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Liquid−Liquid Equilibria Measurements for Ternary System of Hexadecane + 1,3,5-Trimethylbenzene + *N*-Methyl-2-pyrrolidone

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

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

Mohamed A. Fahim

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

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In this paper, experimental data on phase equilibria of the ternary system: hexadecane (cetane) + 1,3,5-trimethylbenzene (mesitylene) + *N*-methyl-2-pyrrolidone (NMP) were measured over a temperature range of (293.2 to 323.2) K and at atmospheric pressure in order to evalute the NMP, as an extractant agent, for process engineering application such as extractive distillation and solvent extraction. 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 liquid−liquid equilibria (LLE) results are reported, and the distribution coefficients as well as selectivities are discussed. The effect of temperature and solute concentration in the feed upon solubility, distribution coefficient, and selectivity are investigated experimentally and theoretically. The ability of NRTL and UNIQUAC models to predict LLE was evaluated. The experimental results of the studied system were regressed to estimate the interaction parameters between each of the three pairs of components using the two models as a function of temperature. Both models satisfactorily correlate the experimental data, and they are equally the same.

Introduction

Separation processes of aromatics from petroleum fractions with direct distillation is impossible because of the difficulties in separating them from naphthenes of similar boiling points and many homogeneous binary azoetropes existing between aliphatic and aromatic hydrocarbons. Since distillation becomes ineffective for separating aromatics, extraction processes will be a better choice. The extractive distillation and solvent extraction processes are an important in petroleum production and are carried out by employing selective solvents. The search for selective solvents to extract aromatic compounds is important.[1] When choosing a solvent, several points must be considered: low vapor pressure, high specific gravity, adaptability to a wide range of feeds, availability at reasonable cost, and stability. Among the usual solvents, *N*-methyl-2-pyrrolidone (NMP) is one of the most used because of its high selectivity toward aromatic compounds. Measuring phase equilibria data at different temperatures can be used to generate the interaction parameters of UNIQUAC and NRTL models, which can be used in the design of extraction columns. Solubilities, distribution coefficients, and selectivities should be known at the operating conditions of the proposed extraction processes. Experimental data on liquid−liquid equilibria (LLE) published for *n*-alkanes + aromatic + NMP systems containing carbon number greater than nine for the alkanes and/or aromatics are limited.[2−6]

This paper continues our previous work,[7−10] which deals with the liquid−liquid-phase equilibria for dearomatization of the Kuwait middle distillate. The purpose of this work is to study LLE of the ternary system: hexadecane (1) + mesitylene (2) + NMP (3). The LLE data, distribution coefficient, and selectivity for the studied ternary system were measured at (293.2, 303.2, 313.2, and 323.2) K and then correlated by the nonrandom two-liquid (NRTL) model of Renon and Prausnitz[11] and the universal quasi-chemical (UNIQUAC) model of Abrams and Prausnitz.[12]

Experimental Section

Chemicals. The determined purity of the chemicals, listed in Table 1, was ascertained by comparing the measured refractive indices of the pure components at 293.2 K with the available literature values.[13] The reported experimental values conform closely to their corresponding literature values, with an average of the absolute value of deviation 10^{-4}. The purity of the chemicals was also determined by gas chromatograph (see below). NMP and mesitylene were stored under 0.4 nm molecular sieve. All chemicals were used without further purification.

Apparatus and Procedure. 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 hexadecane, and different known masses (0 to 8 g) of mesitylene were placed in the extraction vessels. The mass measurements were performed using an electronic balance (Mettler AT460) with a stated precision of $\pm 10^{-4}$ g. 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 hexadecane (1) + mesitylene (2) + NMP (3) over a temperature range of (293.2 to 323.2) K and at atmospheric pressure were performed.

Measurements of Phase Compositions. Hexadecane (1), mesitylene (2), and NMP (3) were analyzed using a Chrompack CP 9000 gas chromatograph equipped with an on-column

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

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

		GC purity	UNIQUAC structural parameter		n_D^{20}	
compound	supplier	%	r	q	exp	lit[a]
hexadecane	Aldrich	99.3	11.244	9.256	1.4344	1.4345
mesitylene	Sigma	99.5	5.393	4.014	1.4992	1.4994
NMP	Fluka	99.5	3.9810	3.200	1.4686	1.4684

[a] Ref 13.

injector, flame ionization detector (FID), and data processor system. The column used was CP SIL 8CB (30 m × $3.2 \cdot 10^{-4}$ m × $2.5 \cdot 10^{-7}$ m film thickness). The column temperature was programmed for initial temperature of 383.15 K maintained for 2 min, and a final temperature of 673.15 K was maintained for 5 min. The heating rate was 10 K/min, and the carrier gas (helium, grade 5.6) flow rate was maintained at $3 \cdot 10^{-5}$ 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.

Models and Correlations

Our experimental data were correlated with the NRTL model of Renon and Prausnitz[11] and the UNIQUAC model of Abrams and Prausnitz.[12]

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

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

where

$$\tau_{ij} = \frac{g_{ij} - g_{jj}}{RT} = \frac{a_{ij}}{T} \qquad (2)$$

$$G_{ij} = \exp(-\alpha_{ij}\tau_{ij}) \qquad (3)$$

where R is the gas constant, T is the absolute temperature, x is mole fraction, g is energy of interaction for each binary pair of compounds, G is binary interaction parameter, τ is adjustable parameter, and α is 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

$$\frac{G^{E}}{RT} = \sum_{i=1}^{3} x_i \ln \frac{\psi_i}{x_i} + 5 \sum_{i=1}^{3} x_i q_i \ln \frac{\theta_i}{\psi_i} - \sum_{i=1}^{3} x_i q_i \ln \left(\sum_{j=1}^{n} \theta_j \tau_{ji} \right) \qquad (4)$$

where

$$\psi_i = \frac{x_i r_i}{\sum_{i=1}^{3} x_i r_i} \qquad (5)$$

$$\theta_i = \frac{x_i q_i}{\sum_{i=1}^{3} x_i q_i} \qquad (6)$$

$$\tau_{\mathrm{ij}} = \exp\left(-\frac{u_{\mathrm{ij}} - u_{\mathrm{jj}}}{RT} \right) \qquad (7)$$

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; 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 hexadecane, mesitylene, and NMP. The NRTL and the UNIQUAC models were fitted to experimental data using an iterative computer program, based on flash calculation method, developed by Sørensen and Arlt.[14] The objective function (F) used in this case was determined by minimizing the square of the difference between the mole fractions correlated by the respective method and these 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.[15] The objective function (F) used is

$$F = \min \sum_{k} \sum_{j} \sum_{i} (x_{ijk,\mathrm{exp}} - x_{ijk,\mathrm{cal}})^2 \qquad (8)$$

where x is mole fraction; 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:

$$\mathrm{rmsd} = 100 \sqrt{\frac{\sum_{k} \sum_{j} \sum_{i} (x_{ijk,\mathrm{exp}} - x_{ijk,\mathrm{cal}})^2}{(n - p)}} \qquad (9)$$

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

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

$$K = \frac{(x_2)_{\mathrm{NMP-rich\ phase}}}{(x_2)_{\mathrm{hexadecane-rich\ phase}}} \qquad (10)$$

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 mesitylene (2) from hexadecane (1), is given by

$$S = \frac{(x_2/x_1)_{\mathrm{NMP-rich\ phase}}}{(x_2/x_1)_{\mathrm{hexadecane-rich\ phase}}} \qquad (11)$$

Table 2. Experimental Equilibrium Mole Fraction (x_i), Distribution Coefficient (K), and Selectivity (S) for {Hexadecane (1) + Mesitylene (2) + NMP (3)} at Different Temperatures

	hexadecane-rich phase		NMP-rich phase			
T/K	x_1	x_2	x_1	x_2	K	S
293.2	0.8769	0.0000	0.0080	0.0000		
	0.8005	0.0482	0.0112	0.0167	0.3465	24.87
	0.6915	0.1094	0.0137	0.0497	0.4543	22.93
	0.6294	0.1697	0.0142	0.0672	0.3960	17.55
	0.5518	0.2262	0.0160	0.0925	0.4089	14.15
	0.4847	0.2638	0.0171	0.1145	0.4340	12.34
	0.4557	0.2831	0.0191	0.1281	0.4525	10.79
	0.3437	0.3296	0.0203	0.1553	0.4712	7.98
	0.3050	0.3401	0.0256	0.1801	0.5296	6.31
	0.2750	0.3502	0.0330	0.2102	0.6002	5.00
303.2	0.7870	0.0000	0.0132	0.0000		
	0.6987	0.0433	0.0162	0.0189	0.4365	18.88
	0.5773	0.1201	0.0204	0.0586	0.4879	13.81
	0.5190	0.1507	0.0237	0.0762	0.5056	11.07
	0.4863	0.1708	0.0272	0.0893	0.5228	9.36
	0.4401	0.1921	0.0290	0.1021	0.5315	8.08
	0.3910	0.2177	0.0396	0.1260	0.5788	5.71
	0.3100	0.2446	0.0474	0.1492	0.6100	3.99
	0.2725	0.2596	0.0574	0.1692	0.6518	3.09
313.2	0.7530	0.0000	0.0184	0.0000		
	0.6723	0.0387	0.0227	0.0193	0.4987	14.80
	0.5464	0.1106	0.0277	0.0583	0.5271	10.42
	0.5041	0.1391	0.0346	0.0771	0.5543	8.09
	0.4501	0.1653	0.0506	0.1001	0.6056	5.39
	0.3921	0.1871	0.0566	0.1160	0.6200	4.29
	0.3431	0.2040	0.0676	0.1330	0.6520	3.31
	0.2900	0.2147	0.0996	0.1650	0.7685	2.24
323.2	0.7161	0.0000	0.0246	0.0000		
	0.6246	0.0429	0.0313	0.0210	0.5460	9.77
	0.5550	0.0761	0.0391	0.0417	0.5600	7.79
	0.5072	0.0987	0.0442	0.0572	0.5795	6.65
	0.4572	0.1187	0.0504	0.0719	0.6057	5.49
	0.3654	0.1512	0.0658	0.0983	0.6501	3.61
	0.3083	0.1674	0.0954	0.1189	0.7103	2.30
	0.2731	0.1760	0.1269	0.1388	0.7886	1.70

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:

$$r^2 = \frac{{\sigma_{\text{exp}}}^2 - {\sigma_{\text{exp,cal}}}^2}{{\sigma_{\text{exp}}}^2} \tag{12}$$

where

$$\sigma_{\text{exp}} = \sqrt{\frac{\sum_{k=1}^{n} (y_{k,\text{exp}} - \bar{y}_{\text{exp}})^2}{n - 1}} \tag{13}$$

$$\sigma_{\text{exp,cal}} = \sqrt{\frac{\sum_{k=1}^{n} (y_{k,\text{exp}} - y_{k,\text{cal}})^2}{n - 1}} \tag{14}$$

$$\bar{y}_{\text{exp}} = \frac{1}{n} \sum_{k=1}^{n} y_{k,\text{exp}} \tag{15}$$

and y represents the distribution coefficient (K) or the selectivity (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), distribution coefficients (K), and selectivities (S) for the studied system are given in Table 2. As the temperature increases, the solubility of NMP in the hexadecane-rich phase increases, while temperature has little effect upon the solubility of hexadecane in the NMP-rich phase. The selectivity values are not constant for the two-phase region as shown in Table 2.

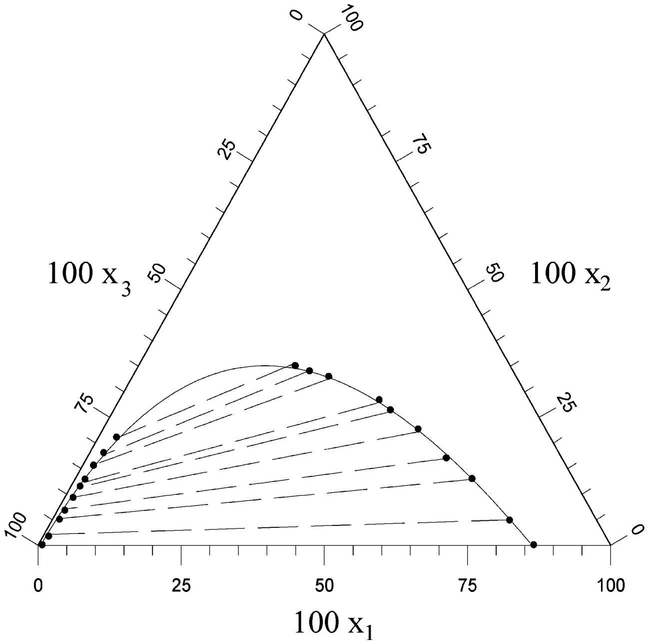

Figure 1. Experimental and predicted LLE data for the ternary system: hexadecane (1) + mesitylene (2) + NMP (3) at T = 293.2 K. ●, experimental; — —, NRTL; — bimodal curve, UNIQUAC.

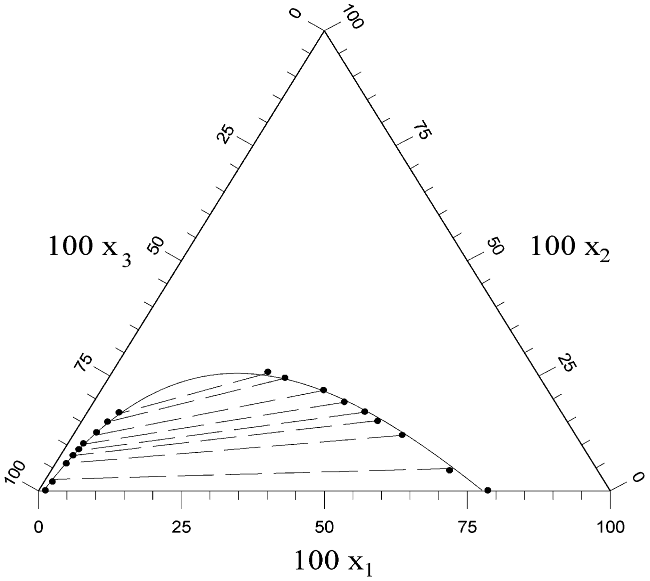

Figure 2. Experimental and predicted LLE data for the ternary system: hexadecane (1) + mesitylene (2) + NMP (3) at T = 303.2 K. ●, experimental; — —, NRTL; — bimodal curve, UNIQUAC.

The experimental and the correlated tie lines for the studied system at (293.2, 303.2, 313.2, and 323.2) K are shown in Figures 1, 2, 3, and 4, respectively. The studied system exhibits type I liquid–liquid-phase diagram. The mutual hexadecane–NMP solubility increased as the concentration of mesitylene in the feed increases. The size of the two-phase region decreases with an increase in temperature and/or mesitylene concentration in the feed.

Data Correlation. The values of interaction parameters and the root mean square deviation (rmsd) for the UNIQUAC and

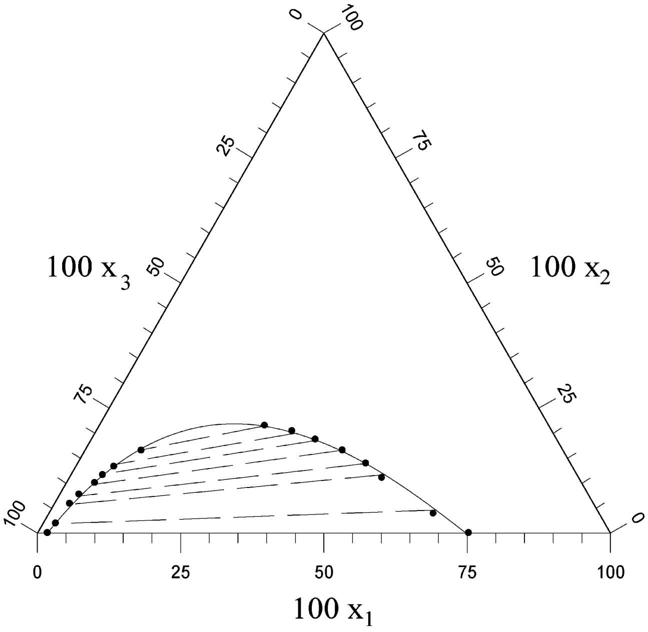

Figure 3. Experimental and predicted LLE data for the ternary system: hexadecane (1) + mesitylene (2) + NMP (3) at T = 313.2 K. ●, experimental; – –, NRTL; — bimodal curve, UNIQUAC.

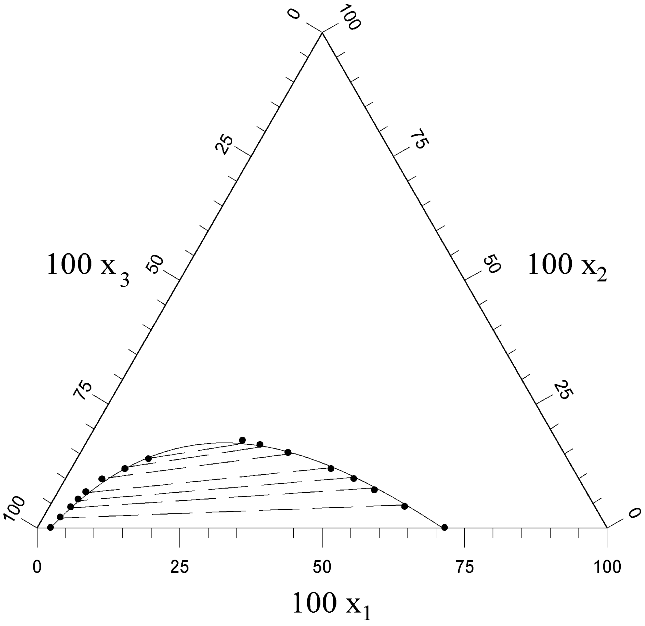

Figure 4. Experimental and predicted LLE data for the ternary system: hexadecane (1) + mesitylene (2) + NMP (3) at T = 323.2 K. ●, experimental; – –, NRTL; — bimodal curve, UNIQUAC.

the NRTL models at different temperatures are shown in Table 3**.** 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, and they are equally the same according to the analysis of the rmsd (average rmsd was 0.447 for UNIQUAC as compared to 0.433 for NRTL).

The distribution coefficients and selectivities were correlated from calculated LLE data by the UNIQUAC model using the interaction parameters generated in Table 3 at different temperatures. Good agreement was shown 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.

Table 3. UNIQUAC and NRTL Interaction Parameters and Root Mean Square Deviation (rmsd) for {Hexadecane (1) + Mesitylene (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	$(g_{ij} - g_{jj})/R$	$(g_{ji}\text{-}\ g_{ii})/R$	rmsd
293.2	1	2	−489.56	25.860		329.52	−116.44	
	1	3	187.34	61.473		149.70	1475.5	
	2	3	−93.509	−313.24	0.6213	341.76	115.91	0.5608
303.2	1	2	−219.89	−121.14		349.99	−80.211	
	1	3	166.23	50.339		12.612	1395.6	
	2	3	−157.41	−125.26	0.4432	865.15	−152.14	0.3013
313.2	1	2	180.23	−107.16		−458.87	−48.892	
	1	3	193.56	21.384		−6.9085	1290.4	
	2	3	−138.25	281.11	0.4027	−248.72	45.164	0.4076
323.2	1	2	425.14	−197.51		−532.89	150.21	
	1	3	198.61	13.395		−37.151	1280.3	
	2	3	−186.62	450.67	0.3188	−391.06	34.014	0.4621

Figure 5 represents the relationship of the mesitylene 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 (293.2 to 323.2) K. The distribution coefficient values increased as the temperature and/or $(x_2)_{\text{NMP-rich phase}}$, increased.

Figure 6 represents the relationship of the mesitylene 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 (293.2 to 323.2) K. The selectivity decreased as the concentration of mesitylene increased, it means the higher the concentration of mesitylene in the feed, 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 6. Since the selectivity in all cases is greater than 1, the extraction is possible. Data of the same system at 298.2 K studied by Letcher and Naicker[2] shows the similar trend behavior for both K and S as shown in Figures 5 and 6, respectively.

As shown in Figure 7, the selectivities (S) and distribution coefficients (K) reflect opposing behavior (i.e., a solvent with particularly high selectivity has often only a limited distribution

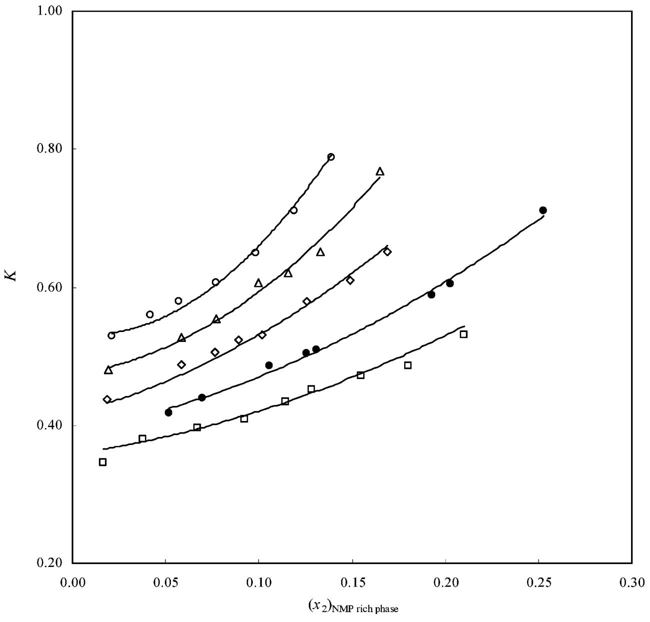

Figure 5. Effect of temperature on measured and correlated distribution coefficient (K) at □, 293.2 K; ●, 298.2 K;[2] ◇, 303.2 K; △, 313.2 K; ○, 323.2 K; —, UNIQUAC.

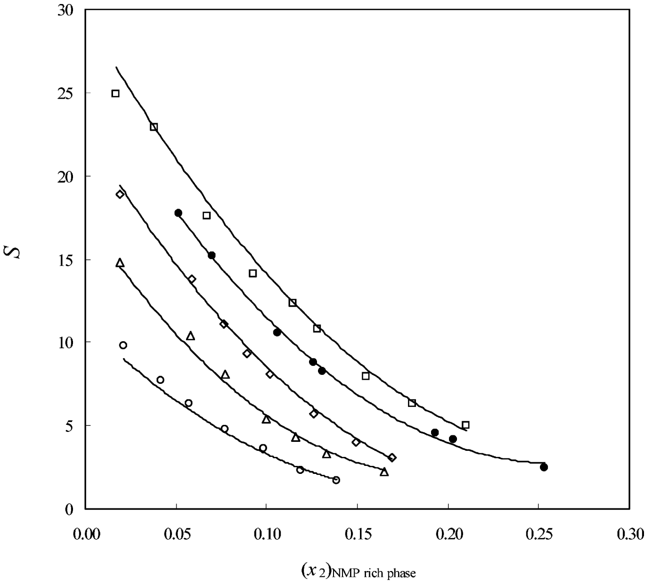

Figure 6. Effect of temperature on measured and correlated selectivity (*S*) at □, 293.2 K; ●, 298.2 K;[2] ◇, 303.2 K; △, 313.2 K; ○, 323.2 K; —, UNIQUAC.

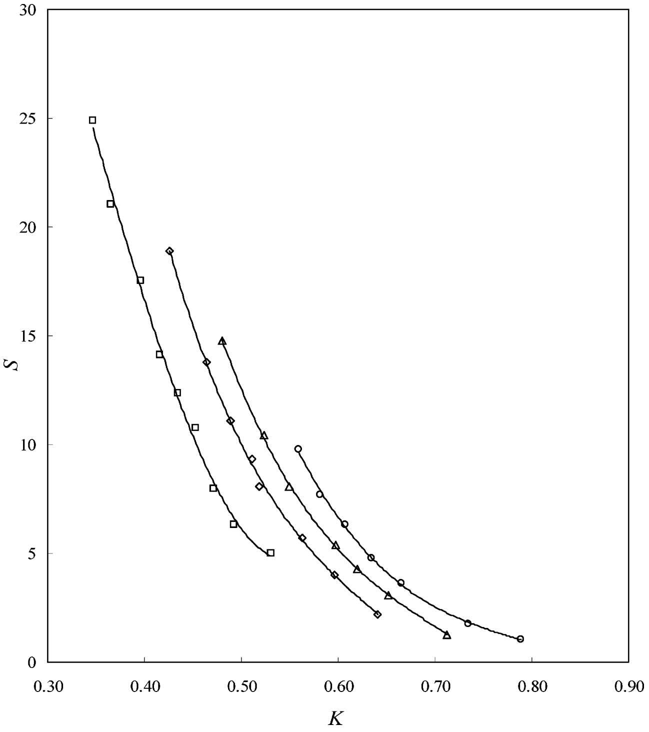

Figure 7. Distribution coefficient (*K*) against selectivity (*S*) at □, 293.2 K; ●, 298.2 K;[2] ◇, 303.2 K; △, 313.2 K; ○, 323.2 K.

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 liquid−liquid {hexadecane (1) + mesitylene (2) + NMP (3)} ternary system is carried out at temperatures of (293.2 to 323.2) K and at atmospheric pressure. The solubility of NMP in hexadecane-rich phase increases as the temperature increases, but it has little effect on the solubility of hexadecane in NMP-rich phase. The mutual NMP−hexadecane solubility increased as the concentration of mesitylene increases. Both the UNIQUAC and the NRTL models satisfactorily correlate the LLE experimental data, and they are equally the same according to the analysis of the rmsd (average rmsd was 0.447 for UNIQUAC as compared to 0.433 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 mesitylene in the feed increased. From the selectivity data, the separation of mesitylene from hexadecane by liquid extraction with NMP is feasible.

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