Measurement and Correlation of Phase Equilibria for Dodecane + *sec*-Butylbenzene + *N*-Methyl-2-pyrrolidone

Adel S. Al-Jimaz,* Mohamed S. Fandary, and Jasem A. Al-Kandary

Chemical Engineering Department, College of Technological Studies, P.O. Box 3242, Salmyiah 22033, Kuwait

Mohamed A. Fahim

Chemical Engineering Department, University of Kuwait, P.O. Box 5969, Safat 13060, Kuwait

Measurement and correlation of phase equilibria for the ternary system dodecane + *sec*-butylbenzene + *N*-methyl-2-pyrrolidone (NMP) were carried out over a temperature range of (288.15 to 318.15) K and at atmospheric pressure. Such a system is found in the extraction of aromatics in the production of middle distillate. The system studied exhibits type I liquid−liquid phase diagram. The values of distribution coefficients and selectivities were calculated from the equilibrium data. The effect of temperature and solute concentration in the feed upon solubility, distribution coefficient, and selectivity were investigated experimentally and theoretically. The experimental results of the studied system was regressed to estimate the interaction parameters between each of the three pairs of components with NRTL and UNIQUAC models as a function of temperature. Both models satisfactorily correlate the experimental data; however, the UNIQUAC fit was slightly better than that obtained with the NRTL model.

Introduction

The feasibility of liquid−liquid extraction depends primarily on the quality of the measured phase equilibrium data. Solubilities, distribution coefficients, and selectivities should be known at the operating conditions of the proposed extraction processes. The separation of aromatic and nonaromatic compounds from their mixtures is an important commercial process and is carried out by liquid−liquid extraction employing a selective solvent. Some of organic solvents have been tried by different workers for aromatics extraction.[1] However, only a few of these solvents are either used industrially or have been tried on pilot plant scale. These solvents, which are offered commercially, include glycols, sulfolane, *N*-methyl-2-pyrrolidone (NMP), and *N*,*N*-dimethylformamide (DMF). NMP is a dipolar aprotic basic solvent used in the well-established AROSOLVAN process as a highly selective extractant for the recovery of aromatic and saturated hydrocarbons from petroleum fractions. Experimental data on liquid−liquid equilibria (LLE) published for NMP + aromatic + *n*-alkanes systems containing carbon number greater than nine for the alkanes and/or aromatics are limited.[2−6] Reliable prediction of these data from the knowledge of limited experimental information is of vital importance for the design and analysis of the aromatics extraction systems.

This paper continues our previous work,[7] which deals with the liquid−liquid-phase equilibria for de-aromatization of the Kuwait middle distilled fraction. The purpose of this work is to study LLE of the ternary system dodecane (1) + *sec*-butylbenzene (2) + NMP (3). The LLE data, distribution coefficient, and selectivity for the studied ternary system were measured at (288.15, 298.15, 308.15, and 318.15) K and then correlated by the nonrandom two-liquid (NRTL) model of Renon and Prausnitz[8] and the universal quasi-chemical (UNIQUAC) model of Abrams and Prausnitz.[9]

Table 1. Details of the Chemicals: Purities, UNIQUAC Structural Parameters, and Refractive Indices

compound	supplier	GC purity %	UNIQUAC structural parameter *r*	*q*	n_D^{20} exp	lit.[a]
dodecane	Aldrich	99.4	8.5462	7.096	1.4220	1.4216
sec-butylbenze	Sigma	99.5	5.9452	4.584	1.4890	1.4891
NMP	Fluka	99.5	3.9810	3.200	1.4686	1.4684

[a] Ref 13.

Experimental Section

Chemicals. The purities and refractive indices of all chemicals used in this study are presented in Table 1. NMP and *sec*-butylbenzene were stored under a 0.4 nm molecular sieve. The purity of the chemicals was determined by gas chromatograph (see below). All chemicals were used without further purification.

Apparatus and Procedure. Determination of Critical Solution Temperature (T_c). To find the operating extraction temperatures, the miscibilities and critical solution temperatures (T_c) of the system studied were measured. The miscibilities of binary mixtures, dodecane (1) + NMP (2), were measured by adding a known mass of NMP to a known mass of dodecane and mixing the two phases completely in a 60 cm^3 glass cell. To maintain a constant temperature, the cell was connected to a Haake K15 water bath fitted with a Haake DC1 thermostat. The mixture's temperature was raised gradually and controlled to within ± 0.2 K. A magnetic stirrer was used to mix the two phases. The miscibility temperature was marked as the point where turbidity of the mixture disappears and the two phases become completely miscible in each other.

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* Corresponding author e-mail: a_jimaz@yahoo.com.

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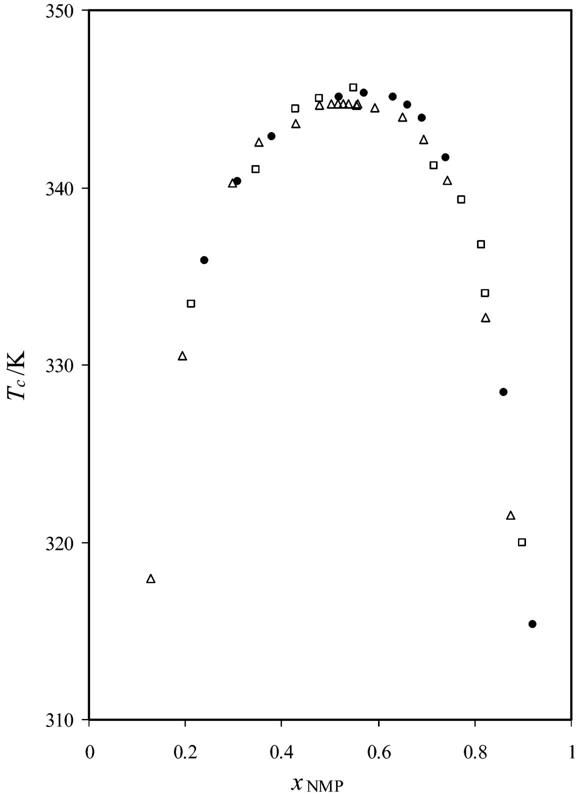

Figure 1. Critical solution temperature T_c/K, for binary system {dodecane (1) + NMP (2)}: ●, this work; □, Al-Jimaz et al.;[7] △, Bittrich et al.[12]

Heating is then cut off, and another reading is then taken when the solution cools and becomes turbid, indicating the beginning of phase separation. The two readings were within ± 0.2 K difference. The mole fraction and the critical solution temperature were measured with an uncertainties ± 0.005 K and ± 0.04 K, respectively. The same procedure was followed to determine the critical solution temperature of ternary mixtures, dodecane (1) + *sec*-butylbenzene (2) + NMP (3), at different phase ratio.

Extraction Runs. The experimental apparatus used for extraction consists of a 60 cm^3 glass cell with a water jacket in order to maintain a constant temperature. The temperature was controlled within ± 0.2 K. The cell was connected to a Haake K15 water bath fitted with a Haake DC1 thermostat. Mixtures, comprised of 20 g of NMP, 20 g of dodecane, and different known masses (0 to 8 g) of *sec*-butylbenzene were placed in the extraction vessel. The mixtures were vigorously stirred for 1 h and then left to settle for 4 h. Samples were taken by a syringe from both the upper and lower layers. A series of LLE measurements for the ternary system dodecane (1) + *sec*-butylbenzene (2) + NMP (3) over a temperature range of (288.15 to 318.15) K and at atmospheric pressure were performed.

Measurements of Phase Compositions. Dodecane (1), *sec*-butylbenzene (2), and NMP (3) were analyzed using a Chrompack CP 9000 gas chromatograph equipped with an on-column injector, a flame ionization detector (FID), and a data processor system. The column used was CP SIL 8CB (30 m × 3.2 × 10^{-4} m × 2.5 × 10^{-7} m film thickness). The column temperature was programmed for initial temperature of 383 K maintained for 2 min, and a final temperature of 673.15 K maintained for 5 min. The heating rate was 10 K/min, and the carrier gas (helium, grade 5.6) flow rate was maintained at 3 × 10^{-5} m^3/min. The injection temperature was 523.15 K, and the detector temperature was 573.15 K. The temperature was controlled with practical accuracy of apparatus ± 0.03 K. The mole fraction was measured with an uncertainty of ± 0.005.

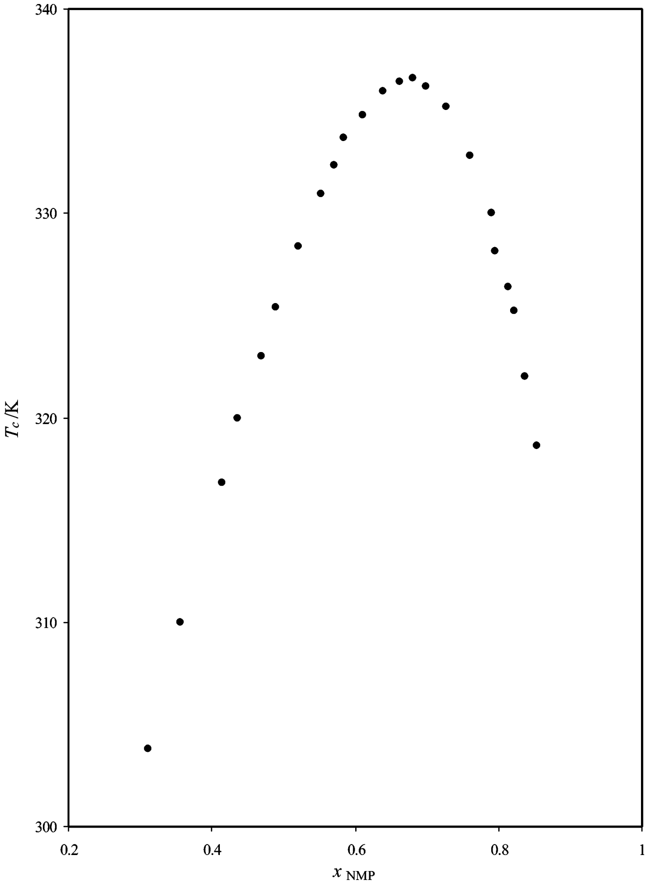

Figure 2. Critical solution temperature T_c/K, for the ternary system dodecane (1) + *sec*-butylbenzene (2) + NMP (3).

Models and Correlations

Our experimental data were correlated with the NRTL model of Renon and Prausnitz[8] and the UNIQUAC model of Abrams and Prausnitz.[9]

NRTL Model. The excess Gibbs energy of mixing (G^E) of the NRTL model is

$$\frac{G^E}{RT} = \sum_{i=1}^{3} x_i \frac{\sum_{j=1}^{n} \tau_{ji} G_{ji} x_j}{\sum_{k=1}^{n} G_{ki} x_k} \tag{1}$$

where

$$\tau_{ij} = \frac{g_{ij} - g_{jj}}{RT} = \frac{a_{ij}}{T} \tag{2}$$

$$\tau_{ji} = \frac{g_{ji} - g_{ii}}{RT} = \frac{a_{ji}}{T} \tag{3}$$

$$G_{ij} = \exp(-\alpha_{ij}\tau_{ij}) \tag{4}$$

$$G_{ji} = \exp(-\alpha_{ji}\tau_{ji}) \tag{5}$$

where R is the gas constant, T is the absolute temperature, x is mole fraction, g is the energy of interaction for each binary pair of compounds, G *the* is binary interaction

Table 2. Critical Solution Temperature (T_c) and Mole Fraction (x_3) for the Ternary System Dodecane (1) + *sec*-Butylbenzene (2) + NMP (3)

x_3	T_c/K	x_3	T_c/K	x_3	T_c/K	x_3	T_c/K
0.311	303.8	0.521	328.4	0.662	336.4	0.796	328.2
0.356	310.0	0.552	331.0	0.681	336.6	0.814	326.4
0.414	316.8	0.571	332.4	0.699	336.2	0.822	325.2
0.436	320.0	0.584	333.7	0.728	335.2	0.837	322.0
0.469	323.0	0.610	334.8	0.760	332.8	0.854	318.6
0.489	325.4	0.639	336.0	0.791	330.0		

Table 3. Experimental Equilibrium Mole Fraction (x_i), Selectivity (S), and Distribution Coefficient (K) for the Ternary System Dodecane (1) + *sec*-Butylbenzene (2) + NMP (3) at Different Temperatures

	dodecane-rich phase		NMP-rich phase			
T/K	x_1	x_2	x_1	x_2	S	K
288.15	0.9343	0.0000	0.0123	0.0000		
	0.8982	0.0333	0.0214	0.0171	21.55	0.5135
	0.8579	0.0513	0.0248	0.0267	18.00	0.5205
	0.7761	0.1077	0.0323	0.0573	12.78	0.5320
	0.6624	0.1577	0.0425	0.0902	8.91	0.5720
	0.5297	0.2017	0.0602	0.1242	5.42	0.6158
	0.4901	0.2128	0.0651	0.1335	4.72	0.6273
	0.4339	0.2286	0.0881	0.1558	3.36	0.6815
298.15	0.8157	0.0000	0.0316	0.0000		
	0.7996	0.0336	0.0358	0.0191	12.70	0.5685
	0.7341	0.0629	0.0399	0.0376	11.00	0.5978
	0.6779	0.1066	0.0509	0.0633	7.91	0.5938
	0.6272	0.1338	0.0574	0.0819	6.69	0.6121
	0.5171	0.1856	0.0827	0.1251	4.21	0.6740
	0.4797	0.1974	0.0951	0.1382	3.53	0.7001
	0.3811	0.2209	0.1225	0.1683	2.37	0.7619
308.15	0.7724	0.0000	0.0409	0.0000		
	0.7249	0.0294	0.0457	0.0193	10.41	0.6565
	0.6613	0.0609	0.0508	0.0402	8.59	0.6601
	0.6182	0.0976	0.0597	0.0662	7.02	0.6783
	0.5791	0.1318	0.0785	0.0928	5.19	0.7041
	0.4598	0.1764	0.1036	0.1312	3.30	0.7438
	0.4215	0.1843	0.1144	0.1417	2.83	0.7689
	0.3377	0.2062	0.1449	0.1691	1.91	0.8201
318.15	0.7346	0.0000	0.0474	0.0000		
	0.6948	0.0258	0.0601	0.0196	8.78	0.7597
	0.6328	0.0581	0.0672	0.0449	7.28	0.7728
	0.5865	0.0853	0.0781	0.0669	5.89	0.7843
	0.4786	0.1257	0.1079	0.1017	3.59	0.8091
	0.3517	0.1694	0.1621	0.1518	1.94	0.8961
	0.3078	0.1807	0.2003	0.1713	1.46	0.9480

parameter, τ is the adjustable parameter, and α is the nonrandomness parameter. The a_{ij} and a_{ji} are the two interaction parameters for each binary pair that we find from correlation.

UNIQUAC Model. The excess Gibbs energy (G^E) of the UNIQUAC model is

$$\frac{G^E}{RT} = \sum_{i=1}^{3} x_i \ln \frac{\psi_i}{x_i} + 5\sum_{i=1}^{3} x_i q_i \ln \frac{\theta_i}{\psi_i} - \sum_{i=1}^{3} x_i q_i \ln \left(\sum_{j=1}^{n} \theta_j \tau_{ji}\right) \tag{6}$$

where

$$\psi_i = \frac{x_i r_i}{\sum_{i=1}^{3} x_i r_i} \tag{7}$$

$$\theta_i = \frac{x_i q_i}{\sum_{i=1}^{3} x_i q_i} \tag{8}$$

$$\tau_{ij} = \exp\left(-\frac{u_{ij} - u_{jj}}{RT}\right) \tag{9}$$

$$\tau_{ji} = \exp\left(-\frac{u_{ji} - u_{ii}}{RT}\right) \tag{10}$$

where q and r represent the UNIQUAC area and volume, while θ_i and ψ_i represent the area fraction and segment fraction of species i, respectively. The u is the energy of interaction for each binary pair of compounds, and τ is an adjustable parameter.

Interaction Parameters. The LLE experimental data were used to determine the optimum NRTL and UNIQUAC binary interaction parameters between dodecane, *sec*-butylbenzene, and NMP. The NRTL and the UNIQUAC

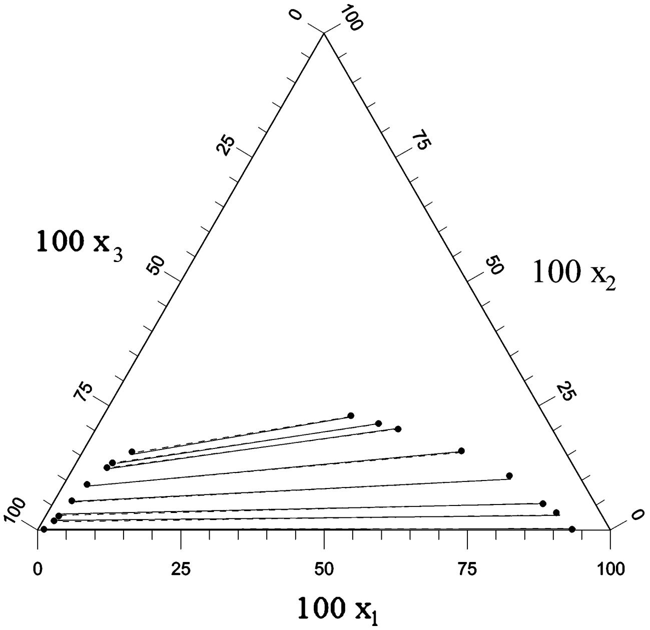

Figure 3. Experimental and correlated LLE data for ternary system dodecane (1) + *sec*-butylbenzene (2) + NMP (3) at T = 288.15 K: ●, experimental; ···, NRTL; —, UNIQUAC.

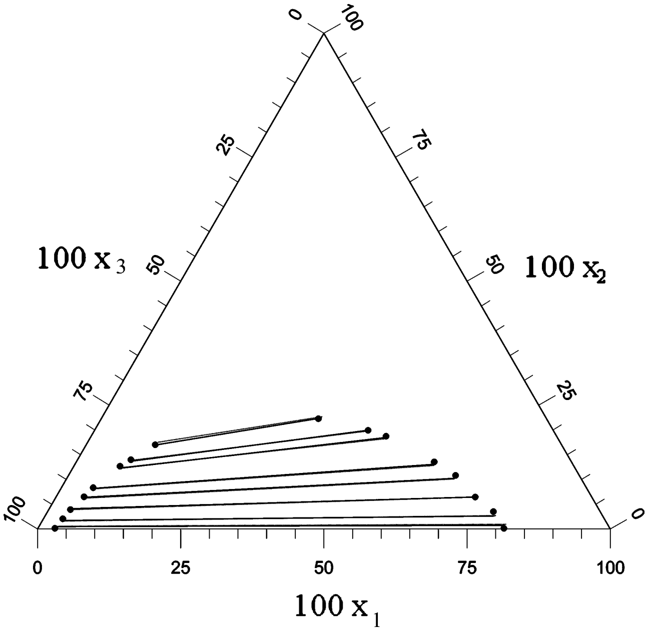

Figure 4. Experimental and correlated LLE data for ternary system dodecane (1) + *sec*-butylbenzene (2) + NMP (3) at T = 298.15 K: ●, experimental; ···, NRTL; —, UNIQUAC.

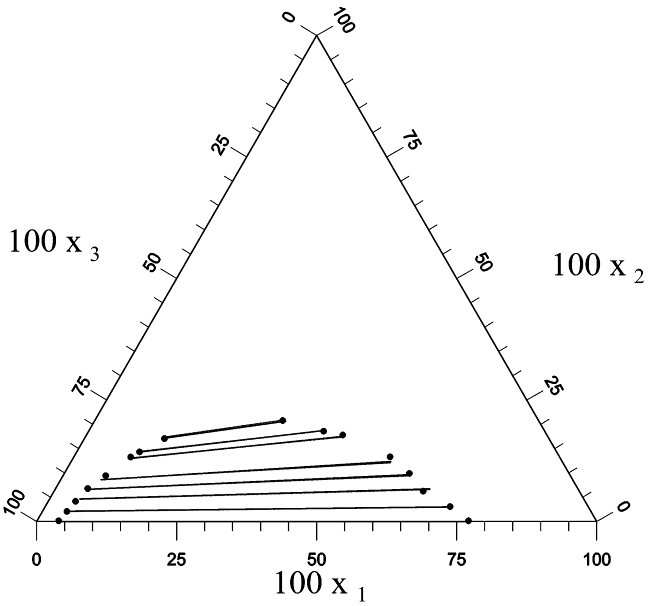

Figure 5. Experimental and correlated LLE data for ternary system dodecane (1) + *sec*-butylbenzene (2) + NMP (3) at T = 308.15 K: ●, experimental; ···, NRTL; —, UNIQUAC.

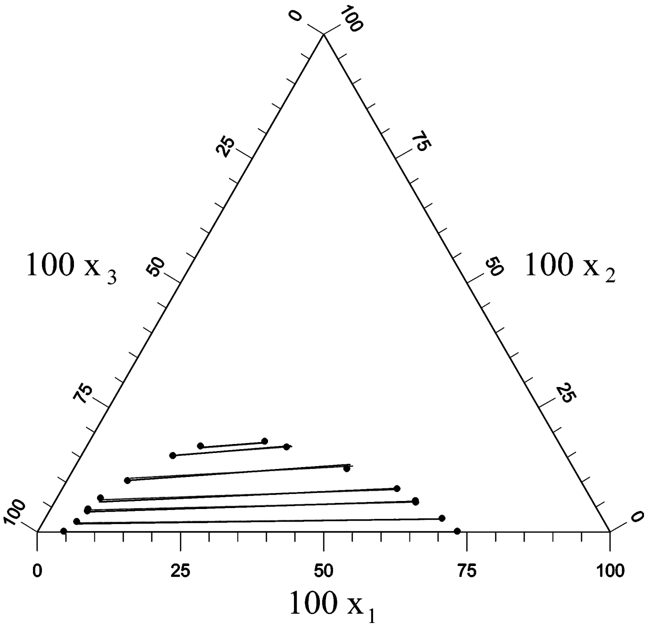

Figure 6. Experimental and correlated LLE data for ternary system dodecane (1) + *sec*-butylbenzene (2) + NMP (3) at T = 318.15 K: ●, experimental; ···, NRTL; —, UNIQUAC.

models were fitted to experimental data using an iterative computer program, based on the flash calculation method, developed by Sørensen.[10] The objective function used in this case was determined by minimizing the square of the difference between the mole fractions correlated by the respective method and those experimentally measured over all the tie lines in the ternary system. For the UNIQUAC correlation, the pure component structural parameters (r and q) listed in Table 1 were calculated from the data published by Magnussen et al.[11] The objective function (F) used is

$$F = \min \sum_k \sum_j \sum_i (x_{ijk,\mathrm{exp}} - x_{ijk,\mathrm{cal}})^2 \tag{11}$$

where x is the mole fraction; the subscripts exp, cal, i, j, and k are experimental, calculated, components, phases and tie lines, respectively.

The NRTL model was fitted with fixed values of the nonrandomness parameter (α_{ij}) for each pair of components. A fixed value of $\alpha_{ij} = 0.2$ between each pair of components was found to be satisfactory.

The optimization results were judged by calculating the corresponding rmsd values using the following equation:

$$\mathrm{rmsd} = 100\sqrt{\frac{\sum_k \sum_j \sum_i (x_{ijk,\mathrm{exp}} - x_{ijk,\mathrm{cal}})^2}{(n-p)}} \tag{12}$$

where n is the number of the experimental data and p is the number of the UNIQUAC or the NRTL interaction parameters.

Results and Discussion

Experimental Data. Figure 1 presents the measured critical solution temperatures (T_c) of binary mixtures dodecane (1) + NMP (2) at different solvent to feed ratios. The equilibrium coexistence curve has a rather horizontal top. Our experimental results are in agreement (rmsd = 0.69) with that obtained by Al-Jimaz et al.[7] and Bittrich et al.[12] as shown in Figure 1.

Figure 2 presents the measured critical solution temperatures (T_c) of ternary mixtures dodecane (1) + *sec*-butylbenzene (2) + NMP (3) at different solvent to feed ratios. The studied system has an upper critical solution temperature due to adding *sec*-butylbenzene. The critical solution temperatures for the ternary mixtures are given in Table 2. All extraction measurements were made at temperatures 20 K below the critical solution temperatures.

Distribution Coefficient and Selectivity. The distribution coefficient of *sec*-butylbenzene (K) for the ternary system {dodecane (1) + *sec*-butylbenzene (2) + NMP (3)}, which is the measure of the solvent power or capacity of the NMP (3), is given by

$$K = \frac{(x_2)_{\mathrm{NMP-rich\ phase}}}{(x_2)_{\mathrm{dodecane-rich\ phase}}} \tag{13}$$

The effectiveness of a solvent can be expressed by the selectivity (S) of the solvent. The selectivity of the NMP (3), which is a measure of the solvent ability to separate *sec*-butylbenzene (2) from dodecane (1), is given by

$$S = \frac{(x_2/x_1)_{\mathrm{NMP-rich\ phase}}}{(x_2/x_1)_{\mathrm{dodecane-rich\ phase}}} \tag{14}$$

The experimental and correlated results of K or S were judged by calculating the corresponding coefficient of determination (r^2) values using the following equation:

$$r^2 = \frac{\sigma_{\mathrm{exp}}^2 - \sigma_{\mathrm{exp,cal}}^2}{\sigma_{\mathrm{exp}}^2} \tag{15}$$

where

$$\sigma_{\mathrm{exp}} = \sqrt{\frac{\sum_{k=1}^{n} (y_{k,\mathrm{exp}} - \bar{y}_{\mathrm{exp}})^2}{n-1}} \tag{16}$$

$$\sigma_{\mathrm{exp,cal}} = \sqrt{\frac{\sum_{k=1}^{n} (y_{k,\mathrm{exp}} - y_{k,\mathrm{cal}})^2}{n-1}} \tag{17}$$

$$\bar{y}_{\mathrm{exp}} = \frac{1}{n}\sum_{k=1}^{n} y_{k,\mathrm{exp}} \tag{18}$$

and y represents the distribution coefficient (K) or selectiv-

Table 4. UNIQUAC and NRTL Interaction Parameters and Root Mean Square Deviation (rmsd) for {Dodecane (1) + *sec*-Butylbenzene (2) + NMP (3)} at Different Temperatures

			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
288.15	1	2	−63.009	−1.7765		−561.89	−12.252	
	1	3	268.45	14.219		422.42	919.75	
	2	3	−99.553	96.312	0.3381	−554.41	355.66	0.3231
298.15	1	2	−473.39	293.44		269.28	−128.76	
	1	3	203.62	25.490		179.78	945.61	
	2	3	19.627	−282.38	0.4264	48.839	206.13	0.4890
308.15	1	2	−404.12	262.69		315.36	31.322	
	1	3	182.557	30.980		96.978	988.11	
	2	3	33.820	−241.25	0.5221	18.449	399.79	0.5323
318.15	1	2	219.02	−69.866		−270.93	26.995	
	1	3	187.36	23.356		64.940	1002.2	
	2	3	−13.225	189.18	0.3913	−37.773	−121.01	0.4648

ity (S), $\bar{y}$ is the arithmetic mean, n is the number of the experimental data, σ is the standard deviation; subscripts exp, cal, and k are experimental, calculated and tie lines, respectively.

The measured equilibrium mole fractions (x), selectivities (S), and distribution coefficients (K) for the studied system are given in Table 3. As the temperature increases, the solubility of NMP in the dodecane-rich phase increases, while temperature has little effect upon the solubility of dodecane in the NMP-rich phase. The selectivity values are not constant for the two-phase region as shown in Table 3.

The experimental and the correlated tie lines for the studied system at (288.15, 298.15, 308.15, and 318.15) K are shown in Figures 3, 4, 5, and 6, respectively. The studied system exhibits type I liquid−liquid-phase diagram. The mutual dodecane NMP solubility increased as the concentration of *sec*-butylbenzene in the feed increases. The size of the two-phase region decreases with an increase in temperature and/or *sec*-butylbenzene concentration in the feed.

Data Correlation. The values of interaction parameters and the relative mean square deviation (rmsd) for the UNIQUAC and the NRTL models at different temperatures are shown in Table 4. These parameters are used to calculate LLE tie lines for the present system. The calculation based on both models gave good representation of the tie lines data for this system. However, the UNIQUAC model, fitted to LLE experimental data, is slightly better than the NRTL model, according to the analysis of the rmsd (the average rmsd was 0.44 for UNIQUAC as compared to 0.48 for NRTL).

The distribution coefficients and selectivities were correlated from calculated LLE data by the UNIQUAC model using the interaction parameters generated in Table 4 at different temperatures. Figures 7 and 8 show that there is good agreement between the experimental and correlated distribution coefficients and selectivities, respectively, with coefficient of determination (r^2) equal to 0.99 for both K and S.

Figure 9 represents the relationship of the *sec*-butylbenzene concentration in the NMP-rich phase, $(x_2)_{\text{NMP−rich phase}}$, with the measured and correlated distribution coefficients (K) for the studied system at temperatures range of (288.15 to 318.15) K. The distribution coefficient values increased as the temperature and/or $(x_2)_{\text{NMP−rich phase}}$, increased.

Figure 10 represents the relationship of the *sec*-butylbenzene concentration in the NMP-rich phase, $(x_2)_{\text{NMP−rich phase}}$, with the measured and correlated selectivity, S, for the studied system at temperatures range of (288.15 to 318.15) K. The selectivity decreased as the concentration of *sec*-butylbenzene increased, it means the higher the concentration of *sec*-butylbenzene in the feed

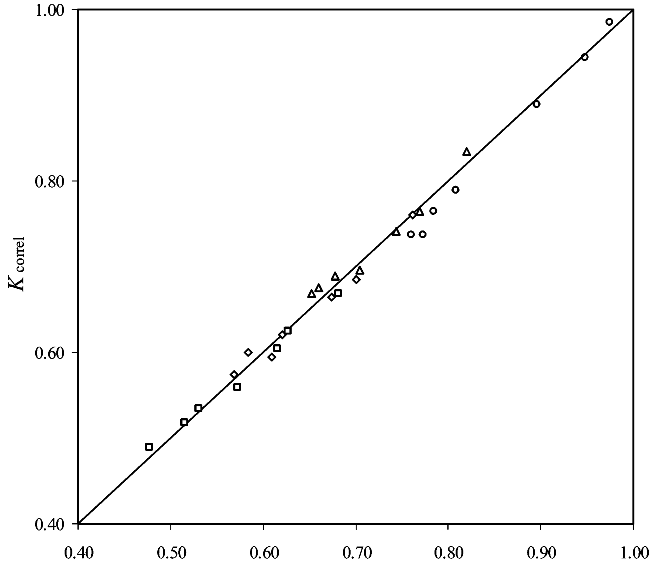

Figure 7. Measured distribution coefficient (K_{exp}) against correlated distribution coefficient (K_{correl}) at □, 288.15; ◇, 298.15; △, 308.15; ○, 318.15 K.

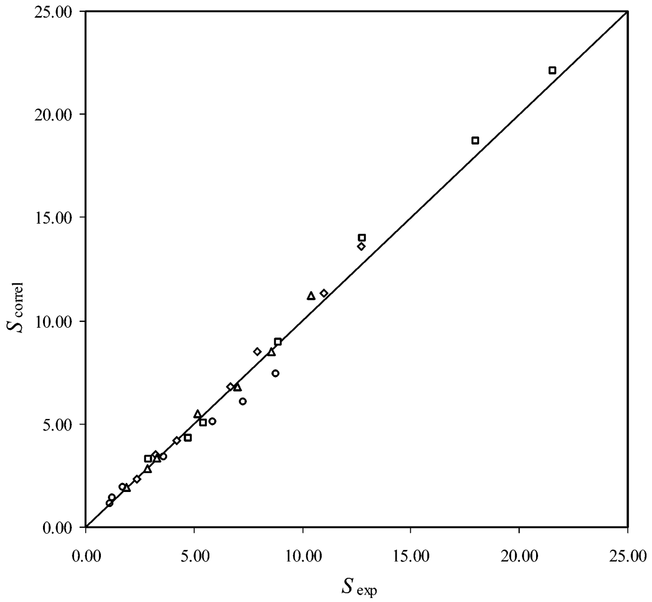

Figure 8. Measured selectivity (S_{exp}) against correlated selectivity (S_{correl}) at □, 288.15; ◇, 298.15; △, 308.15; ○, 318.15 K.

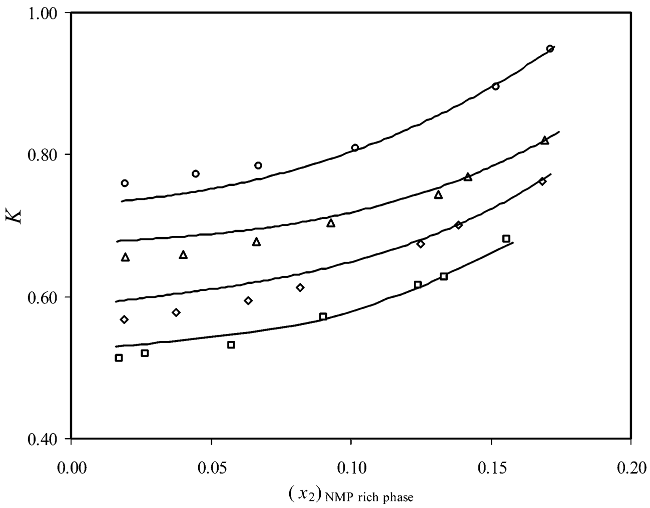

Figure 9. Effect of temperature on measured and correlated distribution coefficient (*K*) at □, 288.15; ◇, 298.15; △, 308.15; ○, 318.15 K; —, UNIQUAC.

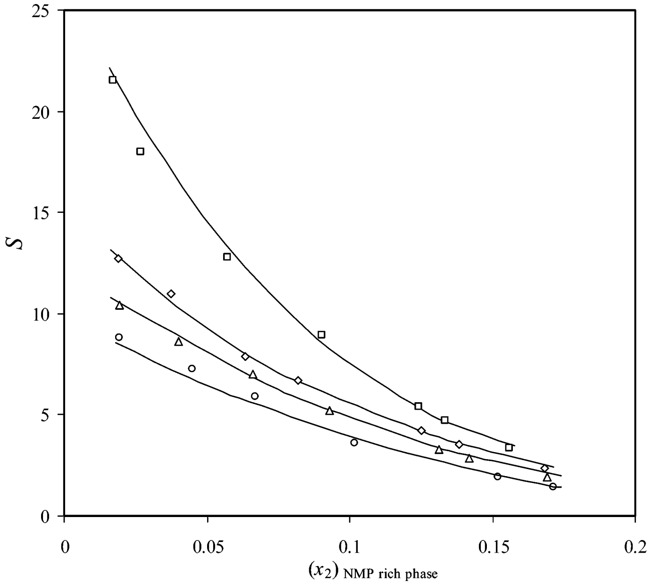

Figure 10. Effect of temperature on measured and correlated selctivity (*S*) at □, 288.15; ◇, 298.15; △, 308.15; ○, 318.15 K; —, UNIQUAC.

the lower the selectivity of solvent. The higher the temperature, the lower the selectivity; the same behavior was also correctly correlated from calculated LLE data using the UNIQUAC model as shown in Figure 10. Since the selectivity in all cases is greater than 1, the extraction is possible.

As shown in Figure 11, the selectivities (*S*) and distribution coefficients (*K*) reflect opposing behavior (i.e., a solvent with particularly high selectivity has often only a limited distribution coefficient and vice versa). While at low temperature selectivity is high and distribution coefficient is low, at high temperature selectivity is low and distribution coefficient is high.

Conclusions

An experimental investigation of equilibrium behavior of the liquid−liquid, dodecane (1) + *sec*-butylbenzene (2)+ NMP (3) ternary system is carried out at temperatures of (288.15 to 318.15) K and at atmospheric pressure. The solubility of NMP in a dodecane-rich phase increases as the temperature increases, but it has little effect on the solubility of dodecane in the NMP-rich phase. The mutual NMP−dodecane solubility increased as the concentration of *sec*-butylbenzene increases. Both the UNIQUAC and the NRTL models satisfactorily correlate the LLE experimental data; however, the former model was more suitable for the studied system (the average rmsd was 0.44 for UNIQUAC as compared to 0.48 for NRTL). The effect of temperature upon distribution coefficient and selectivity were correlated satisfactorily using the UNIQUAC model. While the distribution coefficient increased as the temperature increased, the selectivity increased as the temperature decreased. The distribution coefficient increased, while the selectivity decreased as the concentration of *sec*-butylbenzene in the feed increased. Since the selectivity in all cases is greater than 1, NMP can be used to extract *sec*-butylbenzene from dodecane.

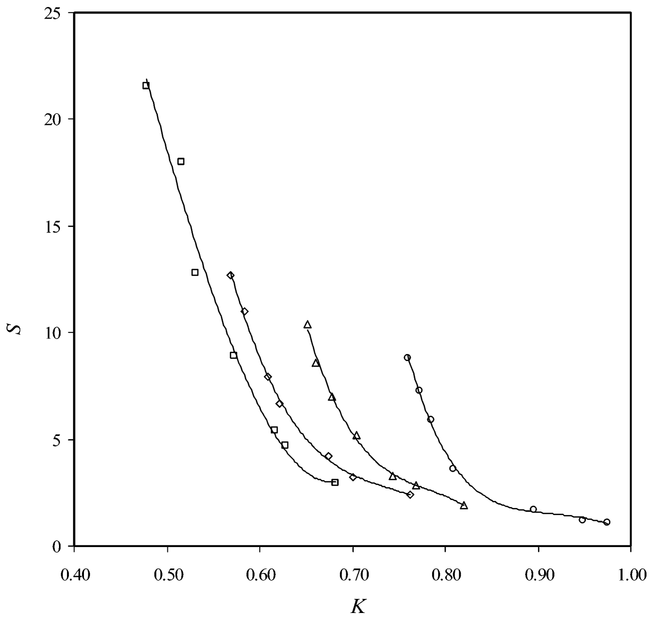

Figure 11. Distribution coefficient (*K*) against selectivity (*S*) at □, 288.15; ◇, 298.15; △, 308.15; ○, 318.15 K.

Literature Cited

(1) Lin, W. Studies on the extraction of aromatics from C9$^+$ oil. *J. Chem. Eng. Jpn.* **2002**, *35*, 1257−1262.

(2) Letcher, T. M.; Naicker, P. K. Ternary liquid−liquid equilibria for mixtures of an *n*-alkane + an aromatic hydrocarbon + *N*-methyl-2-pyrrolidone at 298.2 K and 1 atm. *J. Chem. Eng. Data* **1998**, *43*, 1034−1038.

(3) Ferreira, P. O.; Barbosa, D.; Medina, A. G. Phase equilibria for the separation of aromatic and nonaromatic compounds using mixed solvents. Part I. The system *n*-heptane-toluene-*N*-methylpyrrolidone/monoethyleneglycol. *Fluid Phase Equilib.* **1984**, *15*, 309−322.

(4) Ferreira, P. O.; Ferreira, J. B.; Medina, A. G. Liquid−liquid equilibria for the system *N*-methylpyrrolidone + toluene + *n*-heptane: UNIFAC interaction parameters for *N*-methylpyrrolidone. *Fluid Phase Equilib.* **1984**, *16*, 369−379.

(5) Nagpal, J. M.; Rawat, B. S. Liquid−liquid equilibria for toluene-heptane-*N*-methyl-pyrrolidone and benzene-heptane solvents. *J. Chem. Technol. Biotechnol.* **1981**, *31*, 146−150.

(6) Gonzalez, J. A.; Cobos, J. C.; Garcia de la Fuente, I. Thermodynamics of liquid mixtures containing a very strongly polar compound: Part 6. DISQUAC characterization of *N*,*N*-dialkylamides. *Fluid Phase Equilib.* **2004**, *224*, 169−183.

(7) Al-Jimaz, A. S.; Fandary, M. S.; Al-Kandary, J. A.; Fahim, M. A. Liquid−liquid equilibria for *n*-alkanes (C_{12}, C_{14}, C_{17}) + propylbenzene + NMP mixtures at temperatures between 298 and 328 K. *Fluid Phase Equilib.* **2005**, *231/2*, 163−170.

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

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

(10) Sørensen, J. M.; Arlt, W. *Liquid−Liquid Equilibrium Collection Data*; Vol. V, Part 2, Dechema Chemistry Data Series: Dechema: Frankfort/Main, Germany, 1980.

(11) Magnussen, T.; Rasmussen, P.; Fredenslund, A. UNIFAC parameter table for prediction of liquid−liquid equilibriums. *Ind. Eng. Chem. Process Des. Dev.* **1981**, *20*, 331−339.

(12) Bittrich, H.-J.; Lempe, D. A.; Reinhardt, K.; Wûstling, J.-U. Liquid−liquid equilibria in binary mixtures of *N*-methyl-α-pyrrolidone and saturated hydrocarbons. Part II. *Fluid Phase Equilib.* **1996**, *126*, 115−125.

(13) *CRC Handbook of Chemistry and Physics*, 72nd ed.; CRC Press: Boca Raton, FL, 1991−1992.

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