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

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Equilibrium tie line data have been determined at (323.15, 348.15, and 373.15) K for the ternary liquid−liquid equilibria (LLE) of three alkane + hexylbenzene + sulfolane systems, where the alkanes studied are decane, dodecane, and tetradecane. The relative mutual solubility of hexylbenzene is higher in decane + sulfolane than in dodecane + 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 distribution coefficients were calculated from the equilibrium data.

Introduction

Ternary liquid−liquid equilibrium (LLE) data are essential for a proper understanding of the solvent extraction process. Sulfolane is widely used in the chemical industry for the extraction of aromatics,[1−4] and many investigators[5−15] have studied the 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 alkanes with carbon number larger than nine[16−18] are scarce.

In this study, decane, dodecane, tetradecane, and hexylbenzene were taken as the model compounds for the kerosene range, combined with sulfolane to generate the data for these systems to aid the correlation of LLE. The LLE data for these ternary systems were measured at (323.15, 348.15, and 373.15) K and correlated using the UNIQUAC model of Abrams and Prausnitz[19] and the NRTL model of Renon and Prausnitz.[20]

Experimental Section

Chemicals. Sulfolane, decane, dodecane, anisole, and carbon disulfide were supplied by E. Merck with a stated purity of 99.0 %. Tetradecane was obtained from Tokyo Kasei Organic Chemical Industry Company with a purity of more than 99.0 %. Hexylbenzene was obtained from the Acros Organics, and further purification was achieved by distillation. The purities of all materials were checked by gas chromatograph and found to be better than 99.0 %. All compounds were stored in a desiccator with a drying agent before use.

Table 1. Experimental LLE Data for the Decane (1) + Hexylbenzene (2) + Sulfolane (3) System

	alkane-rich phase			sulfolane-rich phase		
T/K	x_{11}	x_{21}	x_{31}	x_{12}	x_{22}	x_{32}
323.15	0.995	0.000	0.005	0.004	0.000	0.996
	0.886	0.108	0.006	0.004	0.007	0.989
	0.735	0.254	0.011	0.004	0.018	0.978
	0.596	0.389	0.015	0.003	0.030	0.967
	0.465	0.510	0.025	0.003	0.042	0.955
	0.304	0.654	0.042	0.002	0.057	0.941
	0.189	0.748	0.063	0.002	0.068	0.930
	0.089	0.825	0.086	0.001	0.082	0.917
	0.000	0.876	0.124	0.000	0.099	0.901
348.15	0.991	0.000	0.009	0.006	0.000	0.994
	0.890	0.100	0.010	0.005	0.008	0.987
	0.771	0.213	0.016	0.005	0.018	0.977
	0.640	0.336	0.024	0.005	0.032	0.963
	0.484	0.481	0.035	0.005	0.046	0.949
	0.352	0.591	0.057	0.004	0.062	0.934
	0.240	0.676	0.084	0.003	0.075	0.922
	0.121	0.752	0.127	0.002	0.090	0.908
	0.000	0.797	0.203	0.000	0.124	0.876
373.15	0.986	0.000	0.014	0.009	0.000	0.991
	0.885	0.100	0.015	0.007	0.011	0.982
	0.741	0.235	0.024	0.007	0.027	0.966
	0.599	0.360	0.041	0.006	0.043	0.951
	0.435	0.496	0.069	0.006	0.060	0.934
	0.335	0.569	0.096	0.005	0.071	0.924
	0.227	0.640	0.133	0.005	0.085	0.910
	0.081	0.670	0.249	0.003	0.114	0.883
	0.000	0.591	0.409	0.000	0.161	0.839

Apparatus and Procedure. The experimental tie line data in the two-phase region was determined by using a 50 cm^3 jacketed glass cell controlled at a temperature of (323.15, 348.15, or 373.15) K ± 0.03 K. Specific amounts of alkane, sulfolane, and hexylbenzene were introduced into the cell and agitated while 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 1100 rpm and then allowed to settle for at least 5 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 the internal standard and diluted with 50 g of carbon disulfide[6] to prepare them for analysis. The accuracy of weighing was ± 0.0001 g. The sample analysis was performed by 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^{-1}, and the flow rate of nitrogen carrier gas was 2.5 × 10^{-5} m^3·min^{-1}. The calibration graphs for all components were prepared prior to the determination of the composition of the two phases. Mass fraction measurements were reproducible

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Table 2. Experimental LLE Data for the Dodecane (1) + Hexylbenzene (2) + Sulfolane (3) System

	alkane-rich phase			sulfolane-rich phase		
T/K	x_{11}	x_{21}	x_{31}	x_{12}	x_{22}	x_{32}
323.15	0.995	0.000	0.005	0.002	0.000	0.998
	0.847	0.147	0.006	0.002	0.009	0.989
	0.689	0.298	0.013	0.001	0.021	0.978
	0.550	0.433	0.017	0.001	0.034	0.965
	0.396	0.576	0.028	0.001	0.048	0.951
	0.244	0.709	0.047	0.001	0.065	0.934
	0.144	0.789	0.067	0.000	0.078	0.922
	0.000	0.876	0.124	0.000	0.099	0.901
348.15	0.990	0.000	0.010	0.004	0.000	0.996
	0.888	0.101	0.011	0.004	0.009	0.987
	0.741	0.245	0.014	0.004	0.022	0.974
	0.601	0.376	0.023	0.004	0.036	0.960
	0.491	0.475	0.034	0.003	0.046	0.951
	0.380	0.573	0.047	0.003	0.057	0.940
	0.289	0.645	0.066	0.003	0.069	0.928
	0.142	0.746	0.112	0.002	0.091	0.907
	0.000	0.797	0.203	0.000	0.124	0.876
373.15	0.983	0.000	0.017	0.005	0.000	0.995
	0.835	0.143	0.022	0.005	0.013	0.982
	0.691	0.276	0.033	0.005	0.029	0.966
	0.576	0.382	0.042	0.005	0.040	0.955
	0.484	0.459	0.057	0.005	0.051	0.944
	0.334	0.577	0.089	0.005	0.069	0.926
	0.230	0.642	0.128	0.004	0.082	0.914
	0.085	0.689	0.226	0.003	0.110	0.887
	0.000	0.590	0.410	0.000	0.161	0.839

Table 3. Experimental LLE Data for the Tetradecane (1) + Hexylbenzene (2) + Sulfolane (3) System

	alkane-rich phase			sulfolane-rich phase		
T/K	x_{11}	x_{21}	x_{31}	x_{12}	x_{22}	x_{32}
323.15	0.994	0.000	0.006	0.001	0.000	0.999
	0.894	0.100	0.006	0.001	0.006	0.993
	0.762	0.229	0.009	0.001	0.016	0.983
	0.589	0.398	0.013	0.001	0.027	0.972
	0.445	0.533	0.022	0.001	0.039	0.960
	0.294	0.667	0.039	0.001	0.055	0.944
	0.135	0.799	0.066	0.000	0.075	0.925
	0.000	0.876	0.124	0.000	0.099	0.901
348.15	0.988	0.000	0.012	0.002	0.000	0.998
	0.882	0.105	0.013	0.002	0.007	0.991
	0.743	0.242	0.015	0.002	0.017	0.981
	0.539	0.434	0.027	0.002	0.035	0.963
	0.392	0.568	0.040	0.001	0.051	0.948
	0.289	0.653	0.058	0.001	0.063	0.936
	0.188	0.728	0.084	0.001	0.078	0.921
	0.090	0.786	0.124	0.001	0.096	0.903
	0.000	0.797	0.203	0.000	0.124	0.876
373.15	0.978	0.000	0.022	0.004	0.000	0.996
	0.879	0.097	0.024	0.004	0.008	0.988
	0.783	0.192	0.025	0.003	0.017	0.980
	0.600	0.369	0.031	0.003	0.036	0.961
	0.489	0.464	0.047	0.003	0.048	0.949
	0.391	0.545	0.064	0.002	0.061	0.937
	0.182	0.679	0.139	0.001	0.092	0.907
	0.091	0.701	0.208	0.001	0.113	0.886
	0.000	0.591	0.409	0.000	0.161	0.839

to within ± 0.005. The greatest error in the material balance in these experiments was found to be less than 2 %.

Results

The experimental tie line data are given in Tables 1 to 3 for the ternary systems formed by sulfolane (3) + hexylbenzene (2) with decane, dodecane, or tetradecane (1), respectively. Concentrations of components i ($i = 1, 2, 3$) in phase L ($L = 1$, alkane-rich phase; $L = 2$, sulfolane-rich phase) are given in mole fraction, x_{iL}. The effect of temperature on the equilibrium for the decane (1) + hexylbenzene (2) + sulfolane (3) system is shown in Figure 1. As expected, the size of the two-phase region decreases with an increase in temperature. Similar behavior was also noticed in the other two ternaries. The three systems studied present a wide two-phase region that is important, together with the slope of the tie lines, when establishing the selectivity of sulfolane.

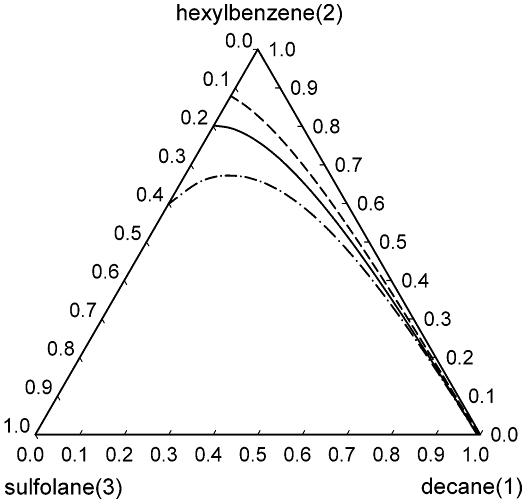

Figure 1. Effect of temperature on the liquid−liquid equilibrium for the decane (1) + hexylbenzene (2) + sulfolane (3) system. Curves calculated by UNIQUAC: − −, 323.15 K; −, 348.15 K; − · −, 373.15 K.

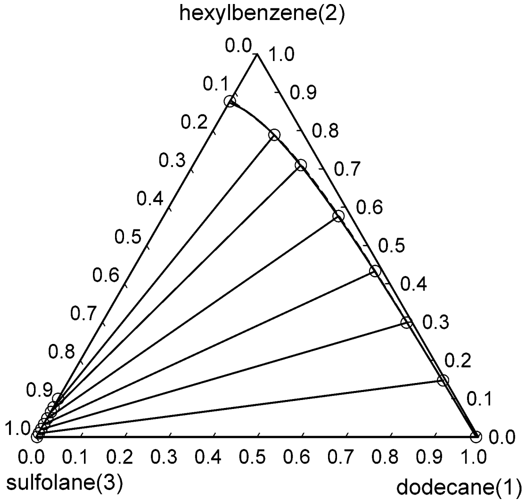

Figure 2. LLE data for the dodecane (1) + hexylbenzene (2) + sulfolane (3) system at 323.15 K. Curves calculated by −, UNIQUAC model; − −, NRTL model; ○−○, experimental tie line.

Data Correlation. The UNIQUAC and NRTL 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

$$F = \min \sum_{i} \sum_{L} \sum_{k} (x_{iLk} - x^{c}_{iLk})^2 \tag{1}$$

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.[8] The parameters calculated are

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

		UNIQUAC parameters/K			NRTL parameters/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	−141.20	176.32	0.00138	−657.68	1251.50	0.00198
	1−3	517.26	50.30		1194.00	1226.30	
	2−3	310.49	−29.32		455.79	577.91	
348.15	1−2	−46.42	55.30	0.00197	−560.31	1042.80	0.00440
	1−3	510.27	54.27		1041.70	1237.800	
	2−3	273.27	−11.05		331.48	670.37	
373.15	1−2	−62.62	97.78	0.00337	−489.44	741.41	0.00505
	1−3	493.18	121.98		1343.20	1351.10	
	2−3	172.86	48.99		128.04	837.67	

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

		UNIQUAC parameters/K			NRTL parameters/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	29.30	−35.24	0.00207	−707.68	1444.70	0.00219
	1−3	515.20	52.70		1161.00	1487.60	
	2−3	303.21	−25.97		446.29	587.75	
348.15	1−2	−132.69	169.43	0.00237	−587.81	932.77	0.00191
	1−3	539.51	48.47		1269.90	1296.30	
	2−3	275.61	−14.81		354.42	650.19	
373.15	1−2	25.26	−4.67	0.00341	−222.89	162.61	0.00810
	1−3	402.47	151.12		1381.00	1228.10	
	2−3	176.22	46.20		156.05	802.77	

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

		UNIQUAC parameters/K			NRTL parameters/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	−2.18	1.32	0.00187	−850.82	1440.10	0.00313
	1−3	526.17	37.22		1155.10	1438.90	
	2−3	315.24	−30.31		442.57	568.26	
348.15	1−2	−186.04	259.81	0.00276	−909.74	1457.50	0.00313
	1−3	520.89	51.77		1129.10	1445.30	
	2−3	277.73	−12.25		345.96	648.61	
373.15	1−2	−19.06	35.24	0.00447	−982.22	1497.70	0.00814
	1−3	549.67	82.87		1268.50	1494.80	
	2−3	175.05	46.19		145.04	822.75	

shown in Tables 4 to 6, together with the root-mean-square deviation (rmsd) values, defined as

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

where N = the number of tie lines.

As can be seen from Tables 4 to 6, the calculation 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 rmsd phase composition error was 0.00263 for UNIQUAC as compared to 0.00422 for NRTL).

Discussion

The slopes of the tie lines presented in Figures 2 to 7 show that hexylbenzene is more soluble in alkanes than in sulfolane. It is observed that the relative mutual solubility of hexylbenzene is higher in decane + sulfolane than in dodecane + sulfolane or tetradecane + sulfolane mixtures at the same temperature. This effect is the most significant at 373.15 K. This solubility effect is reflected in the size of the two-phase region, increasing slightly in the order tetradecane > dodecane > 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:

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

where subscript 2 represents hexylbenzene and subscript 1 represents decane, dodecane, or tetradecane.

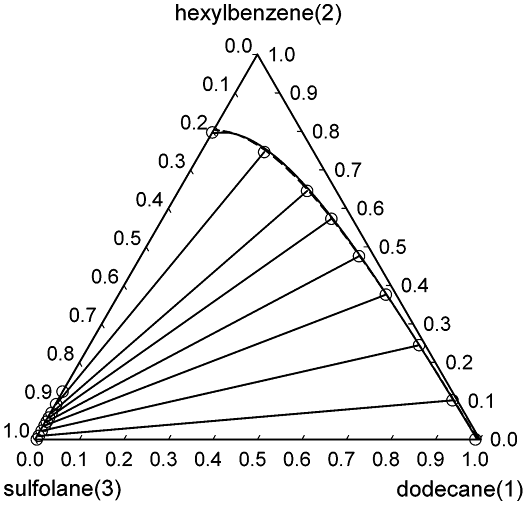

Figure 3. LLE data for the dodecane (1) + hexylbenzene (2) + sulfolane (3) system at 348.15 K. Curves calculated by —, UNIQUAC model; – –, NRTL model; ○–○, experimental tie line.

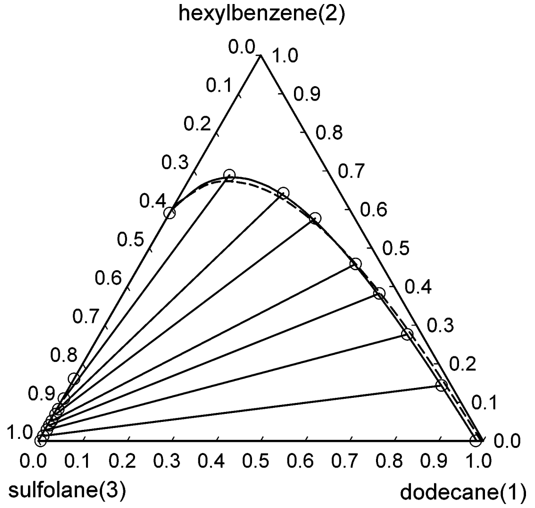

Figure 4. LLE data for the dodecane (1) + hexylbenzene (2) + sulfolane (3) system at 373.15 K. Curves calculated by —, UNIQUAC model; – –, NRTL model; ○—○, experimental tie line.

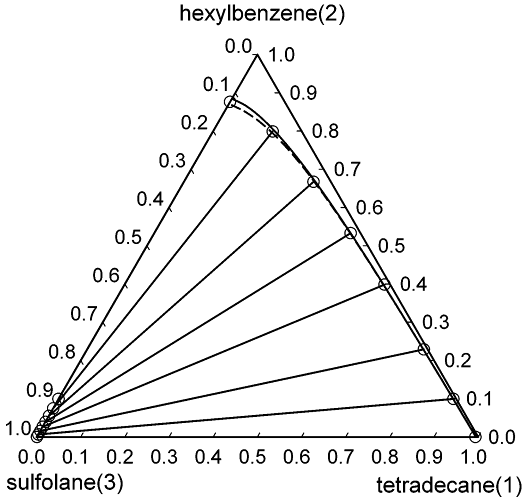

Figure 5. LLE data for the tetradecane (1) + hexylbenzene (2) + sulfolane (3) system at 323.15 K. Curves calculated by —, UNIQUAC model; – –, NRTL model; ○—○, experimental tie line.

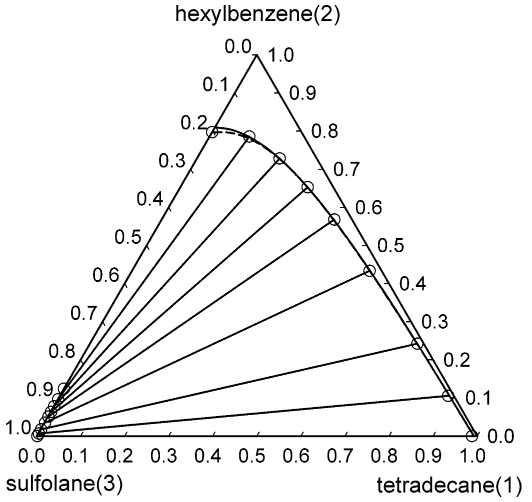

Figure 6. LLE data for the tetradecane (1) + hexylbenzene (2) + sulfolane (3) system at 348.15 K. Curves calculated by —, UNIQUAC model; – –, NRTL model; ○—○, experimental tie line.

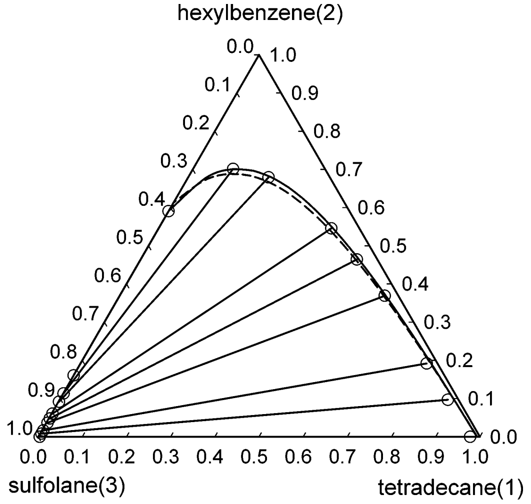

Figure 7. LLE data for the tetradecane (1) + hexylbenzene (2) + sulfolane (3) system at 373.15 K. Curves calculated by —, UNIQUAC model; – –, NRTL model; ○—○, experimental tie line.

Table 7. Experimental Selectivity Values *S* for Each Tie Line

S for the system	323.15 K	348.15 K	373.15 K
decane	15.1	14.5	12.9
	14.7	13.4	12.4
	14.2	12.6	10.8
	13.8	10.3	9.0
	12.1	9.5	8.0
	10.2	7.8	6.1
	9.8	6.3	3.9
dodecane	36.4	19.2	14.2
	36.2	16.8	14.0
	35.5	15.2	12.7
	30.0	13.1	11.1
	24.8	11.4	8.5
	23.7	10.3	7.0
		8.3	4.4
tetradecane	64.9	30.7	21.0
	58.8	29.8	20.6
	49.3	24.1	19.1
	46.8	23.4	18.6
	0.3	23.3	18.8
	25.3	22.3	17.5
		18.4	16.3

This quantity is not constant over the whole two-phase region. Table 7 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 system, the order of the selectivity of sulfolane to hexylbenzene is tetradecane > dodecane > decane. Since the selectivity in all cases is greater than one, it means that extraction is possible.

The distribution coefficient of hexylbenzene over the two liquid phases in equilibrium is defined as

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

This coefficient is related to the number of theoretical stages that are necessary for a given extraction. The lower the number of theoretical stages is necessary for the larger κ values. The experimental values of κ in this study is presented in Table 8. We can find the tendency that for the same system, the higher the temperature, the larger the κ value. Also in our three different systems, there are not obvious differences between the κ values at the same temperature.

Conclusions

LLE data of the ternary systems decane (1) + hexylbenzene (2) + sulfolane (3), dodecane (1) + hexylbenzene (2) + sulfolane (3), and tetradecane (1) + hexylbenzene (2) +

Table 8. Experimental Distribution Coefficient Values κ for Each Tie Line

κ for the system	323.15 K	348.15 K	373.15 K
decane	0.065	0.083	0.105
	0.070	0.085	0.114
	0.076	0.094	0.119
	0.083	0.096	0.121
	0.087	0.105	0.124
	0.091	0.110	0.133
	0.100	0.120	0.170
dodecane	0.064	0.089	0.089
	0.068	0.091	0.105
	0.077	0.096	0.106
	0.083	0.096	0.112
	0.091	0.099	0.120
	0.098	0.106	0.128
		0.122	0.159
tetradecane	0.065	0.063	0.084
	0.069	0.072	0.087
	0.067	0.081	0.099
	0.074	0.089	0.103
	0.082	0.097	0.111
	0.093	0.107	0.135
		0.123	0.162

sulfolane (3) were determined at (323.15, 348.15, and 373.15) K, respectively.

From the selectivity data, the separation of hexylbenzene from decane, dodecane, or tetradecane by extraction with sulfolane is feasible. 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 for the systems studied here were drawn to investigate the temperature dependence. The size of the two-phase region decreases with increasing temperature.

Literature Cited

(1) Broughton, D. B.; Asselin, G. F. Production of high purity aromatics by the sulfolane process. *Seventh World Pet. Congr. Proc.* **1967**, *4*, 65−73.

(2) Evans, H. D. Extraction process. U.S. Patent 3,222,416, 1965.

(3) Guccione, E. Largest aromatics plant is on stream. *Chem. Eng.* **1965**, *72*, 112−114.

(4) Wheeler, T. *Handbook of Petroleum Refining Processes*; McGraw-Hill: New York, 1986.

(5) Ashour, I.; Abu-Eishah, S. I. Liquid−liquid equilibria of ternary and six-component systems including cyclohexane, benzene, toluene, ethylbenzene, cumene, and sulfolane at 303.15 K. *J. Chem. Eng. Data* **2006**, *51*, 1717−1722.

(6) Cassell, G. W.; Dural, N.; Hines, A. L. Liquid−liquid equilibria of sulfolane−benzene−pentane and sulfolane−toluene−pentane. *Ind. Eng. Chem. Res.* **1989**, *28*, 1369−1374.

(7) Cassell, G. W.; Hassan, M. M.; Hines, A. L. Correlation of the phase equilibrium data for the heptane−toluene−sulfolane and heptane−xylene−sulfolane systems. *J. Chem. Eng. Data* **1989**, *34*, 434−438.

(8) Cassell, G. W.; Hassan, M. M.; Hines, A. L. Phase equilibria of the cyclohexane−toluene−sulfolane and hexane−toluene−sulfolane ternary systems. *Chem. Eng. Commun.* **1989**, *85*, 233−243.

(9) Chen, J.; Li, Z.; Duan, L. Liquid−liquid equilibria of ternary and quaternary systems including cyclohexane, 1-heptene, benzene, toluene, and sulfolane at 298.15 K. *J. Chem. Eng. Data* **2000**, *45*, 689−692.

(10) De Fré, R. M.; Verhoeye, L. A. The prediction of the ternary liquid−liquid equilibrium by means of the NRTL-equation. *J. Appl. Chem. Biotechnol.* **1977**, *27*, 667−679.

(11) Lee, S.; Kim, H. Liquid−liquid equilibria for the ternary systems sulfolane + octane + benzene, sulfolane + octane + toluene and sulfolane + octane + *p*-xylene. *J. Chem. Eng. Data* **1995**, *40*, 499−503.

(12) Lee, S.; Kim, H. Liquid−liquid equilibria for the ternary systems sulfolane + octane + benzene, sulfolane + octane + toluene and sulfolane + octane + *p*-xylene at elevated temperatures. *J. Chem. Eng. Data* **1998**, *43*, 358−361.

(13) Letcher, T. M.; Redhi, G. G.; Radloff, S. E. Liquid−liquid equilibria of the ternary mixtures with sulfolane at 303.15 K. *J. Chem. Eng. Data* **1996**, *41*, 634−638.

(14) Lin, W. C.; Kao, N. H. Liquid−liquid equilibria of octane + (benzene or toluene or *m*-xylene) + sulfolane at 323.15, 348.15, and 373.15 K. *J. Chem. Eng. Data* **2002**, *47*, 1007−1011.

(15) Tripathi, R. P.; Ram, A. R.; Rao, P. B. Liquid−liquid equilibria in ternary system toluene−*n*-heptane−sulfolane. *J. Chem. Eng. Data* **1975**, *20*, 261−264.

(16) Kao, C. F.; Lin, W. C. Liquid−liquid equilibria of alkane (C10−C14) + butylbenzene + sulfolane. *J. Chem. Eng. Data* **1999**, *44*, 803−808.

(17) Lin, W. C.; Yang, C. H.; Tsai, T. H. Influence of the temperature on the liquid−liquid equilibria of tridecane + butylbenzene + sulfolane and tridecane + 1,4-diisopropylbenzene + sulfolane. *J. Chem. Eng. Data* **2002**, *47*, 245−249.

(18) Masohan, A.; Nanoti, S. M.; Sharma, K. G.; Puri, S. N.; Gupta, P.; Rawat, B. S. Liquid−liquid equilibria studies on hydrocarbon (C10−C20)-sulfolane systems. *Fluid Phase Equilib.* **1990**, *61*, 89−98.

(19) Abrams, D. S.; Prausnitz, J. M. Statistical thermodynamics of liquid mixtures: a new expression for the excess Gibbs energy of partly or completely miscible systems. *AIChE J.* **1975**, *21*, 116−128.

(20) Renon, H.; Prausnitz, J. M. Local compositions in thermodynamic excess functions for liquid mixtures. *AIChE J.* **1968**, *14*, 135−144.

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