J. Chem. Eng. Data **2006,** *51,* 859−863

Liquid−Liquid Equilibria for Cyclohexane + Ethylbenzene + Sulfolane at (303.15, 313.15, and 323.15) K

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Liquid−liquid equilibrium for cyclohexane + ethylbenzene + sulfolane have been measured at the temperatures (303.15, 313.15, and 323.15) K and at atmospheric pressure. The reliability of the experimental data was tested using the Othmer−Tobias correlation. The liquid−liquid equilibrium (LLE) data were then analyzed using a UNIFAC model with group interaction parameters extracted from the LLE data bank (UNIF-LL) and a NRTL version with temperature-dependent binary parameters determined from the experimental LLE data (NRTL/2); both as programmed by the Aspen Plus simulator. On the basis of the analysis of these data, both models represented the experimental data with sufficient accuracy as revealed from the very small values of the root-mean-square error (RMSE) and the average absolute deviation (AAD) in composition.

Introduction

Extraction of aromatics from catalytic reformates pyrolysis naphtha, kerosene, and superior kerosene has potential commercial importance in the oil refining industry. There are many processes used to separate aromatics, for instance, utilizing transition metals.[1] The most widely used process for separating aromatics from different paraffins is liquid extraction. In 1976, Rawat et al.[2] studied 19 organosulfur solvents as potential solvents for the extraction of aromatics using gas chromatography. Solvents for the extraction should have high selectivity for aromatics, high capacity, high density, low viscosity, and partial miscibility with the hydrocarbon mixtures at reasonably low temperatures.[3] They also must have good thermal stability, low reactivity, and minimum corrosion characteristics in addition to being environmentally friendly. Many organic solvents have been investigated for extracting aromatics, for example, sulfolane,[4−22] diethylene glycol,[23,24] triethylene glycol,[25,26] tetraethylene glycol,[27−30] propylene carbonate,[26,31] dimethyl sulfoxide,[32] *N*-methylpyrrolidone,[33] ethylene carbonate,[34] γ-butyrolactone,[35] and ionic liquids.[36,37] Combinations of solvents to balance selectivity and solvency have also been investigated.[38−40]

Accurate phase equilibrium data are important parameters for the design and evaluation of industrial unit operations for the extraction processes. Liquid−liquid equilibrium (LLE) data for cyclohexane + ethylbenzene + sulfolane systems are scarce in the literature. Although the technical literature is very rich on the subject of solvent extraction of some aromatics such as benzene, toluene, and xylene ternary systems, Table 1 reveals that, in general, studies involving ethylbenzene are scarce. Moreover, ternary phase equilibrium data are essential for the proper understanding of the solvent extraction processes, selection of solvents, and design of extractors.

The objective of the present work is to measure the LLE data for the ternary system cyclohexane + ethylbenzene + sulfolane at the temperatures (303.15, 313.15, and 323.15) K under atmospheric pressure conditions. Additionally, a predictive activity coefficient model (UNIF-LL) will be used to demonstrate its predictive capacity for the resulting data. This model has group interaction parameters extracted from the LLE data bank.[41] In addition, a Non-Random Two-Liquid model (called NRTL/2) will be used to correlate the experimental LLE data. This model is usually suitable for highly non-ideal systems and has temperature-dependent binary parameters determined from the LLE data.[41] The UNIF-LL model gave accurate predictions in comparison with other models used in previous studies.[23,42] Julia et al.[43] stated that it is very risky to employ the NRTL parameters from any data bank in predicting the phase equilibria of other ternary mixtures that are not included in obtaining such parameters in those data banks. The statement of Julia et al.[43] should apply to any thermodynamic model, not only the NRTL activity coefficient model.

Experimental Section

Synthetic-grade chemicals were used in this work and supplied as follows: sulfolane by Merck with a stated purity of 99 % (< 0.2 % H_2O), ethylbenzene by BDH with a stated purity of 99 %, and cyclohexane by Riedel-DeHaen with a stated purity of 99.5 % (< 0.01 % H_2O). All materials were used as received without any further purification.

The equilibrium experimental data were determined using a tightly closed, jacketed equilibrium cell with 100 mL volume. The temperature was measured with a mercury-in-glass thermometer with uncertainty of ± 0.1 K. The temperature in the jacket of the cell was kept constant by circulating water from a water bath (Julabo Labortechnik GmbH, Germany) equipped with a temperature controller (Julabo PC) capable of maintaining

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10.1021/je050227f CCC: $33.50

Table 1. Liquid−Liquid Equilibrium Studies of Systems Containing Sulfolane (3)

substance (1)	substance (2)	t/°C	ref
benzene	pentane	17, 25, 50	4
benzene	hexane	9, 50, 75, 100	8,9,10
benzene	cyclohexane	25	8
benzene	heptane	25, 30	7,26
benzene	octane	25, 35, 40, 45, 50, 70.2, 75, 99.2, 100, 129.2	8,9,13−15
benzene	decane	30	7
benzene	dodecane	30	7
toluene	pentane	17, 25, 50	4
toluene	hexane	17, 25, 35, 40, 50	5,6,9,13
toluene	cyclohexane	17, 25, 50	5,6,8
toluene	2-methylpentane	25	6
toluene	1-hexene	25	6
toluene	heptane	25	8,32
toluene	octane	25, 35, 40, 45, 50 70.2, 75, 99.2, 100, 129.2	9,13−15
p-xylene	cyclohexane	35, 50	12
p-xylene	hexane	35, 50	12
p-xylene	heptane	30	7
p-xylene	octane	25, 35, 45, 70.2, 99.2, 129.2	7,13,14
m-xylene	heptane	30, 40	16
m-xylene	heptane	25	8
m-xylene	octane	50, 75, 100	15
ethylbenzene	cyclohexane	30, 40, 50	This work
butylbenzene	decane	50, 75, 100	17
butylbenzene	tetradecane	50, 75, 100	17
butylbenzene	dodecane	60, 100	22
butylbenzene	undecane	50, 75, 100	17
butylbenzene	tridecane	50, 60, 75, 87.5, 100	21
1,4-diisopropylbenzene	decane	50, 75, 100	18
1,4-diisopropylbenzene	tridecane	50, 60, 75, 87.5, 100	21
1,4-diisopropylbenzene	dodecane	50, 75, 100	18
1,4-diisopropylbenzene	tetradecane	50, 75, 100	18
octylbenzene	decane	50, 75, 100	19
octylbenzene	cetane	60, 100	22
octylbenzene	dodecane	50, 60, 75, 100	19, 22
octylbenzene	tetradecane	50, 75, 100	19
hexylbenzene	cetane	60, 100	22
hexylbenzene	dodecane	60, 100	22
tetralin	cetane	60, 100	20
butyltetralin	cetane	60, 100	20
hexyltetralin	cetane	60, 100	20

Table 2. Experimental LLE Data of Cyclohexane (1) + Ethylbenzene (2) + Sulfolane (3) System at (303.15, 313.15, and 323.15) K

feed mass fractions			mass fractions in upper layer (cyclohexane-rich phase)			mass fractions in lower layer (sulfolane-rich phase)		
w_1	w_2	w_3	w_1	w_2	w_3	w_1	w_2	w_3
				T = 303.15 K				
0.3876	0.0	0.6124	0.9978	0.0	0.0022	0.0290	0.0	0.9710
0.3654	0.0407	0.5940	0.9186	0.0757	0.0057	0.0292	0.0169	0.9539
0.3539	0.0801	0.5660	0.8425	0.1489	0.0086	0.0315	0.0334	0.9351
0.3296	0.1470	0.5234	0.7286	0.2574	0.0140	0.0304	0.0606	0.9090
0.3058	0.2053	0.4889	0.6238	0.3533	0.0228	0.0332	0.0869	0.8800
0.2885	0.2574	0.4545	0.5494	0.4167	0.0339	0.0326	0.1044	0.8630
0.2686	0.2994	0.4320	0.4856	0.4766	0.0377	0.0308	0.1335	0.8357
				T = 313.15 K				
0.3812	0.0	0.6188	0.9947	0.0	0.0053	0.0269	0.0	0.9731
0.3634	0.0416	0.5951	0.9090	0.0834	0.0076	0.0308	0.0186	0.9506
0.3474	0.0776	0.5749	0.8369	0.1528	0.0103	0.0321	0.0347	0.9333
0.3200	0.1479	0.5321	0.7214	0.2604	0.0181	0.0324	0.0638	0.9038
0.3093	0.1794	0.5110	0.6661	0.3122	0.0217	0.0327	0.0780	0.8893
0.2993	0.2047	0.4956	0.6237	0.3488	0.0275	0.0346	0.0901	0.8752
0.2790	0.2572	0.4638	0.5466	0.4139	0.0394	0.0355	0.1152	0.8493
0.2617	0.3022	0.4361	0.4747	0.4786	0.0467	0.0321	0.1386	0.8292
				T = 323.15 K				
0.3847	0.0	0.6153	0.9946	0.0	0.0054	0.0314	0.0	0.9686
0.3661	0.0420	0.5919	0.9069	0.0837	0.0094	0.0332	0.0186	0.9482
0.3531	0.0800	0.5669	0.8318	0.1526	0.0157	0.0371	0.0360	0.9269
0.3271	0.1473	0.5257	0.7106	0.2610	0.0285	0.0408	0.0683	0.8909
0.3184	0.1761	0.5056	0.6620	0.3095	0.0285	0.0365	0.0786	0.8849
0.3067	0.2021	0.4912	0.6162	0.3441	0.0398	0.0403	0.0944	0.8653
0.2854	0.2570	0.4576	0.5319	0.4093	0.0588	0.0430	0.1236	0.8333
0.2667	0.2999	0.4334	0.4774	0.4605	0.0621	0.0349	0.1382	0.8269

the temperature at a fixed value (within ± 0.1 K). Mixtures of known masses of sulfolane, ethylbenzene, and cyclohexane were introduced into the cell and stirred for 2 h and then left for 8 h to equilibrate and settle down into a lower layer (sulfolane-rich phase) and an upper layer (cyclohexane-rich phase) under the same temperature.

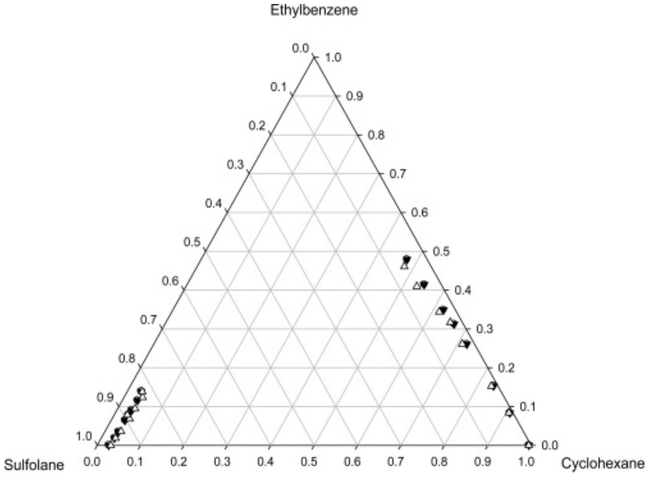

Figure 1. Experimental LLE data equilibrium molar compositions of the ternary system cyclohexane (1) + ethylbenzene (2) + sulfolane (3): ○, 303.15 K; ▼, 313.15 K; △, 323.15 K.

Table 3. Constants of the Othmer−Tobias Correlation and the Correlation Factor, R^2, for the Cyclohexane (1) + Ethylbenzene (2) + Sulfolane (3) System as a Function of Temperature

T/K	a	b	R^2
303.15	20.0348	1.7791	0.9956
313.15	16.7735	1.7073	0.9961
323.15	15.0023	1.6928	0.9913

Samples from both layers were carefully taken and analyzed using a gas chromatograph (Chrompack CP 9001) with a flame ionization detector (FID). Chromatographic separation of the mixture constituents was achieved using a 50 m long × 0.32 mm i.d. WCOT (wall-coated-open-tube) fused-silica capillary column coated with a 1.2 μm stationary film (CP-Sil 5CB). The inlet pressure of the carrier nitrogen gas was set to 30 kPa, and the temperatures of the detector and the injector were set to (300 and 275) °C, respectively. The oven temperature was programmed as follows: the initial temperature was set to 100 °C for 2 min followed by a constant heating rate of 20 K/min until a final temperature of 250 °C was attained. The final temperature was kept for 8 min, and then the cycle was repeated. Mixtures of known compositions of reagents were used to calibrate the gas chromatograph. Mass fraction measurements were reproducible to within ± 0.1 %. The greatest error in the material balance in these experiments was found to be less than 1 %.

Results and Discussion

A summary of citations of LLE studies of ternary systems involving sulfolane (including this work) are given in Table 1. The cited literature data span a temperature range of (17 to 130) °C in 120 isothermal data sets with more than 1200 experimental data points.

The experimental LLE data for the ternary system cyclohexane + ethylbenzene + sulfolane measured at (303.15, 313.15, and 323.15) K and at atmospheric pressure are shown in Table 2 and displayed on the triangular diagram shown in Figure 1. As expected, the size of the two-phase region decreases with the increase in temperature. It is clear from the data shown in Figure 1 (and also in Table 2) that the ethylbenzene has a much higher affinity toward cyclohexane (upper layer) than sulfolane (lower layer), while the lower layer is almost free of cyclohexane.

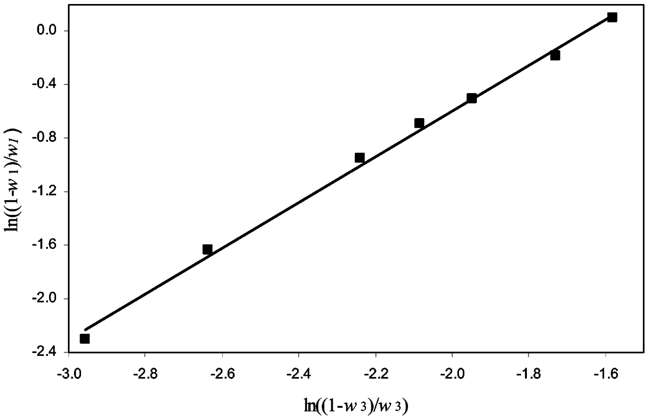

Figure 2. Othmer−Tobias plot of the cyclohexane (1) + ethylbenzene (2) + sulfolane (3) system at 313.15 K: ■, experimental; solid line, best linear fit.

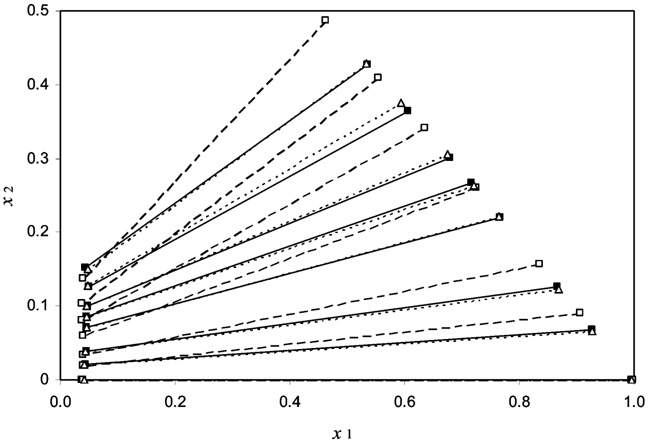

Figure 3. Experimental vs predicted LLE for cyclohexane (1) + ethylbenzene (2) + sulfolane (3) at 313.15 K. Data points: ■, experimental; □, predicted by UNIF-LL; △, correlated by NRTL/2. Tie lines: solid, experimental; dashed, UNIF-LL; dotted, NRTL/2.

Table 4. NRTL/2 Binary Parameters, $\{(g_{ij} - g_{jj})/R\}$ in Kelvin, for Cyclohexane (1) + Ethylbenzene (2) + Sulfolane (3) System as a Function of Temperature

component	$j = 1$	$j = 2$	$j = 3$
	$T = 303.15$ K		
$i = 1$	0	−26.9227	2120.03
$i = 2$	163.6422	0	278.2845
$i = 3$	1069.601	342.4102	0
	$T = 313.15$ K		
$i = 1$	0	278.509	1988.112
$i = 2$	−144.717	0	411.5768
$i = 3$	1107.662	244.5993	0
	$T = 323.15$ K		
$i = 1$	0	72.58506	2039.86
$i = 2$	61.52949	0	239.3701
$i = 3$	1106.816	386.8545	0

The reliability of the experimental data can be ascertained by applying the Othmer−Tobias correlation,[44] depicted in eq 1, at each temperature:

$$\ln\left(\frac{1 - w_{3L}}{w_{3L}}\right) = a + b\ln\left(\frac{1 - w_{1U}}{w_{1U}}\right) \tag{1}$$

or

$$\left(\frac{1 - w_{3L}}{w_{3L}}\right) = a\left(\frac{1 - w_{1U}}{w_{1U}}\right)^{b} \tag{2}$$

Table 5. RMSE and AAD in Liquid Mole Fractions as Obtained from UNIF-LL and NRTL/2 Models for the Cyclohexane (1) + Ethylbenzene (2) + Sulfolane (3) System at (303.15, 313.15, and 323.15) K

	$T = 303.15$ K						$T = 313.15$ K						$T = 323.15$ K					
	cyclohexane		ethylbenzene		sulfolane		cyclohexane		ethylbenzene		sulfolane		cyclohexane		ethylbenzene		sulfolane	
model	RMSE	AAD	RMSE	AAD	RMSE	AAD	RMSE	AAD	RMSE	AAD	RMSE	AAD	RMSE	AAD	RMSE	AAD	RMSE	AAD
upper layer (cyclohexane-rich phase)																		
UNIF-LL	0.043	0.035	0.040	0.038	0.006	0.004	0.042	0.037	0.041	0.039	0.005	0.004	0.054	0.048	0.058	0.055	0.003	0.002
NRTL/2	0.007	0.006	0.009	0.008	0.004	0.002	0.005	0.004	0.005	0.004	0.001	0.001	0.007	0.005	0.009	0.007	0.003	0.002
lower layer (sulfolane-rich phase)																		
UNIF-LL	0.008	0.007	0.015	0.013	0.021	0.019	0.007	0.007	0.015	0.013	0.021	0.018	0.011	0.001	0.008	0.007	0.017	0.015
NRTL/2	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.001	0.001	0.002	0.001	0.004	0.003	0.002	0.002	0.004	0.003

where w_{3L} = mass fraction of sulfolane (3) in the lower layer (sulfolane-rich phase), w_{1U} = mass fraction of cyclohexane (1) in the upper layer (cyclohexane-rich phase), and a and b are the fitting parameters of Othmer−Tobias correlation. The first data point, where no ethylbenzene exists in the mixture (i.e., $w_2 = 0$) is usually not included in this correlation. The values of a, b, and R^2 are given in Table 3 at (303.15, 313.15, and 323.15) K for reference. Figure 2 demonstrates the Othmer−Tobias plot at 313.15 K, as an example. The Othmer−Tobias plots are almost linear, and the values of the correlation factor R^2 are very close to unity.

The experimental data of this work were also used to examine the LLE predictive capability of some liquid-phase models. One version of the UNIFAC equation was examined; the UNIF-LL (with group interaction parameters extracted from the LLE data bank). In addition, NRTL/2 model, which has temperature-dependent binary parameters determined from the LLE data, was also used to correlate the LLE data. Both models are programmed in the Aspen Plus simulator.[41] The availability of a rich data bank of the required interaction parameters for the models employed by many simulators such as Aspen Plus provides, on one side, a good means to test for the cross-consistency of the emerging experimental LLE data[23] (i.e., agreement between different data sets when treated by the same model which uses the same interaction parameters for the different data sets). On the other side, the experimental LLE data for systems containing species of very limited solubility, like the system studied in this work, represents a tough test for the predictive models. Figure 3 depicts the experimental LLE data for the cyclohexane + ethylbenzene + sulfolane at 313.15 K along with those predicted by the UNIF-LL model and those correlated using the NRTL/2 model. Figure 3 also shows the experimental and predicted tie lines connecting the mole fractions in the two liquid phases. On the other hand, Table 4 shows the NRTL/2 binary parameters, $A_{ij} = \{(g_{ij} - g_{jj})/R$, in SI units, for each pair of components in the mixture with $A_{ii} = A_{jj} = 0$ and $A_{ij} \neq A_{ji}$. R is the universal gas constant, and g_{ij} is the energy parameter in the NRTL equation, K. The Aspen Plus simulator default values of the non-randomness factor, α_{ij}, were used: $\alpha_{12} = \alpha_{23} = 0.3$, $\alpha_{13} = 0.2$, with $\alpha_{ij} = \alpha_{ji}$.

Table 5 shows the root-mean-square error (RMSE) and the average absolute deviation (AAD) in composition (mole fractions) obtained using UNIF-LL (predictive) model and NRTL/2 (correlative) model. The RMSE and AAD are defined as follows:

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_i (x_i^{\mathrm{exp}} - x_i^{\mathrm{pred}})^2} \qquad (3)$$

$$\mathrm{AAD} = \frac{1}{N}\sum_i |x_i^{\mathrm{exp}} - x_i^{\mathrm{pred}}| \qquad (4)$$

where N is the number of data points and x_i is the mole fraction of component i. For the three LLE data sets of cyclohexane + ethylbenzene + sulfolane system of this work, both UNIF-LL and NRTL/2 models represent the experimental data quite well, and the predictions are accurate enough as demonstrated by the very small values of the RMSE and the AAD presented in Table 5. Last, by increasing the temperature, the representation of the experimental LLE data is slightly decreasing for both models; the NRTL/2 correlative model performs better than the predictive UNIF-LL model.

Conclusions

The liquid−liquid equilibrium data for the cyclohexane + ethylbenzene + sulfolane system were measured at the temperatures (303.15, 313.15, and 323.15) K and at atmospheric pressure. The linearity of the Othmer−Tobias plots and the values of the correlation factor (R^2 very close to 1.0) proved the consistency of the experimental measurements. The LLE data of this work were then analyzed using the UNIF-LL predictive model and the NRTL/2 correlative model as programmed by the Aspen Plus simulator. On the basis of the analysis of these data, both models represented the experimental data with sufficient accuracy as revealed from the very small RMSE and AAD values for composition.

Acknowledgment

The contributions of Dr. Ali Dowaidar in the analysis of the experimental data and the chemist Hasan Kamal in helping with the running of the experiments are highly appreciated.

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Received for review June 14, 2005. Accepted February 3, 2006. This work was financially supported by the Research Affairs at the United Arab Emirates University under Contract 06-02-7-11/05.

JE050227F