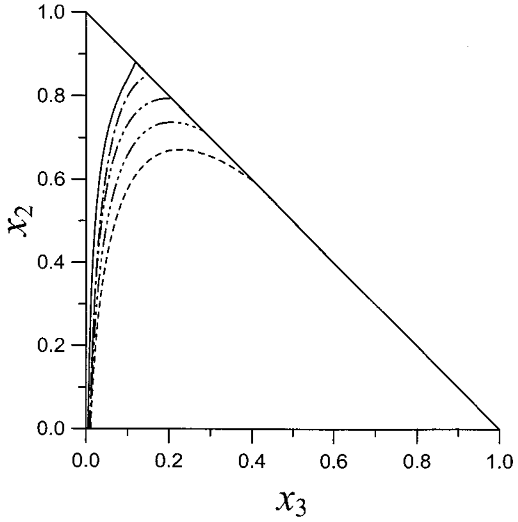

Figure 1. Effect of temperature on the liquid–liquid equilibrium for the tridecane (1) + 1,4-diisopropylbenzene (2) + sulfolane (3): curves calculated by UNIQUAC; (—) 323.15 K; (–•–) 335.65 K; (–••–) 348.15 K; (–•••–) 360.65 K; (- - -) 373.15 K.

Data Correlation. The NRTL and UNIQUAC models were used to correlate and predict the LLE data in the present work. The corresponding sets of binary interaction parameters were determined by minimizing the differences between the experimental and calculated concentrations over all the tie lines for each ternary system using the Simplex Search method. The objective function (F) used is

$$F = \min \sum_i \sum_L \sum_k (x_{iLk} - x^{c}_{iLk})^2 \qquad (1)$$

where x and x^c are the experimental and calculated mole fractions, respectively, and the subscripts i, L, and k denote the number of components, phases, and tie lines, respectively.

For the NRTL model, the third nonrandomness parameter, α_{ij}, was set at a value of 0.2.[7] The parameters calculated are shown in Tables 4 and 5, together with the root-mean-square deviation (rmsd) values, defined as

$$\text{rmsd} = 100[\sum_i \sum_L \sum_k (x_{iLk} - x^{c}_{iLk})^2/6N]^{1/2} \qquad (2)$$

where N = number of tie lines.

Table 4. UNIQUAC and NRTL Parameters for the System Tridecane (1) + Butylbenzene (2) + Sulfolane (3) at (323.15, 335.65, 348.15, 360.65, and 373.15) K, as Well as the Calculated Root Mean Square Deviation, rmsd

		UNIQUAC parameters/K		NRTL parameters/K ($\alpha_{ij} = 0.2$)	
T/K	i–j	$(u_{ij} - u_{jj})/R$	$(u_{ji} - u_{ii})/R$	$(g_{ij} - g_{jj})/R$	$(g_{ji} - g_{ii})/R$
323.15	1–2	−150.08	176.74	−117.74	−283.99
	1–3	540.82	158.81	1194.20	1383.10
	2–3	89.52	90.31	430.91	306.84
	rmsd	0.2802		0.7745	
335.65	1–2	−82.93	61.09	−550.86	516.03
	1–3	602.67	−36.19	1355.90	1289.10
	2–3	229.87	−11.52	334.64	423.77
	rmsd	0.2858		0.2923	
348.15	1–2	−338.84	544.84	1.51	−45.46
	1–3	513.64	20.39	1075.40	1405.80
	2–3	274.11	−44.73	377.65	383.40
	rmsd	0.6542		0.7277	
360.65	1–2	−398.60	659.74	180.57	−307.47
	1–3	519.88	−12.44	1194.60	1319.80
	2–3	339.53	−88.93	364.78	404.00
	rmsd	0.4990		0.4456	
373.15	1–2	31.37	−19.61	−132.44	69.12
	1–3	500.81	51.82	1302.50	1286.20
	2–3	78.51	102.92	155.03	588.51
	rmsd	0.4462		0.4450	

Table 5. UNIQUAC and NRTL Parameters for the System Tridecane (1) + 1,4-Diisopropylbenzene (2) + Sulfolane (3) at (323.15, 335.65, 348.15, 360.65 and 373.15) K, as Well as the Calculated Root Mean Square Deviation, rmsd

		UNIQUAC parameters/K		NRTL parameters/K ($\alpha_{ij} = 0.2$)	
T/K	i–j	$(u_{ij} - u_{jj})/R$	$(u_{ji} - u_{ii})/R$	$(g_{ij} - g_{jj})/R$	$(g_{ji} - g_{ii})/R$
323.15	1–2	−242.92	348.56	−609.98	776.57
	1–3	535.43	38.20	1156.40	1425.80
	2–3	311.98	−29.41	452.15	571.64
	rmsd	0.2228		0.2029	
335.65	1–2	−139.72	164.67	−477.20	734.31
	1–3	499.85	21.71	1045.50	1467.70
	2–3	298.09	−23.22	403.08	626.09
	rmsd	0.2468		0.2653	
348.15	1–2	−199.71	275.89	−682.14	1067.70
	1–3	496.83	57.84	1107.00	1414.10
	2–3	275.55	−15.26	338.12	655.89
	rmsd	0.2283		0.1931	
360.65	1–2	−16.44	29.37	−615.12	974.24
	1–3	540.76	24.45	1150.30	1474.10
	2–3	234.59	7.92	240.98	739.97
	rmsd	0.3267		0.3415	
373.15	1–2	−32.36	55.48	−352.20	310.37
	1–3	506.04	64.34	1310.90	1382.80
	2–3	168.08	52.53	127.65	842.11
	rmsd	0.4694		0.8362	

The rmsd is a measure of the agreement between the experimental data and the calculated values. As can be seen from Tables 4 and 5, the calculation based on both the UNIQUAC and the NRTL models gave a good representation of the tie line data for these systems. However, the UNIQUAC model, fitted to the experimental data, is more accurate than the NRTL model, according to the analysis of the rmsd (the average root-mean-square deviation phase composition error was 0.3659 for UNIQUAC as compared to 0.4524 for NRTL). At a temperature of 323.15 K or 335.65 K, the values of the rmsd (for UNIQUAC) are smaller than those at higher temperature. This means that the lower the temperature, the higher the accuracy of the predictions by the UNIQUAC model for the systems studied here.

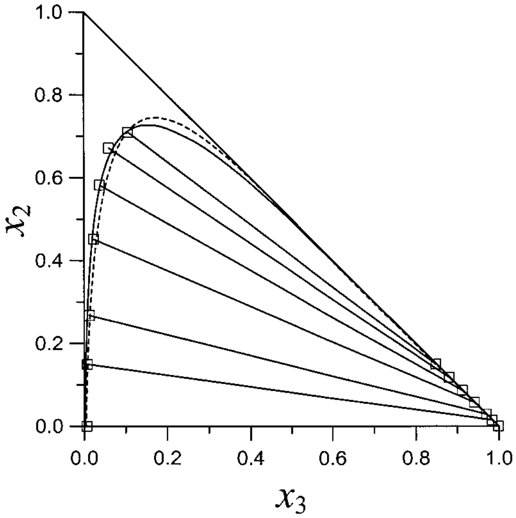

Figure 2. LLE data for the tridecane (1) + butylbenzene (2) + sulfolane (3) system at 323.15 K: curves calculated by (—) the UNIQUAC model and (- - -) the NRTL model; experimental tie line (□–□).

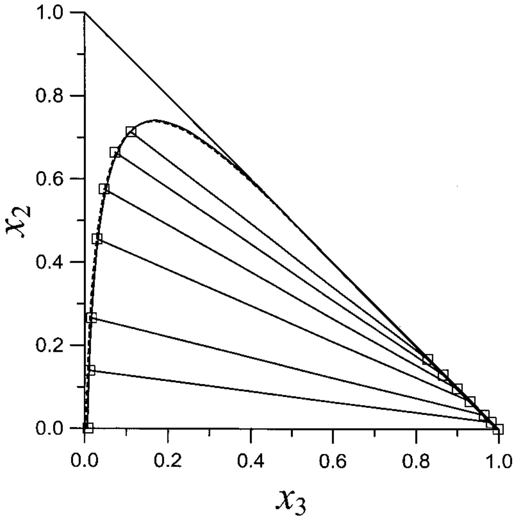

Figure 3. LLE data for the tridecane (1) + butylbenzene (2) + sulfolane (3) system at 335.65 K: curves calculated by (—) the UNIQUAC model and (- - -) the NRTL model; experimental tie line (□–□).

The calculated values using both the UNIQUAC and NRTL models for the tridecane (1) + butylbenzene (2) + sulfolane (3) system at 323.15 K, 335.65 K, 348.15 K, 360.65 K, and 373.15 K are compared with the experimental data in Figures 2–6. It was observed that the slopes of the tie lines show that butylbenzene is more soluble in tridecane than in sulfolane. It is observed that the relative mutual solubility of butylbenzene is higher than those of 1,4-diisopropylbenzene in tridecane + sulfolane mixtures at the same temperature. This solubility effect is reflected in the size of the two-phase region, increasing slightly in the order 1,4-diisopropylbenzene > butylbenzene at the same temperature. The ternary system tridecane (1) + butylbenzene (2) + sulfolane (3) at any given temperature of this study is a type 1 system,[19] and the system tridecane (1) + 1,4-diisopropylbenzene (2) + sulfolane (3) is a type 2 system. It is seen from Table 3 that there were two partially miscible pairs in each different temperature system.

Selectivity and Distribution Coefficient. The effectiveness of extraction of an aromatic compound by

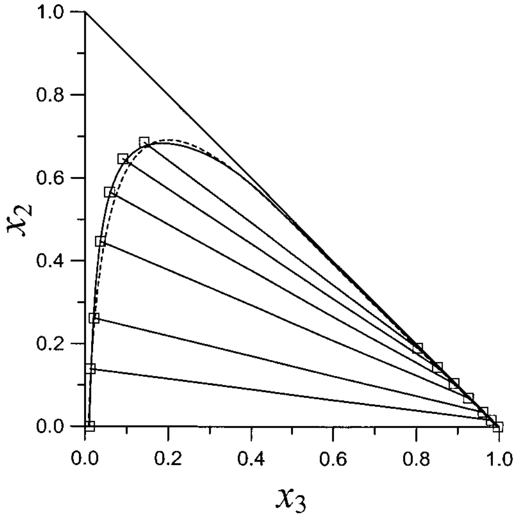

Figure 4. LLE data for the tridecane (1) + butylbenzene (2) + sulfolane (3) system at 348.15 K: curves calculated by (—) the UNIQUAC model and (- - -) the NRTL model; experimental tie line (□—□).

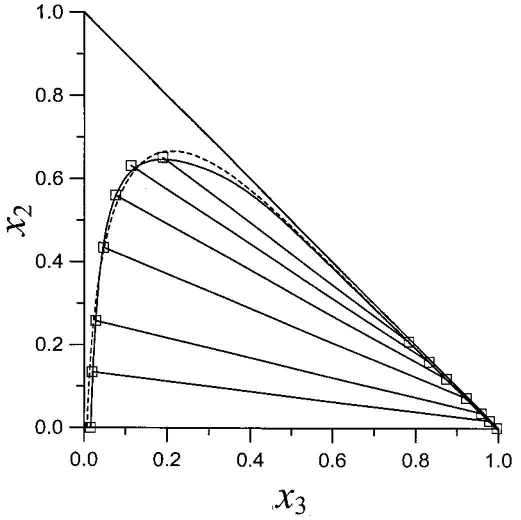

Figure 5. LLE data for the tridecane (1) + butylbenzene (2) + sulfolane (3) system at 360.65 K: curves calculated by (—) the UNIQUAC model and (- - -) the NRTL model; experimental tie line (□—□).

sulfolane is given by its selectivity (S), which is a measure of the ability of sulfolane to separate aromatics from alkane:

$$S = (x_2/x_1)_{\text{sulfolane-rich phase}}/(x_2/x_1)_{\text{tridecane-rich phase}} \quad (3)$$

where the subscript 2 represents butylbenzene or 1,4-diisopropylbenzene and 1 represents tridecane.

This quantity is not constant over the whole two-phase region. Table 6 lists experimental values of S. From the data, we find the tendency that, for the same system, the higher the temperature, the lower the selectivity. At the same temperature for the different systems, the order of the selectivity of sulfolane to aromatic is butylbenzene > 1,4-diisopropylbenzene. And as seen, S decreases when going through the tie lines from low concentration to high concentration of aromatic. It means the higher the concentration of aromatic in the feed, the lower the selectivity of sulfolane to aromatic. Since the selectivity in all cases is greater than 1, it means that extraction is possible.

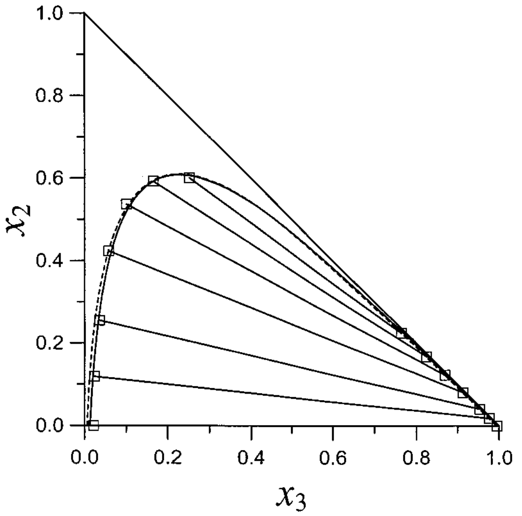

Figure 6. LLE data for the tridecane (1) + butylbenzene (2) + sulfolane (3) system at 373.15 K: curves calculated by (—) the UNIQUAC model and (- - -) the NRTL model; experimental tie line (□—□).

Table 6. Experimental Selectivity Values, S

T/K	sample no.	S for the system butylbenzene	sample no.	S for the system 1,4-diisopropylbenzene
323.15	2	53	37	36
	3	44	38	35
	4	32	39	28
	5	24	40	24
	6	17	41	V.L.[a]
	7	14	42	V.L.
335.65	9	48	45	31
	10	39	46	28
	11	27	47	22
	12	19	48	19
	13	13	49	16
	14	9	50	13
348.15	16	35	53	22
	17	30	54	22
	18	21	55	17
	19	15	56	13
	20	10	57	12
	21	7	58	10
360.65	23	27	61	20
	24	21	62	17
	25	16	63	16
	26	11	64	13
	27	9	65	11
	28	6	66	10
373.15	30	25	69	15
	31	18	70	14
	32	14	71	12
	33	10	72	11
	34	8	73	10
	35	5	74	9

[a] V.L. denotes very large.

The capacity or dissolving ability of a solvent is a measure of the ratio of solvent to feed required for the desired recovery of aromatics. The distribution coefficient for aromatic, which is the measure of the solvent power or capacity of sulfolane, is given as

$$\mathcal{K} = (x_2)_{\text{sulfolane-rich phase}}/(x_2)_{\text{tridecane-rich phase}} \quad (4)$$

The experimental values of $\mathcal{K}$ of this study are presented in Table 7. We can find the tendency that, for the same system, the higher the temperature, the larger the $\mathcal{K}$ value. However, an increase in the solvent capacity of sulfolane leads to a decrease in its selectivity or vice versa. To choose

Table 7. Experimental Distribution Coefficient Values, κ

T/K	sample no.	κ for the system butylbenzene	sample no.	κ for the system 1,4-diisopropylbenzene
323.15	2	0.10	37	0.06
	3	0.11	38	0.07
	4	0.13	39	0.07
	5	0.15	40	0.08
	6	0.18	41	0.08
	7	0.21	42	0.09
335.65	9	0.12	45	0.07
	10	0.13	46	0.07
	11	0.15	47	0.08
	12	0.17	48	0.08
	13	0.20	49	0.09
	14	0.24	50	0.10
348.15	16	0.12	53	0.07
	17	0.14	54	0.08
	18	0.16	55	0.09
	19	0.18	56	0.10
	20	0.22	57	0.11
	21	0.28	58	0.12
360.65	23	0.13	61	0.08
	24	0.14	62	0.08
	25	0.17	63	0.10
	26	0.21	64	0.10
	27	0.25	65	0.12
	28	0.32	66	0.13
373.15	30	0.15	69	0.09
	31	0.16	70	0.10
	32	0.19	71	0.10
	33	0.23	72	0.12
	34	0.28	73	0.13
	35	0.37	74	0.14

the optimum values of selectivity and capacity is therefore a compromise between the two values which can be adjusted either by changing the temperature and/or by adding a second component like water to the solvent.[20] At the same temperature for the different systems, the $\mathscr{K}$ values are larger for the system of butylbenzene than those for the system of 1,4-diisopropylbenzene. This result is similar to the trend of S values.

Conclusions

Liquid−liquid equilibrium data of the ternary systems tridecane (1) + butylbenzene (2) + sulfolane (3) and tridecane (1) + 1,4-diisopropylbenzene (2) + sulfolane (3) were determined at 323.15 K, 335.65 K, 348.15 K, 360.65 K, and 373.15 K, respectively.

The calculation based on the UNIQUAC and NRTL models showed that the best results are given by the UNIQUAC model. The binodal curves calculated by the UNIQUAC model or NRTL model for the systems studied here show that the size of the two-phase region decreases with increasing temperature. For the same system, the higher the temperature, the larger the distribution coefficient but the lower the selectivity. From the selectivity values, the separation of butylbenzene/1,4-diisopropylbenzene from tridecane by extraction with sulfolane is feasible. Not only the selectivity data but also the distribution coefficient data showed that sulfolane is more extractive for butylbenzene than for 1,4-diisopropylbenzene at a given temperature.

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