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Analysis and Evaluation of the Liquid−Liquid Equilibrium Data of the Extraction of Aromatics from Hydrocarbons by Tetraethylene Glycol

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Liquid−liquid equilibrium (LLE) data for the systems heptane + *o*-xylene + tetraethylene glycol (TTEG) have been experimentally studied over the temperature range (293 to 313) K. The experimental data of this work, in addition to 22 isothermal sets of LLE data (from the literature) for the extraction of aromatics from hydrocarbon mixtures using TTEG, are analyzed using two models. The models used are the empirical Othmer−Tobias correlation and the thermodynamic UNIQUAC model as programmed in the Aspen Plus simulator. For each data set, the analysis performed by the Othmer−Tobias correlation involves the determination of the model's parameters by regressing each set of data. The predictive capability of the UNIQUAC model has been investigated in terms of deviations for the mole fraction of the target aromatic species in the extract phase. Direct fitting of the data of this work using the Othmer−Tobias model gives an average rms (root-mean-square) of 0.002 in TTEG mass fraction in the extract phase, whereas prediction using UNIQUAC gives an average rms of 0.15.

1. Introduction

Separation of aromatic compounds from multicomponent hydrocarbon mixtures, such as reformed naphtha, is of potential commercial importance in the oil refining industry. Along with aromatics, reformed naphtha is comprised of paraffins, cycloparaffins, and isoparaffins. The most widely used process for separating aromatics from different paraffins is liquid extraction. In such a process, a solvent, such as tetraethylene glycol, dissolves selectively one of the components of the hydrocarbon mixture (the aromatic species in our case), resulting in two partially miscible liquid phases. Solvents for extraction should have high selectivity for aromatics, high capacity, high density, low viscosity, and partial miscibility with the hydrocarbon mixture at reasonably low temperature.[1] They also must have a good thermal stability, low reactivity, and minimal corrosion characteristics.[1,2] Among the most widely used extracting solvents for aromatics are sulfur dioxide, sulfolane, dimethyl sulfoxide, morpholine (*N*-formylmorpholine), *N*-methylpyrrolidone, γ-butyrolactone, glycols, ethylene carbonate, and propylene carbonate.[1−11] Among the glycol family, that is, ethylene glycol (EG), diethylene glycol (DEG), triethylene glycol (TEG), and tetraethylene glycol (TTEG), the latter was found to be the best in terms of the extraction capacity toward aromatics.[12] To optimize the balance between capacity and selectivity, mixed solvents, such as tetraethylene glycol + *N*-formylmorpholine, have also been explored by some investigators.[13]

The design and evaluation of industrial unit operations for extraction processes require reliable phase equilibrium data of the different mixtures involved in a given process. Because of the important industrial applications of tetraethylene glycol (TTEG), several studies dealing with the phase equilibria of TTEG-related systems have been carried out.[11−21] Although the technical literature is very rich in solvent extraction of some aromatics such as benzene and toluene, ternary studies involving xylenes in general and *o*-xylene in particular are relatively scarce. This is probably because of the difficulty of extracting xylenes from other hydrocarbons such as paraffins.[19] Ternary phase equilibrium data are also essential for the proper understanding of solvent extraction processes, selection of solvents, and design of extractors.

The purpose of the present study is to measure LLE data of the ternary system heptane + *o*-xylene + tetraethylene glycol over the temperature range (293 to 313) K at atmospheric pressure and to analyze and evaluate the experimental data (including the data of this work) available in the literature for the extraction of aromatics using TTEG. The literature data considered here involve binary,[16] ternary,[13,16,20] and quaternary mixtures[12,13,19,21] and mixtures with six species[19] covering the temperature range (293 to 413) K. The analysis will be performed using the empirical, two-parameter correlation of Othmer−Tobias[22] and the thermodynamic UNIQUAC model[23] as programmed in the Aspen Plus simulator.[24] The latter model will be used in the predictive, rather than the correlative, mode.

2. Experimental Section

Tetraethylene glycol (TTEG) used in this study was supplied by Riedel−deHaen with a stated purity of 98%. *o*-Xylene and heptane were supplied by Fluka with a purity

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Table 1. Experimental LLE Mole Fractions of Heptane (A) + *o*-Xylene (C) + Tetraethylene Glycol (B) at 293.1, 303.1, and 313.1 K

raffinate (upper, A-rich phase)		extract (lower, B-rich phase)	
x_A	x_C	x_A	x_C
	293.1 K		
0.901	0.099	0.015	0.028
0.819	0.181	0.011	0.048
0.671	0.328	0.010	0.081
0.514	0.486	0.008	0.109
0.430	0.568	0.011	0.148
	303.1 K		
0.807	0.192	0.017	0.053
0.699	0.301	0.001	0.084
0.660	0.338	0.014	0.091
0.516	0.481	0.008	0.121
0.467	0.532	0.013	0.146
0.410	0.584	0.015	0.162
	313.1 K		
0.889	0.110	0.022	0.033
0.810	0.189	0.018	0.057
0.673	0.325	0.020	0.091
0.566	0.428	0.019	0.133
0.484	0.508	0.016	0.157
0.422	0.568	0.015	0.179

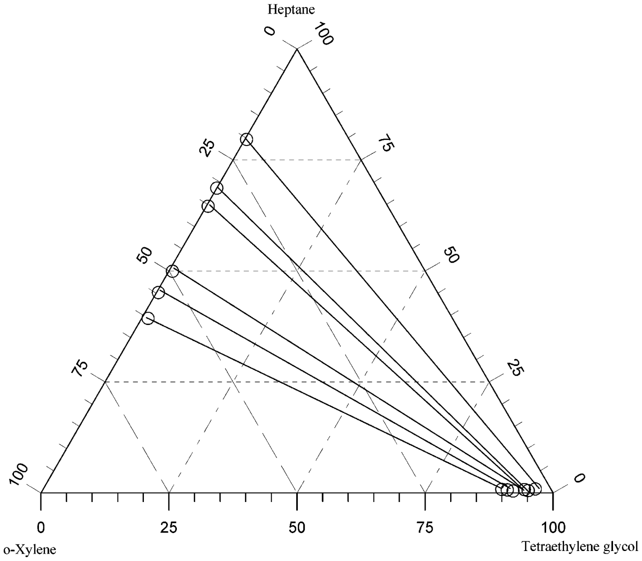

Figure 1. Equilibrium compositions of the ternary system heptane + *o*-xylene + tetraethylene glycol at 303.1 K.

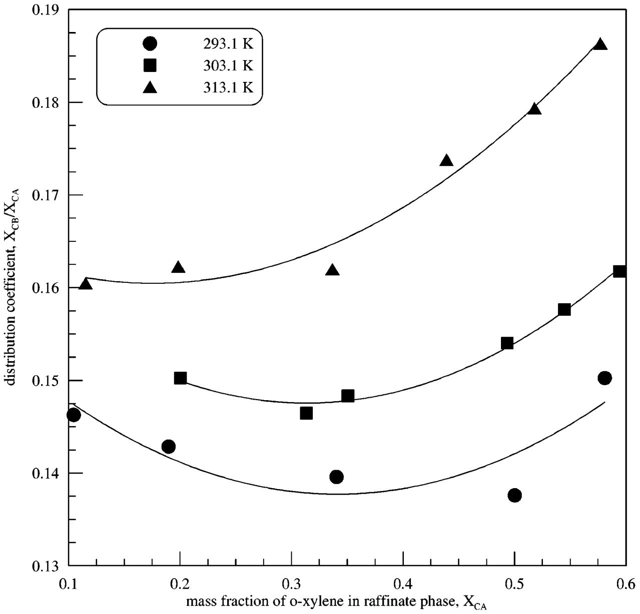

Figure 2. Distribution coefficient of *o*-xylene between the raffinate and the extract phases in the ternary system heptane (A) + *o*-xylene (C) + TTEG (B) at 293.1, 303.1, and 313.1 K (continuous lines represent a second-degree polynomial fit).

of 99%. Materials were used as received without further purification.

The equilibrium data were determined using an experimental apparatus consisting of an 85 cm^3 glass cell with a water jacket to maintain isothermal conditions. The temperature was measured by a mercury-in-glass thermometer with a precision better than 0.1 K. The temperature inside the jacketed cell was kept constant by circulating water from a water bath (Julabo Labortechnik GMBH—Germany), which is equipped with a temperature controller (Julabo PC) capable of maintaining the temperature within ±0.1 K. Different amounts of heptane, *o*-xylene, and TTEG were introduced into the extraction cell and were stirred for 2 h and then left for 6 h to equilibrate and settle down into a raffinate and extract layers under the same controlled temperature. No attempt was made to measure the initial feed composition of the mixture.

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 is achieved by a capillary column, 50 m × 0.32 mm i.d., of WCOT (wall-coated-open-tube) fused silica coated with a 1.2 μm stationary film (CP-Sil 5 CB). The inlet pressure of the carrier (nitrogen) gas was set at 45 kPa, and the temperatures of both detector and injector were set at 573.1 K. Oven temperature was programmed as follows: the initial temperature was set at 348.1 K for 5 min, followed by a constant heating rate of 15 K/min until a final temperature of 513.1 K was attained. This final temperature was held for 9 min, and the cycle was repeated. Mixtures of known compositions of the reagents were used to calibrate the gas chromatograph. The reproducibility of composition measurements was better than 0.1%.

3. Results and Discussion

3.1. New Experimental Data of This Work. The experimental LLE data at 293.1, 303.1, and 313.1 K for the system heptane + *o*-xylene + TTEG, studied in this work, are shown in Table 1. It is evident that *o*-xylene (the target species to be extracted) is distributed between the raffinate (heptane-rich phase) and the extract (TTEG-rich phase). A typical triangular diagram for the 303.1 K isotherm is displayed in Figure 1 (other isotherms plotted on the same figure will render it crowded and unclear). The slight mutual solubility of TTEG and heptane is rather obvious from both the data in Table 1 and the plot in Figure 1. The distribution coefficient of *o*-xylene (the ratio of the mass fraction of *o*-xylene (C) in the extract (B) to that in the raffinate (A)), ω_{CB}/ω_{CA}, plotted versus mass percent of *o*-xylene in the raffinate phase (ω_{CA}) is shown in Figure 2. For values of ω_{CA} below 35%, the distribution coefficient at a given temperature changes only slightly with ω_{CA}, whereas, for values of ω_{CA} above 35%, the distribution coefficient tends to increase with feed mass fraction of the target species (Figure 2). Employing the error propagation formula[25] and assuming 0.1% reproducibility in the measured ω_{CA} and ω_{CB}, the uncertainties in the reported distribution coefficients have been computed, and the highest uncertainty obtained is used to generate the error bars shown in Figure 2 for the 313.1 K isotherm. As shown in Figure 2, the distribution coefficient increases with

Table 2. Correlation of LLE Data for the Extraction of Aromatics Using Tetraethylene Glycol (TTEG) over the Temperature Range (293 to 413) K Using the Othmer−Tobias Correlation:[22] $\ln[(1-\omega_{BB})/\omega_{BB}] = \ln\alpha + \beta \ln[(1-\omega_{AA})/\omega_{AA}]$

T/K	points	$-\ln\alpha$	β	MAXD[a]	AAD[b]	rms[c]
Heptane + *o*-Xylene + TTEG (This Work)						
293.1	5	2.532	0.581	0.005	0.002	0.003
303.1	6	2.415	0.592	0.002	0.001	0.001
313.1	6	2.259	0.613	0.002	0.001	0.001
Decane + Ethylbenzene + TTEG (ref 16)						
298.5	3	2.615	1.042	0.014	0.009	0.312
312.0	4	3.004	0.707	0.006	0.004	0.052
323.0	5	2.951	0.696	0.015	0.006	0.026
Decane + Benzene + TTEG (ref 16)						
302.0	4	1.387	2.642	0.019	0.0084	0.860
318.0	5	2.023	1.652	0.029	0.014	1.076
327.0	3	1.765	1.064	0.01	0.007	0.036
Heptane + *p*-Xylene + (98 mass % TTEG + 2 mass % Water) (ref 19)						
333.1	6	2.801	0.434	0.012	0.005	0.020
Heptane + *p*-Xylene + (95 mass % TTEG + 5 mass % Water) (ref 19)						
333.1	7	2.448	0.636	0.017	0.008	0.017
413.1	5	1.402	0.440	0.036	0.016	0.048
Heptane + Benzene + Toluene + *p*-Xylene + (98 mass % TTEG + 2 mass % Water) (ref 19)						
333.1	10	2.601	0.283	0.015	0.005	0.0175
Cyclohexane + Benzene + Toluene + *p*-Xylene + TTEG + 2 mass % Water (ref 19)						
333.1	7	1.842	0.120	0.019	0.008	0.010
Heptane + Benzene + (95 mass % TTEG + 5 mass % Water) (ref 21)						
393.1	6	1.612	0.679	0.048	0.04	0.0003
Heptane + Toluene + TTEG (ref 13)						
313.1	6	1.937	0.556	0.0219	0.009	0.009
Heptane + Toluene + (70 mass % TTEG + 30 mass % *N*-Formylmorpholine) (ref 13)						
313.1	6	1.592	0.693	0.01244	0.005	0.001
Heptane + Toluene + (70 mass % TTEG + 30 mass % *N*-methylpyrrolidone) (ref 13)						
313.1	7	1.262	0.703	0.004	0.002	0.0003
Heptane + Benzene + TTEG (ref 20)						
298.1	4	1.627	0.801	0.007	0.004	0.001
Heptane + Ethylbenzene + TTEG (ref 20)						
298.1	4	2.372	0.615	0.014	0.011	0.029
Heptane + Benzene + (96.1 vol % TTEG + 3.9 vol % Water) (ref 20)						
373.1	5	1.237	0.739	0.04	0.034	0.024

[a] MAXD = maximum absolute deviation. [b] AAD = average absolute deviation, $\sum|\text{Dev}|/n$. [c] rms = root-mean-square deviation $(\sum \text{Dev}^2/n)^{1/2}$.

temperature. However, in view of the high uncertainty used, not much can be concluded about the effect of temperature on the distribution coefficient of *o*-xylene in the studied ternary system.

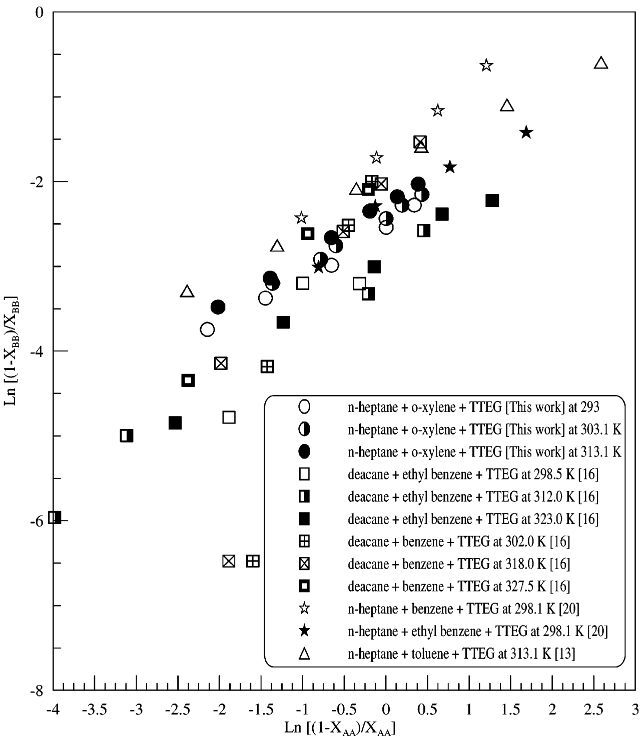

Figure 3. Othmer−Tobias correlation of liquid−liquid equilibrium data for the extraction of aromatics from ternary systems using tetraethylene glycol.

3.2. Modeling and Analysis of Available Literature Data. As mentioned before, the experimental data of this work, in addition to those found in the literature, were first analyzed using the Othmer−Tobias model.[22] This is a two-parameter correlation, which has the following linearized form

$$\ln\left(\frac{1-\omega_{BB}}{\omega_{BB}}\right) = \ln\alpha + \beta\ln\left(\frac{1-\omega_{AA}}{\omega_{AA}}\right) \tag{1}$$

where ω_{AA} stands for the mass fraction of the diluent (the hydrocarbon from which the aromatic species is to be extracted, such as heptane) in the raffinate phase, ω_{BB} is the mass fraction of TTEG in the extract phase, both at equilibrium, and α and β are two adjustable parameters. Other empirical models, such as the Bachman correlation and the Hand correlation,[13] can also be used. The Othmer−Tobias model, as shown in eq 1 above, makes the correlation in terms of the compositions of the diluent and the extracting phase (TTEG) but not the aromatic species. This makes it more appropriate for cases where more than one aromatic species are extracted simultaneously, as encountered in many literature data considered in this study. The results of analysis using this model for data sets of this work and those found in the literature are summarized in Table 2. In this table values of the optimum model parameters (ln α and β), maximum deviation (MAXD), and root-mean-square (rms) deviation in ω_{BB} are presented. The model parameters were obtained by regressing each set of experimental data employing the linearized form of the model (eq 1) and using the least-squares method as implemented by a commercial piece of software.[26]

The ternary and quaternary data sets considered here are adequately fitted by the Othmer−Tobias correlation. Data of this work sufficiently lend itself to this correlation with an rms deviation of 0.003, 0.001, and 0.001 in ω_{BB} at 293.1, 303.1, and 313.1 K, respectively. MAXD and AAD (average of absolute deviations) values are also the lowest among all data sets considered. Some data sets are shown to be totally disobedient to the Othmer−Tobias model. For example, data of the six-component system of Wang et al.[19] are shown not to follow any trend on the Othmer−Tobias coordinates. Quaternary LLE data of the same authors, however, are shown to be adequately represented by the Othmer−Tobias correlation (Table 2). This could point to the deficiency of the Othmer−Tobias model in describing LLE systems with more than four species.

Graphical representation of the Othmer−Tobias correlation for all LLE data sets considered in this study is shown in Figures 3 and 4. While ternary and quaternary LLE data

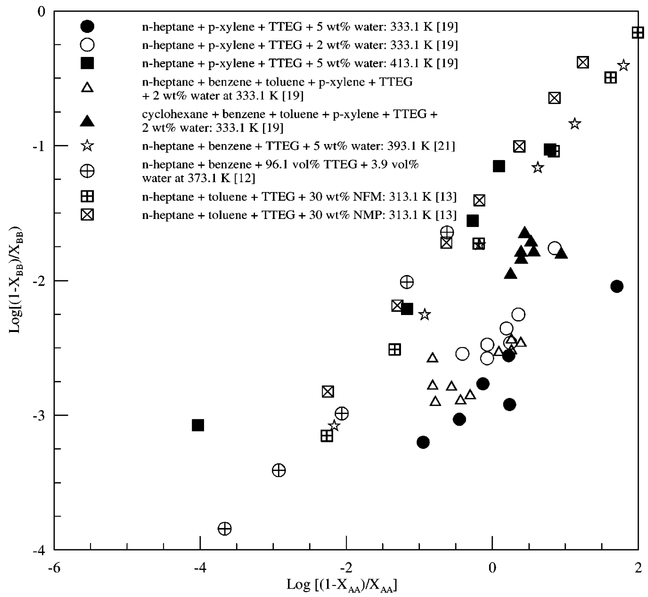

Figure 4. Othmer−Tobias correlation of liquid−liquid equilibrium data for the extraction of aromatics from multicomponent systems using tetraethylene glycol.

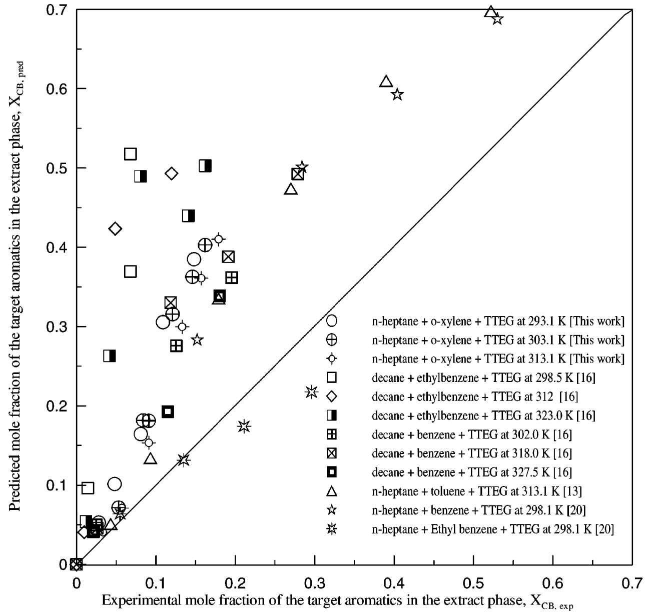

Figure 5. Comparison of experimental and predicted mole fractions of the target aromatic in the extract phase for ternary systems containing tetraethylene glycol (TTEG) using UNIQUAC.

are shown to satisfy the Othmer−Tobias correlation with varying degrees, there are some data that do not follow the correlation. In particular, LLE systems with six species are very clearly shown not to obey the correlation. Among the other data sets, there are some points that could be considered “outliers”. For example, the 302 K and the 318 K isotherms of Al Qattan et al.[16] are shown to have such outliers, as evident in Figure 3.

The other model that has been utilized in this study is the UNIQUAC model. This model has been used in the predictive mode as programmed in the Aspen Plus simulator.[24] The results of analysis for all data sets studied here are summarized in Tables 3−5. Comparisons between the predicted mole fraction of the target aromatic component in the extract phase, x_{CB}(pred), and the experimental one, x_{CB}(exp), are also shown in Figures 5−7. It is interesting to note that, for all LLE systems considered here (except two points that belong to the ternary system heptane + ethyl benzene + TTEG at 298.1 K[20] shown in Figure 5), the UNIQUAC model overpredicts the composition of the target aromatic in the extract phase, as evident from Figures 5−7. It is also clear from these figures that, in general, the prediction capability of UNIQUAC, using the interaction parameters existing in the Aspen library, is better over low concentration ranges of the target aromatic. Data of this work, when processed altogether, are predicted with rms values of 0.17 and 0.15 for x_{CA} and x_{CB}, respectively (Table 3). For all LLE ternary systems studied, rms values lie in the range (0.10 to 0.18) for the predicted x_{CB} in the raffinate phase and (0.15 to 0.29) for the predicted

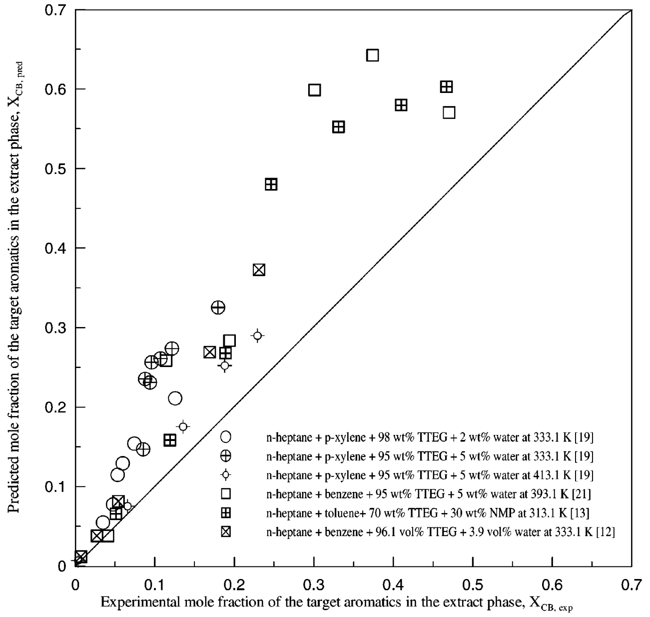

Figure 6. Comparison of experimental and predicted mole fractions of the target aromatic in the extract phase for quaternary systems containing tetraethylene glycol (TTEG) using the UNIQUAC model.

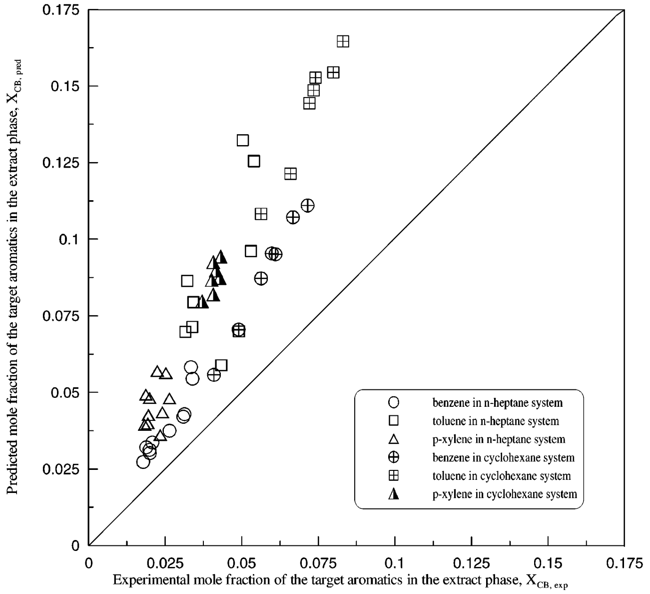

Figure 7. Comparison of experimental and predicted mole fractions of the target aromatic species in the extract phase for the systems heptane + benzene + toulene + *p*-xylene + 98 wt % TTEG + 2 wt % water and cyclohexane + benzene + toulene + *p*-xylene + 98 wt % TTEG + 2 wt % water, both at 333.1 K[19] using the UNIQUAC model.

Table 3. Prediction Results Given by Aspen Simulator[24] for the LLE of Aromatics Extraction by Tetraethylene Glycol from Ternary Systems Using the UNIQUAC Model

raffinate (diluent-rich) phase						extract (TTEG-rich) phase					
diluent			target (aromatics)			target (aromatics)			TTEG		
rms	AAD	MAXD	rms	AAD	MAXD	rms	AAD	MAXD	rms	AAD	MAXD
Heptane + *o*-Xylene + TTEG, 17 points, 293 to 313 K (This Work)											
0.177	0.171	0.233	0.166	0.157	−0.222	0.152)	0.126	0.241	0.148	0.120	−0.236
Decane + Ethylbenzene + TTEG, 12 points, 298 to 323 K[16]											
0.108	0.093	0.148	0.106	0.081	−0.215	0.289	0.244	0.450	0.289	0.243	−0.450
Decane + Benzene + TTEG, 12 points, 302.0 to 327.5 K[16]											
0.199	0.104	0.248	0.064	0.058	−0.103	0.146	0.124	0.214	0.134	0.104	−0.217
Heptane + Toluene + TTEG, 6 points, 313.1 K[13]											
0.095	0.085	0.142	0.107	0.102	−0.141	0.157	0.134	0.220	0.150	0.128	−0.213
Heptane + Benzene + TTEG, 4 points, 298.1 K[20]											
0.114	0.111	0.137	0.101	0.098	−0.133	0.177	0.174	0.217	0.168	0.164	−0.208
Heptane + Ethylbenzene + TTEG, 4 points, 298.1 K[20]											
0.165	0.143	0.245	0.180	0.176	−0.240	0.247	0.227	0.346	0.243	0.220	−0.345

Table 4. Prediction Results Given by Aspen Simulator[24] for the LLE of Aromatics Extraction by Tetraethylene Glycol from Quaternary Systems Using the UNIQUAC Model

raffinate (diluent-rich) phase						extract (TTEG-rich) phase					
diluent			target (aromatics)			target (aromatics)			TTEG		
rms	AAD	MAXD	rms	AAD	MAXD	rms	AAD	MAXD	rms	AAD	MAXD
Heptane + *p*-Xylene + (98 mass % TTEG + 2 mass % Water) at 333.1 K, 13 points[19]											
0.186	0.166	0.337	0.185	0.162	−0.339	0.112	0.100	0.160	0.130	0.119	−0.176
Heptane + *p*-Xylene + (95 mass % TTEG + 5 mass % Water) at 413.1 K, 5 points[19]											
0.267	0.235	0.355	0.271	0.236	−0.351	0.043	0.036	0.064	0.203	0.180	0.303
Heptane + Benzene + (95 mass % TTEG + 5 mass % Water) at 393.1 K, 6 points[21]											
0.203	0.170	−0.347	0.201	0.153	0.391	0.182	0.151	0.298	0.126	0.117	−0.168
Heptane + Toluene + (70 mass % TTEG + 30 mass % *N*-Methylpyrrolidone) at 313.1 K, 7 points[13]											
0.066	0.052	−0.125	0.063	0.055	0.096	0.151	0.128	0.234	0.093	0.072	−0.145
Heptane + Benzene + (96.1 vol % TTEG + 3.9 vol % Water) at 373.1 K, 5 points[12]											
0.092	0.086	0.122	0.043	0.037	−0.072	0.079	0.057	0.142	0.054	0.050	0.088

Table 5. Prediction Results Given by Aspen Simulator[24] for the LLE of Aromatics Extraction by Tetraethylene Glycol from Binary Systems and Systems with Six Species using the UNIQUAC Model

raffinate (diluent-rich) phase						extract (TTEG-rich) phase					
diluent			target (aromatics)			target (aromatics)			TTEG		
rms	AAD	MAXD	rms	AAD	MAXD	rms	AAD	MAXD	rms	AAD	MAXD
Heptane + Benzene + Toluene + *p*-Xylene + (98 wt % TTEG + 2 wt % Water) at 333.1 K, 10 points[19]											
0.015	0.091	−0.174	0.023	0.017	−0.079	0.029	0.027	0.082	0.210	0.192	−0.295
Cyclohexane + Benzene + Toluene + *p*-Xylene + (98 wt % TTEG + 2 wt % Water) at 333.1 K, 7 points[19]											
0.120	0.120	−0.140	0.022	0.020	−0.054	0.050	0.049	0.082	0.437	0.436	−0.481
Heptane + TTEG at 293.0, 302.5, 312.0, and 322.0 K, 4 points[16]											
0.055	0.044	−0.089	0.055	0.044	0.089	0.017	0.016	−0.020	0.017	0.0161	−0.02
trans-Decaline + TTEG at 303.0, 313.0, 321.0, and 322 K, 4 points[16]											
0.402	0.402	−0.410	0.402	0.402	0.410	0.348	0.348	0.363	0.348	0.348	−0.363

x_{CB} in the extract phase, respectively (Table 3). Except for the system decane + ethyl benzene + TTEG[16] (which has a much higher predicted x_{CB} than those of other systems), Figure 5 shows that UNIQUAC gives comparable predictions for the different ternary systems. For the extraction of aromatics from quaternary LLE systems using TTEG, Table 4 shows that rms values lie in the range (0.04 to 0.27) for the predicted x_{CA} in the raffinate phase and (0.04 to 0.18) for the predicted x_{CB} in the extract phase, respectively. Surprisingly, it is evident from Table 4, and also from Figure 6, that UNIQUAC prediction capability is better for quaternary systems than for ternary systems. The lowest AAD for x_{CB} in the extract phase for the quaternary systems shown in Table 4 is 0.04 (for heptane + *p*-xylene + (95% TTEG + 5% water at 413.1 K[19]), and the highest AAD is 0.15 (for heptane + benzene + (95% TTEG + 5% water at 393.1 K[21]). Results of analysis for two multicomponent LLE systems having six species[19] are shown in Table 5 and Figure 7. Shown also in Table 5 are the results of analyses for two binary systems involving TTEG found in the literature.[16] Root-mean-square values associated with the multicomponent systems are shown to be lower than those associated with the other binary, ternary, and quaternary systems. However, the composition of the aromatic component encountered in these two multicomponent systems covers only the dilute region where UNIQUAC has been shown to perform better even for ternary and quaternary systems. This is evident from Figure 7, where x_{CB}(exp) values are all below 0.1.

4. Conclusions

LLE data for the ternary system heptane + *o*-xylene + TTEG have been studied over the temperature range (293 to 313) K at atmospheric pressure. The experimental data, together with 22 isothermal LLE data sets from the literature for the extraction of aromatics from hydrocarbon mixtures using TTEG, are analyzed using the Othmer−Tobias empirical correlation and the thermodynamic UNIQUAC model. The latter is used in the predictive mode as programmed in the Aspen Plus simulator. The ternary and quaternary LLE data sets considered here are adequately represented by the Othmer−Tobias correlation. LLE systems with six species, however, do not obey the correlation. The experimental data of this work are correlated with this model with rms values of 0.003, 0.001, and 0.001 in ω_{BB} at 293.1, 303.1, and 313.1 K, respectively. LLE systems with more than four species besides TTEG were found not be correlated by this empirical correlation. On the other hand, the UNIQUAC model is found to overpredict the composition of the target aromatic in the extract phase for all LLE systems considered. The predictive capability of UNIQUAC deteriorates at higher concentration of the aromatic species in the system. Experimental data of this work, when processed all together using UNIQUAC, were predicted with an rms deviation and an AAD of 0.15 and 0.13 for x_{CB}, respectively.

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