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Liquid−Liquid Equilibria for the Ternary Systems of (Water + Tetrahydrofuran + Polar Solvent) at 298.15 K

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Liquid−liquid equilibrium data and tie-line end compositions are presented for mixtures of [water (1) + tetrahydrofuran (2) + trichloroethylene or + 1-hexanol or + 3-methylbutyl ethanoate (3)] at $T = 298.15$ K and $P = (101.3 \pm 0.7)$ kPa. Among the studied solvents, 3-methylbutyl ethanoate represents the best performance for the extraction of tetrahydrofuran. The properties and liquid−liquid equilibria (LLE) of the associated ternaries containing polar components capable of hydrogen bonding or dipole−dipole interaction have been estimated using a solvatochromic approach (SERLAS). The tie lines were also correlated using the UNIFAC-original model. The reliability of the models has been analyzed against the LLE data with respect to the distribution ratio and separation factor. The proposed solvatochromic model appears to be an improvement in data fit for the ternary systems, yielding a mean error of 15% for all the systems considered.

Introduction

The efficient separation of ring-containing compounds (e.g., cyclic ethers, cyclic alcohols or hydrocarbons, and aromatics) from aqueous solutions is an important concept in the chemical industry where many solvents have been tested to improve such recovery.[1−8] Sometimes it may be desirable to use a high-boiling solvent that does not have to be distilled so long as no azeotropes appear. Three major factors have been found to influence the equilibrium characteristics of solvent extraction of cyclic ethers from aqueous solutions (i.e., the nature and concentration of solute and the type of organic solvent). Simultaneously, the impact of additional controlling factors such as the third-phase formation can also modify the equilibrium. Process considerations dealing with the physical extraction of cyclic ethers through hydrogen bonding or dipole−dipole interaction still remain a challenging problem because such systems show extremely nonideal behavior.

Regarding the technical and economic merits of high-boiling solvents during the regeneration by distillation, the selection of extracting agents from various classes of polar, protic, or nonprotic type was made. They all have higher boiling temperatures than water, except trichloroethylene.

The main purpose of this study is to generate new LLE data for the extraction of tetrahydrofuran from water using trichloroethylene, 1-hexanol and 3-methylbutyl ethanoate (isoamyl acetate), as polar and proton-donating and -accepting solvents of low vapor pressure and to correlate the data by a solvatochromic approach and UNIFAC model. Such studies, besides other purposes, are indispensable to the calibration and verification of analytical models. Liquid−liquid equilibrium (LLE) data for the extraction of a cyclic ether from water are scarce in the literature.[7−9] A survey of the literature indicated that no dependable LLE results were available for the present ternaries.

In this study, attempts have also been made to estimate the properties and liquid−liquid equilibria of associated mixtures on the basis of a solvatochromic approach, SERLAS (solvation energy relation for liquid associated systems), which combines the modified solvatochromic parameters of the linear solvation energy relationship, LSER,[10,11] with the thermodynamic factors (of activity coefficients) derived from the UNIFAC-Dortmund model[12] in a relation including expansion terms and two correction factors for the limiting conditions of extraction. The LLE data have been determined for each of the systems (water + tetrahydrofuran + trichloroethylene or + 1-hexanol or + 3-methylbutyl ethanoate) at 298.15 K. The tie lines were correlated using the UNIFAC-original model.[13,14] Finally, experimental separation factors were compared with the predictions from the SERLAS model.

Experimental Section

Tetrahydrofuran of analytical grade (≥99%, GC) and the organic solvents (99%, GC) were supplied by Fluka. All of the chemicals were used as received without further purification. Mass fractions of impurities detectable by GC were found to be <0.0020. HPLC-grade methanol from Merck was used as an internal substance in gas chromatographic analysis. Deionized and redistilled water was used throughout all experiments.

The binodal (solubility) curves were determined by the cloud point method using an equilibrium glass cell with a water jacket to maintain isothermal conditions.[7,8] The temperature in the cell was kept constant by circulating water from a water bath (Julago Labortechnik GMBH-Germany) that is equipped with a temperature controller capable of maintaining the temperature within ±0.1 K. The major central part of the solubility curves was obtained by titrating heterogeneous mixtures of water + solvent with tetrahydrofuran until the turbidity had disappeared. For the water-side and solvent-side limited regions in which the curve and the sides of the triangle are close and exhibit similar slopes, binary mixtures of either (water + tetrahydrofuran) or (solvent + tetrahydrofuran) were titrated against the third component until the transition

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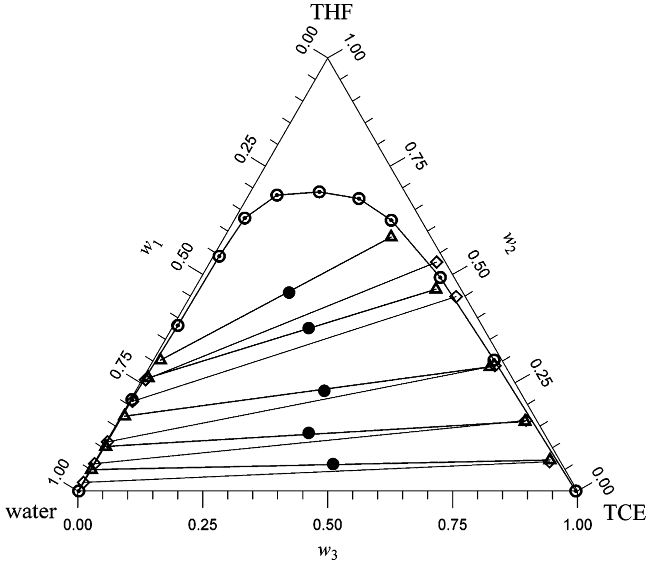

Figure 1. Liquid−liquid equilibria (mass fraction) for the system (w_1 water + w_2 tetrahydrofuran (THF) + w_3 trichloroethylene (TCE)) at 298.15 K: ⊙, solubility (binodal curve) data; △, experimental tie lines (solid line); ◇, UNIFAC-predicted end compositions (dashed line); ●, initial compositions.

from homogeneity to cloudiness was observed. All mixtures were prepared by mass with a Mettler scale accurate to within $\pm 10^{-4}$ g. Mutual solubility values of the (water + solvent) binaries were measured using the method based on the detection of the cloud point.[8] The transition point between the homogeneous and heterogeneous zones was determined visually. The reliability of the method depends on the precision of the Metrohm microburet with an uncertainty of ± 0.01 cm^3 and is limited by the visual inspection of the transition across the apparatus. The concentration determinations were made with an uncertainty of ± 0.001 mass fraction. End-point determinations of the tie lines were based upon the independent analysis of the conjugate phases that were regarded as being in equilibrium. Mixtures of known masses of water, tetrahydrofuran, and a polar solvent lying within the heterogeneous gap were introduced into the extraction cell and were stirred vigorously for at least 2 h and then left for 5 h to settle down into raffinate (aqueous) and extract (solvent) layers. The compositions of liquid samples withdrawn from the conjugate phases were analyzed using a Hewlett-Packard GC analyzer (model 6890) equipped with flame ionization (FI) and thermal conductivity (TC) detectors. HPLC-grade methanol was used as an internal standard. A 15-m-long HP Plot Q column (0.32 mm i.d., 0.2 μm film thickness) for TCD and an HP-Innowax poly(ethylene glycol) capillary column (30 m × 0.32 mm × 0.5 μm) for FID were used to separate organic components of samples at tailorized oven programs suitable for each ternary. The detector temperature was kept at $T = 523.15$ K, and the injection port temperature was held at $T = 473.15$ K. Injections were performed on the split $^1/_{100}$ mode. Nitrogen was used as a carrier at a rate of 6 cm^3/min. The composition of water was determined by means of a thermal conductivity detector (TCD).

Results and Discussion

Distribution Behavior of Tetrahydrofuran. The compositions of mixtures on the binodal curve and the mutual binary solubilities of water and a polar solvent at 298.15 K are given in Figures 1−3, in which w_i denotes the mass fraction of the ith component. Table 1 summarizes the experimental tie-line compositions of the equilibrium phases, for which w_i' and w_i'' refer to the mass fractions of the ith component in the aqueous and solvent phases, respectively. The experimental and calculated tie lines through UNIFAC-original and solubility isotherms of the studied ternaries are plotted on equilateral triangular diagrams in Figures 1−3. The shape of the binodal curves and the slopes of the tie lines in Figures 1−3 show that the distribution of tetrahydrofuran in the (water + polar solvent) mixture is very much dependent on the structure and polarity of the solvents of proton-donating and -accepting types. In the ternary systems, water is most soluble in the system containing 1-hexanol. Figures 1−3 show that the area of the two-phase heterogeneous region for the studied mixtures decreases in the order 1-hexanol < 3-methylbutyl ethanoate (MBE) < trichloroethylene (TCE). This implies that a decrease in the polarity of the extracting

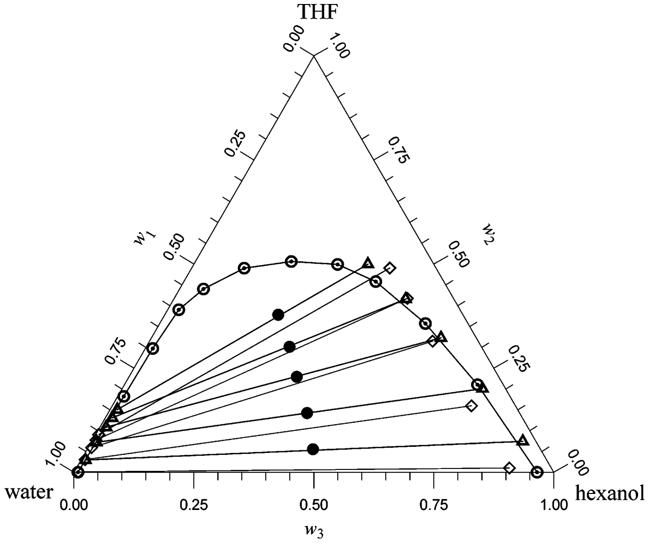

Figure 2. Liquid−liquid equilibria (mass fraction) for the system (w_1 water + w_2 tetrahydrofuran (THF) + w_3 1-hexanol) at 298.15 K: ⊙, solubility (binodal curve) data; △, experimental tie lines (solid line); ◇, UNIFAC-predicted end compositions (dashed line); ●, initial compositions.

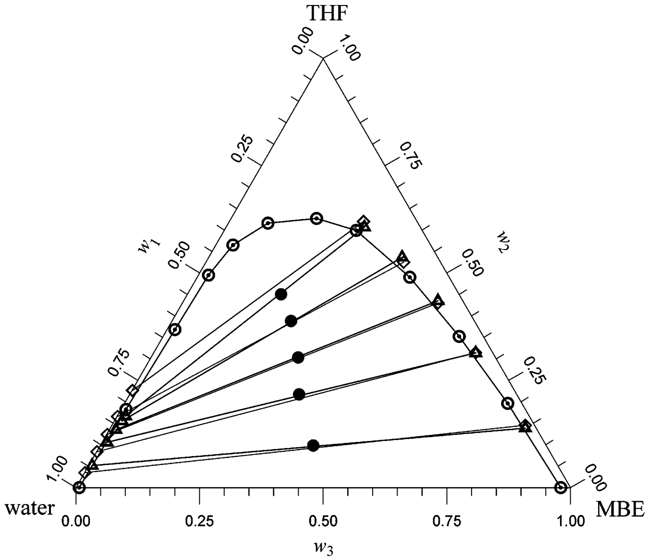

Figure 3. Liquid−liquid equilibria (mass fraction) for the system (w_1 water + w_2 tetrahydrofuran (THF) + w_3 3-methylbutyl ethanoate (MBE)) at 298.15 K: ⊙, solubility (binodal curve) data; △, experimental tie lines (solid line); ◇, UNIFAC-predicted end compositions (dashed line); ●, initial compositions.

Table 1. Thermodynamic Factors (Γ_L) and Experimental Tie-Line Compositions (Mass Fraction) of the Conjugate Solutions w_1', w_2', w_1'', and w_2'' at T = 298.15 K

water-rich		solvent-rich			G^E [b]
w_1'	w_2'	w_1''	w_2''	Γ_L[a]	J/mol
Water (1) + Tetrahydrofuran (2) + Trichloroethylene (3)					
0.9982[c]	0	0.0032[c]	0		
0.9483	0.0492	0.0193	0.0714	0.9980	956.9
0.8930	0.1025	0.0247	0.1603	0.9985	999.8
0.8203	0.1726	0.0315	0.2865	1.0017	1033.4
0.7288	0.2610	0.0504	0.4658	1.0114	1244.2
0.6839	0.3018	0.0798	0.5861	1.0223	1487.8
Water (1) + Tetrahydrofuran (2) + 1-Hexanol (3)					
0.9914[c]	0	0.0347[c]	0		
0.9611	0.0294	0.0275	0.0742	1.0042	688.9
0.9172	0.0718	0.0482	0.2006	1.0078	1084.3
0.8787	0.1080	0.0736	0.3225	1.0093	1383.6
0.8548	0.1305	0.1007	0.4158	1.0116	1572.0
0.8342	0.1503	0.1374	0.4996	1.0180	1703.8
Water (1) + Tetrahydrofuran (2) + 3-Methylbutyl Ethanoate (3)					
0.9935[c]	0	0.0197[c]	0		
0.9419	0.0511	0.0223	0.1384	0.9894	1299.7
0.8846	0.1052	0.0348	0.3136	0.9732	822.8
0.8520	0.1347	0.0505	0.4351	0.9590	589.7
0.8295	0.1550	0.0722	0.5363	0.9438	471.0
0.8166	0.1663	0.1137	0.6065	0.9253	431.6

[a] Thermodynamic factors of tetrahydrofuran in terms of eq 3. [b] Excess Gibbs free energy function for the organic phase due to UNIFAC-Dortmund, $G^E = RT \sum_i x_i \ln \gamma_i$. [c] Mutual solubility value.

solvent (dielectric constants $\epsilon_H = 13.3$, $\epsilon_{MBE} = 4.63$, $\epsilon_{TCE} = 3.42$)[20] results in an increase in the area of the two-phase region (i.e., the mutual solubility of the components is reduced) and also that water is most soluble in the (1-hexanol + tetrahydrofuran) mixture and least soluble in the (trichloroethylene + tetrahydrofuran) mixture. The slope of the tie lines (i.e., the distribution coefficient defined as the ratio of the mass fraction of tetrahydrofuran in the solvent-rich phase to that in the water-rich phase ($D = w_2''/w_2'$)) shows that tetrahydrofuran is more soluble in the organic phase than in the aqueous phase ($D > 1$), yielding the largest D for 3-methylbutyl ethanoate. From the tested polar solvents, the lowest D values show tetrahydrofuran in the (water + trichloroethylene) mixture, whereas 3-methylbutyl ethanoate gives a D that is about 2 times larger as compared to those of other solvents.

This could be attributable to the solubilizing effect of the ethylene (C=C) group for trichloroethylene having the lowest R-chain structure as well as to a lower dipole moment ($\mu_{TCE} = 0.3 \times 10^{-12}$ C·m), categorizing this solvent structure as less capable of association with tetrahydrofuran through hydrogen bonding or dipole−dipole interaction. However, the existence of a large number of methyl groups, as well as the oxygenated (acetate and carboxyl) groups on 1-hexanol and 3-methylbutyl ethanoate, makes both solvent structures of high polarity, favoring the dipole−dipole interaction with tetrahydrofuran. Therefore, it is expected that the dipole moment of the solvent ($\mu_{TCE} = 0.3 \times 10^{-12}$ C·m, $\mu_H = 5.4 \times 10^{-12}$ C·m, $\mu_{MBA} = 6.0 \times 10^{-12}$ C·m)[20] will affect the extraction equilibria. These concepts can be verified by the results from Figures 1−3 and Table 1, which manifest the fact that the controlling factor for the physical extraction is the polarity of the solvent, indicative of the change in the degree of extraction of tetrahydrofuran in the polar solvents ordered as trichloroethylene < 1-hexanol < 3-methylbutyl ethanoate.

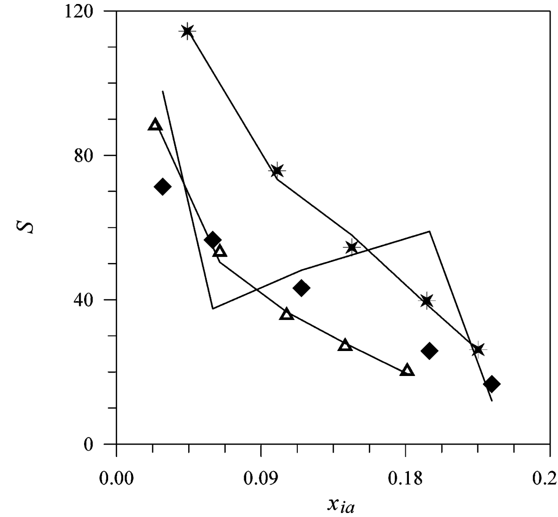

Figure 4. Plot of the separation factor (S) against the initial tetrahydrofuran mole fraction for the ternary systems water + tetrahydrofuran + trichloroethylene (◆) or 1-hexanol (△) or 3-methylbutyl ethanoate (*); experimental and theoretical through SERLAS, (solid line) eq 1.

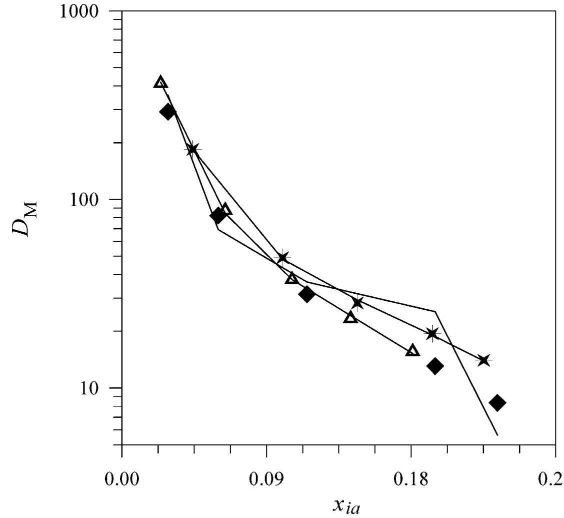

Figure 5. Plot of the distribution ratio (D_M) against the initial tetrahydrofuran mole fraction for the ternary systems water + tetrahydrofuran + trichloroethylene (◆) or 1-hexanol (△) or 3-methylbutyl ethanoate (*); experimental and modeled through SERLAS, (solid line) eq 1.

The effectiveness of the extraction of tetrahydrofuran (2) by the polar solvent is indicated by its selectivity (or separation factor, S) defined on the mole fraction scale as the ratio of distribution coefficients of the solute (2) to water (1), $S = D_2/D_1 = (x_2''/x_2')/(x_1''\}/x_1')$, and is presented in Figure 4. The prime refers to the water-rich phase, and the double prime refers to the solvent-rich phase. From the selectivity data, it can be concluded that the separation of tetrahydrofuran from water by extraction with a polar solvent is feasible. Trichloroethylene is a less favorable solvating agent for tetrahydrofuran. It is also apparent from Figures 4 and 5 that 3-methylbutyl ethanoate is the most appropriate solvent for the separation of mixtures of water and tetrahydrofuran.

The end compositions of the tie lines for the studied ternaries were predicted using the UNIFAC-original model along with LLE-UNIFAC parameters.[13,14] A program of multivariate (Levenberg−Marquardt) convergence developed by Magnussen and Michelsen (Fredenslund et al.[15]) was used to solve the implicit LLE equations. Consequently, the UNIFAC model proved to be moderately accurate, yielding a mean relative error $\bar{e}$ % with regard to the tetrahydrofuran mole fraction (x_2) variable of 42% considering all of the systems studied.

Correlation of LLE Data Using SERLAS

The separation factor (the ratio of distribution coefficients of tetrahydrofuran (2) to water (1) rearranged as $S = (x_2''/x_1'')/(x_2'/x_1')$, where x'' and x' designate solvent-rich and water-rich compositions, respectively) and the modified distribution ratio (i.e., the ratio of the two-phase composition quantities including the mole fraction of overall components in the mixture, $D_M = [(x_2'' + x_3'')/(1 - x_3'')]/[(x_2' + x_3')/(1 - x_3')]$), all defined as a property (Pr) in a logarithmic mean, can be fitted using a log-basis equation consisting of two composition-dependent parts (i.e., a part accounting for the properties at the composition limit of tetrahydrofuran $x_2 = 0$, Pr_0(log mean) and another one considering the influence of an overall interaction in the organic phase and its nonideality, covering the expansion terms with respect to the thermodynamic factor (Γ_L), the Hildebrand solubility parameter [$\delta_H/(J/cm^3)^{1/2}$], and the modified solvatochromic parameters π^*, α^*, and β^*.) D_M was selected instead of D to eliminate dealing with a zero log value for $D = 1$.

$$Pr = F_1 Pr_0 + F_2 \sum_k [C_{\Gamma,k}(\Gamma_L)^k + C_{H,k}(\delta^*_H)^k + C_{\pi,k}(\pi^*)^k + C_{\beta,k}(\beta^*)^k + C_{\alpha,k}(\alpha^*)^k] \quad (1)$$

Pr_0 represents the properties in the log mean attributed to the mutual solubility region (at $x_2 = 0$) defined as $S_0 = (x_{03}''/x_{01}'')/(x_{03}'/x_{01}')$ and $D_{M0} = (x_{03}''/1 - x_{03}'')/(x_{03}'/1 - x_{03}')$, where x_{03} and x_{01} denote the mole fractions of mutual solubility of solvent and water, respectively. Two composition-dependent correction factors F_1 and F_2 should be incorporated into Pr_0 and the expansion term to account for limiting conditions when either the physical interaction is zero for $x_2 = 0$ (i.e., the end points of binodal curve reflecting the mutual solubility of both water and solvent in the absence of solute for which $Pr = Pr_0$) or the plait point of the binodal curve at which the water-rich side composition is equal to the solvent-rich one, $x' = x''$, and extraction factors $S = 1$ and $D_M = 1$. Estimations were performed assuming the composition-dependent correction factors (F) to represent a solvent-basis composition ratio (F_1) and a water-free correction factor (F_2), respectively. x_3 and x_{03} designate the mole fractions of organic solvent relative to the ternary system and the solute-free mutual solubility region ($x_2 = 0$), respectively.

$$F_1 = \frac{\Delta x_3}{\Delta x_{3,\max}} = \frac{x_3'' - x_3'}{x_{03}'' - x_{03}'} \qquad F_2 = \frac{x_3''}{x_2'' + x_3''} - \frac{x_3'}{x_2' + x_3'} \quad (2)$$

Accordingly, for the plait point both F_1 and F_2 are equal to 0, and S and D_M are equal to 1. However, for the solute-free region ($x_2 = 0$), $F_1 = 1$, $F_2 = 0$, and the $Pr = Pr_0$ (i.e., $S = S_0$ and $D_M = D_{M0}$).

Table 2. Hildebrand Solubility Parameter (δ_H) and Solvatochromic Parameters of Compounds

compound	$\pi^{a,b}$	$\beta^{a,b}$	$\alpha^{a,b}$	$\delta_H^{c,d}$ MPa$^{0.5}$	$\delta'^{a,b}$
tetrahydrofuran	0.58	0.55	0.10	18.6	0.0
trichloroethylene	0.53	0.05	0.0	18.8	0.5
1-hexanol	0.40	0.45	0.33	21.9	0.0
3-methylbutyl ethanoate	0.49	0.45	0.0	16.0	0.0
water	1.09	0.47	1.17	47.9	0.0

[a] Kamlet et al.[10] [b] Markus[11] [c] Barton[19] [d] Riddick et al.[20]

The definition of thermodynamic factor $\Gamma_L^{i,j}$ for an n-component system is given by Taylor and Kooijman.[16] Mori et al.[17] extended the application of this approach to ASOG and UNIFAC-Dortmund group contribution methods. For a three-component system, Γ_L in terms of the transferring solute (tetrahydrofuran) composition (x_2) that refers to the organic phase is obtained from eq 3 as

$$\Gamma_L = 1 + x_2 \frac{\partial(\ln \gamma_2)}{\partial x_2}\Big|_\Sigma \quad (3)$$

where the symbol Σ (constrained condition) means that the differentiation with respect to the tetrahydrofuran composition x_2 is to be carried out while keeping all other mole fractions x_k ($k \neq j$, $k = 1...n - 1$) constant except the nth. The mole fraction of species n must be eliminated using the fact that the x_i sum to unity when the partial derivative of $\ln \gamma_i$ is evaluated. In this study, Γ_L values were estimated from UNIFAC-Dortmund model using the derivative approaches for the activity coefficient (γ_i) of Mori et al.[17] The variation of Γ_L and excess Gibbs free energy function (G^E) with composition pertaining to the organic phase species are shown in Table 1.

Modified solvatochromic terms are evaluated as

$$\delta^*_H = \delta_{H,2}\delta_{H,m}/1000 \qquad \pi^* = (\pi_2 - 0.35\delta_2)\pi_m \qquad \beta^* = \beta_2\beta_m \qquad \alpha^* = \alpha_2\alpha_m \quad (4)$$

Estimates were performed assuming the degree of expansion $k = 1$. Index 2 designates the properties of the distributed (extracted) solute component. Subscript m denotes the parameters related to the mixture in terms of x composition in the organic phase, assuming the additional parameter estimation rule:

$$\delta_{H,m} = \sum_i x_i \delta_{H,i} \qquad \pi_m = \sum_i x_i(\pi_i - 0.35\delta_i) \qquad \beta_m = \sum_i x_i \beta_i \qquad \alpha_m = \sum_i x_i \alpha_i \quad (5)$$

δ_H is the Hildebrand solubility parameter. π and δ are the solvatochromic parameters that measure the component dipolarity/polarizability (i.e., the dipole−dipole and dipole−induced dipole interactions of the component in the mixture, respectively). The hydrogen-bonding terms α and β measure the hydrogen-bond donating and hydrogen-bond accepting abilities of the component, respectively (Table 2). Therefore, the implications for the complementary effects of hydrogen bonding, solubility, and thermodynamic factors assuming a mean value estimation rule for the solvatochromic parameters have been taken into account. The coefficients C_i of eq 1 were obtained by the application of multivariable regression procedures of the linpack algorithm,[18] using the parameters from Table 2, and the thermodynamic factors according to eq 3 applied to the UNIFAC-Dortmund model by Mori et al. The resulting C coefficients corresponding to S and D_M properties as well as a comparison with the observed performance in terms

Table 3. Coefficients C_i of Equation 1 and Root-Mean-Square Deviation (σ) and Mean Relative Error ($\bar{e}$ %)[a] Evaluated for Different Properties Pr of the Ternary Systems Water + Tetrahydrofuran (THF) + Solvent

ternary system	C_Γ	C_H	C_π	C_β	C_α
$Pr = \ln(S)$; $Pr_0 = \ln(S_0)$; $\sigma(S)$; $\bar{e}$ % (S)					
trichloroethylene/ THF (σ = 21.63; % = 45.1)	1595.94	0.00666	−8056.72	3129.12	21 197.5
1-hexanol/THF (σ = 1.53; $\bar{e}$ % = 3.3)	24.32	−0.00001	60.45	−214.90	190.10
MBE/THF[b] (σ = 1.94; $\bar{e}$ % = 2.7)	−8.76	−0.00007	186.11	−223.94	38.05
$Pr = \ln(D_M)$; $Pr_0 = \ln(D_{M0})$; $\sigma(D_M)$; $\bar{e}$ % (D_M)					
trichloroethylene/ THF (σ = 55.93; $\bar{e}$ % = 34.2)	1994.22	0.00824	−10 029.5	3876.37	26 209.0
1-hexanol/THF (σ = 2.92; $\bar{e}$ % = 2.2)	−76.70	−0.00004	−111.73	256.89	1010.77
MBE/THF[b] (σ = 0.65; $\bar{e}$ % = 1.7)	13.48	−0.00014	171.92	−285.78	−12.30

[a] $\bar{e}\ \% = (100/N)\sum_{i=1}^{N} |(Y_{i,\mathrm{obsd}} - Y_{i,\mathrm{mod}})/Y_{i,\mathrm{obsd}}|$. [b] MBE, 3-methylbutyl ethanoate; THF, tetrahydrofuran.

of the mean relative error ($\bar{e}$ %) and root-mean-square deviation (σ) are presented in Table 3.

Model Reliability Analysis. Distribution data of tetrahydrofuran obtained for the ternary systems (water + tetrahydrofuran + polar solvent) have been used to establish the basis for the model reliability analysis. Figures 4 and 5 and Table 3 present a quantitative assessment of the predictions achieved for the proposed approach (SERLAS) in terms of S and D_M variables. Referring to Figures 4 and 5, it can be concluded that SERLAS matches the distribution data of tetrahydrofuran for the (water + tetrahydrofuran + polar solvent) system reasonably over the entire composition range, yielding the overall mean relative errors and root-mean-square deviations of $\bar{e}(S)$ = 17% and $\sigma(S)$ = 8.37 and $\bar{e}(D_M)$ = 13% and $\sigma(D_M)$ = 19.85 considering all of the systems studied. The reliability of eq 1 proved to be slightly less accurate for trichloroethylene in terms of the S variable, yielding $\bar{e}(S)$ = 45% ($\sigma(S)$ = 21.63). This would call for the assumption that a lower solvation efficiency of trichloroethylene, regarding its polarity and R-chain structure, should be responsible for a lower precision of the model predictions. The same remarks hold for the UNIFAC model reproducing the distribution behavior of tetrahydrofuran slightly less accurately with mean errors and deviations of $\bar{e}(S)$ = 64% ($\sigma(S)$ = 51.19) and $\bar{e}(D_M)$ = 63% ($\sigma(D_M)$ = 142.13) considering all of the ternary systems studied.

In fact, besides the accuracy of the model prediction, an important concern is whether the proposed equation (eq 1) actually tracks the trend in extraction equilibrium, sensitively depending on the hydrogen bonding, solubility, and thermodynamic factors of components as well as on the solvation effect of the polar solvent. However, it is essential that this phenomenon will have a significant impact on the implementation of a simulation algorithm incorporating the prediction by SERLAS. Consequently, the proposed approach, eq 1, appears to be an improvement in the data fit for the associated systems including components capable of dipole−dipole interaction and hydrogen-bond formation.

Conclusions

Liquid−liquid equilibrium data for the three ternary mixtures [water (1) + tetrahydrofuran (2) + trichloroethylene or + 1-hexanol or + 3-methylbutyl ethanoate (3)] were determined at T = 298.15 K. It is apparent from the distribution and selectivity data that the separation of tetrahydrofuran from water by extraction with a polar solvent is feasible. The isothermal equilibrium distribution of tetrahydrofuran onto a (water + polar solvent) two-phase system is better for 3-methylbutyl ethanoate and 1-hexanol than trichloroethylene. The difference among S and D_M factors varying with the initial solute concentration makes the studied solvents appropriate separation agents for tetrahydrofuran (Figures 4 and 5).

The way to formulate the distribution behaviors of tetrahydrofuran including the design variables characterizing physical interaction has been discussed. The solvatochronmic approach (SERLAS) is expected to be an improvement in data fit clarifying the simultaneous impact of hydrogen bonding, solubility, and thermodynamic factors of components on the extraction equilibria of (water + tetrahydrofuran + polar solvent) systems. Tie lines were also estimated using the UNIFAC-original model. From the two tested models, UNIFAC predicts the extraction equilibria of the ternary systems slightly less accurately, yielding a mean error and deviation of $\bar{e}$ = 63% and σ = 96.66, as compared to $\bar{e}$ = 15% and σ = 14.11 for the SERLAS model, eq 1, in terms of S and D_M factors, respectively.

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