J. Chem. Eng. Data **1999,** *44,* 803−808 **803**

Liquid−Liquid Equilibria of Alkane (C10−C14) + Butylbenzene + Sulfolane

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Equilibrium tie line data have been determined at 323.15 K, 348.15 K, and 373.15 K for the ternary liquid−liquid equilibria (LLE) of three alkane + butylbenzene + sulfolane systems, where the alkanes studied are decane, undecane, and tetradecane. The relative mutual solubility of butylbenzene is higher in decane + sulfolane than in undecane + sulfolane or tetradecane + sulfolane mixtures. The tie line data were correlated with the UNIQUAC and NRTL models. The calculated values based on the UNIQUAC model were found to be better than those based on the NRTL model. The values of selectivity and the distribution coefficient were derived from the equilibrium data.

Introduction

Ternary phase equilibrium data are essential to the proper understanding of the solvent extraction process. Sulfolane is used widely in the chemical industry for the extraction of aromatic hydrocarbons (Wheeler, 1986), and many investigators (Cassell et al., 1989a−c; Lee and Kim, 1995, 1998; Letcher et al., 1996; Mondragón-Garduño et al., 1991) have studied the liquid−liquid equilibria (LLE) of 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 9 (Masohan et al., 1990) are few.

The purpose of this study is to obtain LLE data of decane + butylbenzene + sulfolane, undecane + butylbenzene + sulfolane, and tetradecane + butylbenzene + sulfolane. The LLE data for these ternary systems were measured at 323.15 K, 348.15 K, and 373.15 K and correlated by the UNIQUAC model of Abrams and Prausnitz (1975) and the NRTL model of Renon and Prausnitz (1968).

Experimental Section

Chemicals. The source and grade 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.

Table 1. Source and Grade of Materials Used in This Study

substance	source	grade
sulfolane[a]	merck	for synthesis
butylbenzene	Acros Organics	for synthesis
decane	Merck	for synthesis
undecane	Merck	for synthesis
tetradecane	Tokyo Kasei Organic Chemicals	GR
anisole	Merck	for synthesis
carbon disulfide	Merck	EP

[a] It is also called tetramethylene sulfone, and the CAS registry number of the chemical is [126-33-0].

Table 2. Experimental LLE Data for Decane (1) + Butylbenzene (2) + Sulfolane (3)

	alkane-rich phase			sulfolane-rich phase		
T/K	x_{11}	x_{21}	x_{31}	x_{12}	x_{22}	x_{32}
323.15	0.9949	0.0000	0.0051	0.0041	0.0000	0.9959
	0.8819	0.1130	0.0051	0.0043	0.0141	0.9816
	0.7593	0.2291	0.0116	0.0047	0.0292	0.9661
	0.5719	0.4060	0.0221	0.0051	0.0567	0.9382
	0.4271	0.5356	0.0373	0.0056	0.0831	0.9113
	0.3136	0.6280	0.0584	0.0060	0.1099	0.8841
	0.2259	0.6879	0.0862	0.0064	0.1376	0.8560
	0.1383	0.7123	0.1494	0.0067	0.1624	0.8309
348.15	0.9903	0.0000	0.0097	0.0063	0.0000	0.9937
	0.9199	0.0739	0.0062	0.0071	0.0106	0.9823
	0.8182	0.1651	0.0167	0.0074	0.0238	0.9688
	0.7258	0.2574	0.0168	0.0079	0.0406	0.9515
	0.6003	0.3678	0.0319	0.0087	0.0597	0.9316
	0.4357	0.5080	0.0563	0.0102	0.0966	0.8932
	0.3119	0.5985	0.0896	0.0118	0.1346	0.8536
	0.2077	0.6476	0.1447	0.0123	0.1776	0.8101
373.15	0.9827	0.0000	0.0173	0.0097	0.0000	0.9903
	0.9269	0.0536	0.0195	0.0105	0.0077	0.9818
	0.8152	0.1573	0.0275	0.0123	0.0261	0.9616
	0.7017	0.2643	0.0340	0.0114	0.0446	0.9440
	0.5964	0.3539	0.0497	0.0110	0.0657	0.9233
	0.4275	0.4807	0.0918	0.0136	0.1079	0.8785
	0.2917	0.5597	0.1486	0.0162	0.1561	0.8277
	0.1636	0.5449	0.2915	0.0129	0.1913	0.7958

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 temperature of 323.15 K, 348.15 K, or 373.15 K. Temperatures were controlled to ±0.03 K. Mixtures, comprised of 11−27 g of sulfolane, 7−16 g of the alkane, and up to 23 g of butylbenzene, were introduced into the cell and agitated while being 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 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 (Cassell et al., 1989a) to prepare them for analysis. The accuracy of weighing was ±0.0001 g. The sample analysis was made 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

10.1021/je990020k CCC: $18.00

Table 3. Experimental LLE Data for Undecane (1) + Butylbenzene (2) + Sulfolane (3)

	alkane-rich phase			sulfolane-rich phase		
T/K	x_{11}	x_{21}	x_{31}	x_{12}	x_{22}	x_{32}
323.15	0.9948	0.0000	0.0052	0.0030	0.0000	0.9970
	0.8477	0.1426	0.0097	0.0031	0.0163	0.9806
	0.7494	0.2395	0.0111	0.0033	0.0296	0.9671
	0.6475	0.3357	0.0168	0.0035	0.0429	0.9536
	0.5606	0.4188	0.0206	0.0037	0.0573	0.9390
	0.4218	0.5439	0.0343	0.0041	0.0826	0.9133
	0.2986	0.6454	0.0560	0.0044	0.1112	0.8844
	0.2063	0.7086	0.0851	0.0047	0.1419	0.8534
348.15	0.9900	0.0000	0.0100	0.0053	0.0000	0.9947
	0.8501	0.1355	0.0144	0.0056	0.0192	0.9752
	0.7479	0.2331	0.0190	0.0057	0.0333	0.9610
	0.6462	0.3271	0.0267	0.0059	0.0507	0.9434
	0.5625	0.4031	0.0344	0.0067	0.0659	0.9274
	0.4112	0.5318	0.0570	0.0075	0.0999	0.8926
	0.2975	0.6130	0.0895	0.0091	0.1385	0.8524
	0.1927	0.6601	0.1472	0.0102	0.1852	0.8046
373.15	0.9819	0.0000	0.0181	0.0074	0.0000	0.9926
	0.8368	0.1433	0.0199	0.0076	0.0208	0.9716
	0.7396	0.2283	0.0321	0.0094	0.0378	0.9528
	0.6315	0.3277	0.0408	0.0099	0.0591	0.9310
	0.5506	0.3954	0.0540	0.0114	0.0772	0.9114
	0.3951	0.5071	0.0978	0.0118	0.1172	0.8710
	0.2631	0.5640	0.1729	0.0098	0.1540	0.8362
	0.1516	0.5602	0.2882	0.0099	0.1935	0.7966

Table 4. Experimental LLE Data for Tetradecane (1) + Butylbenzene (2) + Sulfolane (3)

	alkane-rich phase			sulfolane-rich phase		
T/K	x_{11}	x_{21}	x_{31}	x_{12}	x_{22}	x_{32}
323.15	0.9936	0.0000	0.0064	0.0000	0.0000	1.0000
	0.9042	0.0897	0.0061	0.0012	0.0098	0.9890
	0.8089	0.1816	0.0095	0.0012	0.0201	0.9787
	0.7044	0.2826	0.0130	0.0013	0.0325	0.9662
	0.5005	0.4759	0.0236	0.0015	0.0632	0.9353
	0.3573	0.6041	0.0386	0.0017	0.0923	0.9060
	0.2529	0.6878	0.0593	0.0020	0.1208	0.8772
	0.1675	0.7421	0.0904	0.0024	0.1531	0.8445
348.15	0.9878	0.0000	0.0122	0.0021	0.0000	0.9979
	0.8954	0.0896	0.0150	0.0023	0.0101	0.9876
	0.7959	0.1851	0.0190	0.0023	0.0214	0.9763
	0.7021	0.2752	0.0227	0.0025	0.0365	0.9610
	0.5081	0.4547	0.0372	0.0032	0.0722	0.9246
	0.3601	0.5801	0.0598	0.0038	0.1078	0.8884
	0.2495	0.6588	0.0917	0.0049	0.1483	0.8468
	0.1621	0.6948	0.1431	0.0061	0.1973	0.7966
373.15	0.9777	0.0000	0.0223	0.0039	0.0000	0.9961
	0.8877	0.0880	0.0243	0.0040	0.0112	0.9848
	0.7843	0.1843	0.0314	0.0045	0.0271	0.9684
	0.6990	0.2618	0.0392	0.0047	0.0402	0.9551
	0.5061	0.4351	0.0588	0.0058	0.0804	0.9138
	0.3560	0.5500	0.0940	0.0077	0.1250	0.8673
	0.2415	0.6200	0.1385	0.0072	0.1702	0.8226
	0.1374	0.6153	0.2473	0.0071	0.2231	0.7698

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 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%.

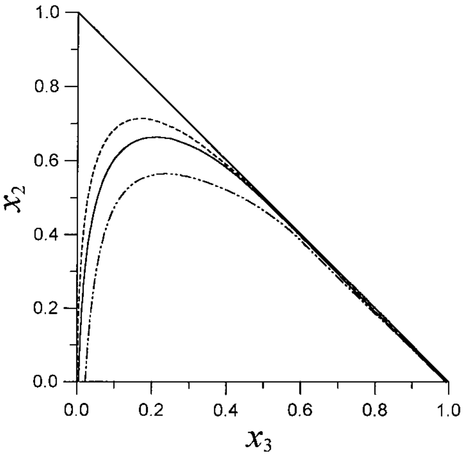

Figure 1. Effect of temperature on the liquid−liquid equilibrium for decane (1) + butylbenzene (2) + sulfolane (3) (curves calculated by the UNIQUAC): (- -) 323.15 K; (—) 348.15 K; (− · · −) 373.15 K .

Table 5. UNIQUAC and NRTL Parameters for Decane (1) + Butylbenzene (2) + Sulfolane (3) at 323.15 K, 348.15 K, and 373.15 K, as Well as the Calculated Root Mean Square Deviation, rmsd

		UNIQUAC param/K			NRTL param/K		
T/K	$i-j$	$(u_{ij} - u_{jj})/R$	$(u_{ji} - u_{ii})/R$	rmsd	$(g_{ij} - g_{jj})/R$	$(g_{ji} - g_{ii})/R$	rmsd
323.15	1−2	−198.90	249.99	0.4323	−629.26	652.94	0.8768
	1−3	637.80	82.02		1282.40	1087.20	
	2−3	151.65	37.63		352.12	369.23	
348.15	1−2	−206.59	298.01	0.3032	241.72	−216.59	0.2733
	1−3	592.55	9.36		1414.30	1105.00	
	2−3	220.02	−2.47		328.35	431.74	
373.15	1−2	−300.85	626.17	0.8170	88.83	−71.57	0.7701
	1−3	406.04	75.63		1340.20	1097.70	
	2−3	225.86	9.29		85.91	669.30	

Table 6. UNIQUAC and NRTL Parameters for Undecane (1) + Butylbenzene (2) + Sulfolane (3) at 323.15 K, 348.15 K, and 373.15 K, as Well as the Calculated Root Mean Square Deviation, rmsd

		UNIQUAC param/K			NRTL param/K		
T/K	$i-j$	$(u_{ij} - u_{jj})/R$	$(u_{ji} - u_{ii})/R$	rmsd	$(g_{ij} - g_{jj})/R$	$(g_{ji} - g_{ii})/R$	rmsd
323.15	1−2	−80.72	19.26	0.6070	−814.24	589.89	0.8613
	1−3	527.83	32.94		973.52	1170.10	
	2−3	208.15	−11.14		425.43	262.35	
348.15	1−2	−272.10	422.12	0.2539	216.03	−258.52	0.2559
	1−3	530.80	19.65		1278.90	1274.80	
	2−3	252.42	−26.96		379.84	385.17	
373.15	1−2	−77.50	103.05	0.4282	119.99	−103.61	0.7213
	1−3	571.72	33.17		1181.40	1192.30	
	2−3	75.26	108.80		143.75	613.01	

Results

The experimental tie line data are given in Tables 2−4 for the ternary systems formed by sulfolane + butylbenzene with decane, undecane, or tetradecane, 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 decane + butylbenzene + sulfolane is shown in Figure 1. As expected, the size of the two-phase region decreases with an increase in temperature. The other two systems have the same result, too. The three 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.

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

Table 7. UNIQUAC and NRTL parameters for the Tetradecane (1) + Butylbenzene (2) + Sulfolane (3) at 323.15 K, 348.15 K, and 373.15 K, as Well as the Calculated Root Mean Square Deviation, rmsd

		UNIQUAC param/K			NRTL param/K		
T/K	$i-j$	$(u_{ij}-u_{jj})/R$	$(u_{ji}-u_{ii})/R$	rmsd	$(g_{ij}-g_{jj})/R$	$(g_{ji}-g_{ii})/R$	rmsd
323.15	1−2	−178.15	163.54	0.3921	−978.19	1278.00	0.5144
	1−3	529.74	25.97		1100.50	1498.70	
	2−3	221.64	−11.33		384.20	340.59	
348.15	1−2	−293.61	335.89	0.5594	−543.20	493.65	0.2784
	1−3	506.24	17.76		1180.80	1373.30	
	2−3	232.19	−36.57		316.61	425.67	
373.15	1−2	−172.17	233.33	0.4929	−275.07	323.11	0.5837
	1−3	496.33	20.18		1043.90	1415.70	
	2−3	172.06	30.53		204.40	563.87	

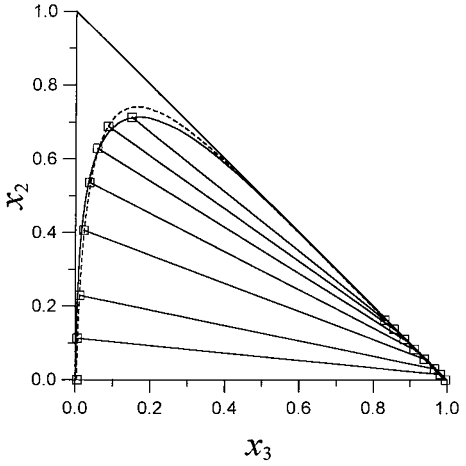

Figure 2. LLE data for decane (1) + butylbenzene (2) + sulfolane (3) at 323.15 K: curves calculated by the (—) UNIQUAC model and (- -) NRTL model; experimental tie line (□ − □).

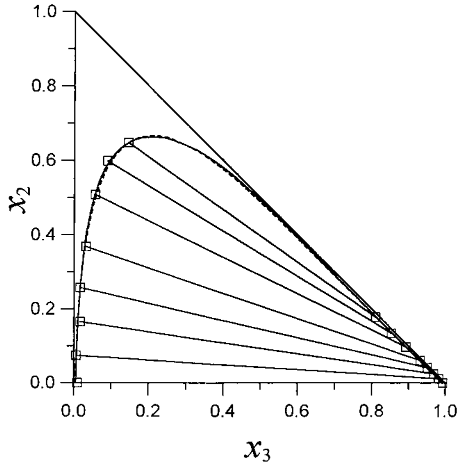

Figure 3. LLE data for the decane (1) + butylbenzene (2) + sulfolane (3) at 348.15 K: curves calculated by the (—) UNIQUAC model and (- -) NRTL model; experimental tie line (□ − □).

Newton−Raphson 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 (Cassell et al., 1989c).

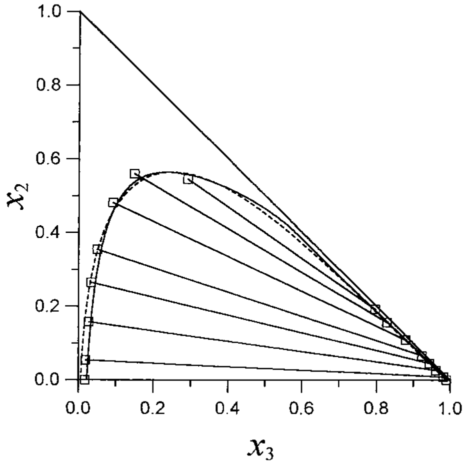

Figure 4. LLE data for the decane (1) + butylbenzene (2) + sulfolane (3) at 373.15 K: curves calculated by the (—) UNIQUAC model and (- -) NRTL model; experimental tie line (□ − □).

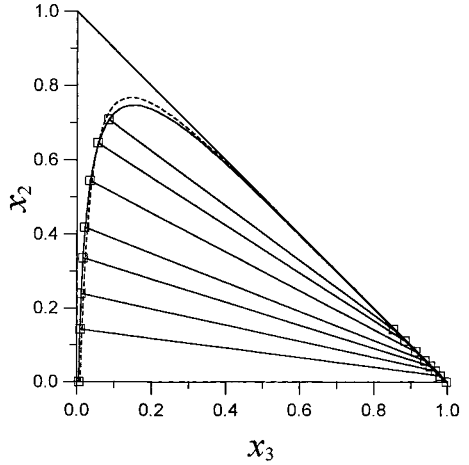

Figure 5. LLE data for undecane (1) + butylbenzene (2) + sulfolane (3) at 323.15 K: curves calculated by the (—) UNIQUAC model and (- -) NRTL model; experimental tie line (□ − □).

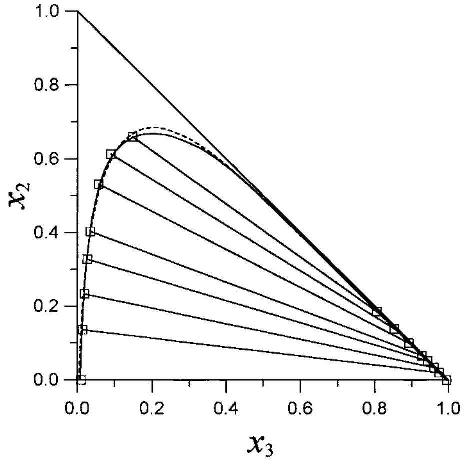

Figure 6. LLE data for undecane (1) + butylbenzene (2) + sulfolane (3) at 348.15 K: curves calculated by the (—) UNIQUAC model and (- -) NRTL model; experimental tie line (□ − □).

The parameters calculated are shown in Tables 5−7, together with the root mean square deviation (rmsd) values, which are defined as

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

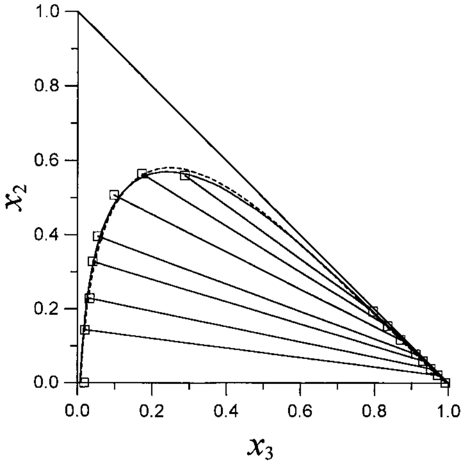

Figure 7. LLE data for undecane (1) + butylbenzene (2) + sulfolane (3) at 373.15 K: curves calculated by the (—) UNIQUAC model and (- -) NRTL model; experimental tie line (□ − □).

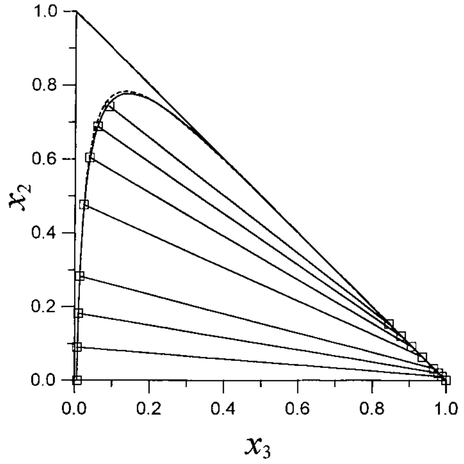

Figure 8. LLE data for the tetradecane (1) + butylbenzene (2) + sulfolane (3) at 323.15 K: curves calculated by the (—) UNIQUAC model and (- -) NRTL model; experimental tie line (□ − □).

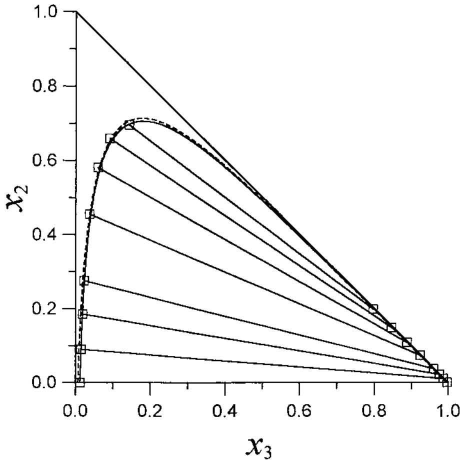

Figure 9. LLE data for the tetradecane (1) + butylbenzene (2) + sulfolane (3) at 348.15 K: curves calculated by the (—) UNIQUAC model and (- -) NRTL model; experimental tie line (□ − □).

As can be seen from Tables 5−7, the calculations based on both the UNIQUAC and the NRTL models gave 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 rmsd (the average root mean square deviations phase composition error was 0.4762 for UNIQUAC as compared to 0.5706 for NRTL).

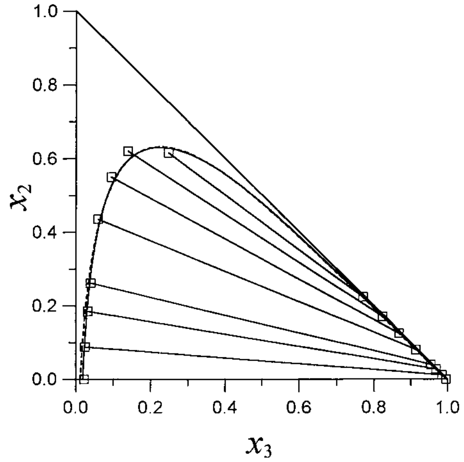

Figure 10. LLE data for the tetradecane (1) + butylbenzene (2) + sulfolane (3) at 373.15 K: curves calculated by the (—) UNIQUAC model and (- -) NRTL model; experimental tie line (□ − □).

Table 8. Experimental Selectivity Values *S* for Each Tie Line

S for the system	323.15 K	348.15 K	373.15 K
decane	25.59	18.58	12.68
	20.59	15.94	11.00
	15.66	14.49	10.39
	11.83	11.20	10.07
	9.15	8.12	7.06
	7.06	5.94	5.02
	4.71	4.63	4.45
undecane	31.26	21.51	15.98
	28.07	18.74	13.03
	23.64	16.98	11.50
	20.73	13.73	9.43
	15.62	10.30	7.74
	11.69	7.39	7.33
	8.79	5.30	5.29
tetradecane	82.32	43.88	28.25
	74.61	40.01	25.63
	62.31	37.25	22.84
	44.31	25.21	16.12
	32.11	17.61	10.51
	22.21	11.46	9.21
	14.40	7.55	7.02

Discussion

The slopes of the tie lines presented in Figures 2−10 show that butylbenzene is more soluble in alkanes than in sulfolane and is more soluble in decane than in undecane or in tetradecane at the same temperature. This solubility effect is reflected in the size of the two-phase region, increasing slightly in the order tetradecane > undecane > decane at the same temperature.

The effectiveness of extraction of aromatic compound by sulfolane is given by its selectivity (*S*), which is a measure of the ability of sulfolane to separate aromatics from alkanes:

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

where the subscript 2 represents butylbenzene and 1 represents decane, undecane, or tetradecane.

This quantity is not constant over the whole two-phase region. Table 8 lists experimental values of *S*. From the data, we find the tendency that for the same system, the

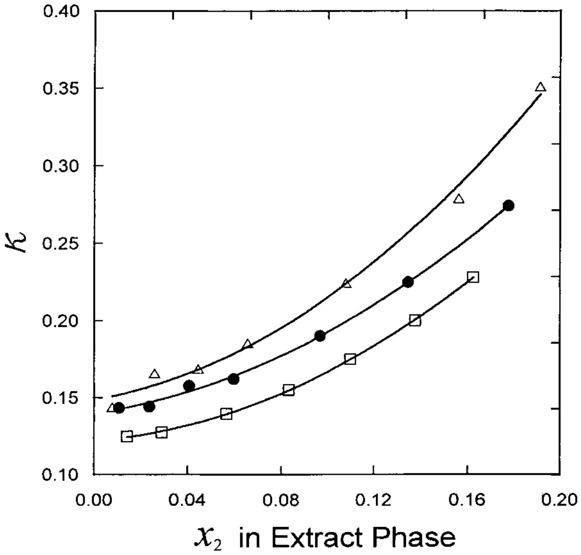

Figure 11. Experimental distribution coefficient of butylbenzene for decane (1) + butylbenzene (2) + sulfolane (3): (□) 323.15 K; (●) 348.15 K; (△) 373.15 K.

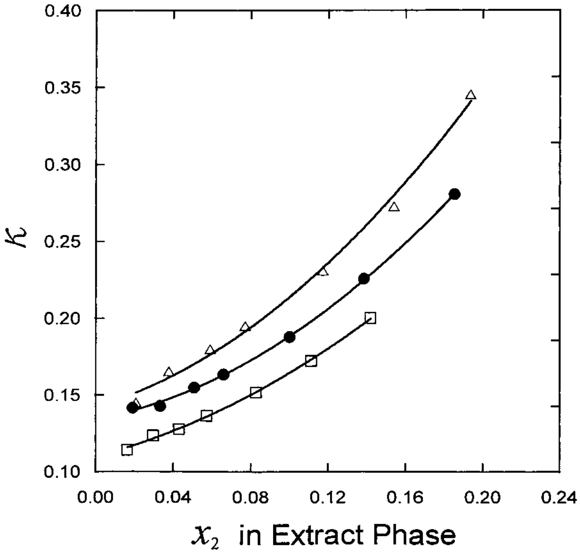

Figure 12. Experimental distribution coefficient of butylbenzene for undecane (1) + butylbenzene (2) + sulfolane (3): (□) 323.15 K; (●) 348.15 K; (△) 373.15 K.

higher the temperature, the lower the selectivity. At the same temperature for the different system, the order of the selectivity of sulfolane to butylbenzene is tetradecane > undecane > decane. Since the selectivity in all cases is greater than 1, it means that extraction is possible.

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 butylbenzene, which is the measure of the solvent power or capacity of sulfolane, is given as

$$\kappa = (x_2)_{\text{sulfolane-rich phase}}/(x_2)_{\text{alkane-rich phase}} \tag{4}$$

The experimental values of κ of this study are presented in Figures 11−13.We can find the tendency that for the same system, the higher the temperature, the larger the κ value. However, an increase in the solvent capacity of sulfolane leads to a decrease in its selectivity or vice versa. To choose 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 (Rawat and Gulati, 1976).

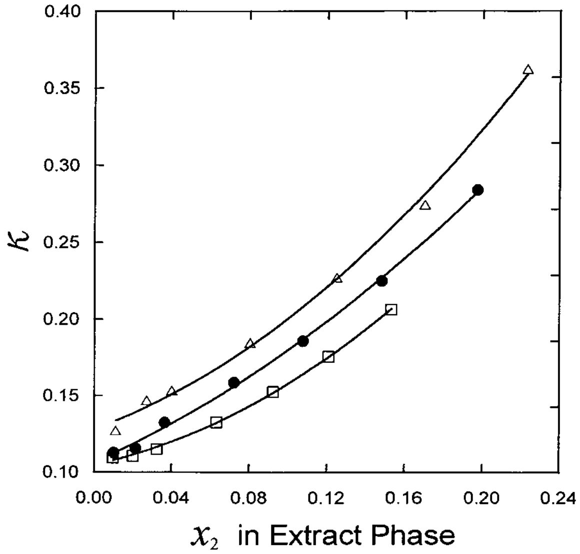

Figure 13. Experimental distribution coefficient of butylbenzene for the tetradecane (1) + butylbenzene (2) + sulfolane (3): (□) 323.15 K; (●) 348.15 K; (△) 373.15 K.

Conclusions

Liquid−liquid equilibrium data of the ternary systems decane + butylbenzene + sulfolane, undecane + butylbenzene + sulfolane, and tetradecane + butylbenzene + sulfolane were determined at 323.15 K, 348.15 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. From the selectivity data, the separation of butylbenzene from decane, undecane, or tetradecane by extraction with sulfolane is feasible.

Nomenclature

F = objective function to minimize (eq 1)
g_{ij} = NRTL parameter, J/mol
N = number of experimental tie lines (eq 2)
R = universal gas constant, J/(mol·K)
rmsd = root mean square deviation (eq 2)
S = selectivity (eq 3)
T = temperature, K
u_{ij} = UNIQUAC parameter, J/mol
x = mole fraction

Greek Letters

α_{ij} = nonrandomness parameter in NRTL model
κ = distribution coefficient (eq 4)

Subscripts

i = component i
j = component j
k = tie line k
L = phase L

Superscripts

c = calculated values

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Received for review January 18, 1999. Accepted March 31, 1999. The authors thank the National Science Council, NSC87-2214-E006-011, for the financial support of this work.

JE990020K