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Liquid—Liquid Phase Equilibria of 1-Propanol + Water + *n*-Alcohol Ternary Systems at 298.15 K and Atmospheric Pressure

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ABSTRACT: Liquid—liquid equilibrium (LLE) data for the ternary systems 1-propanol + water + *n*-alcohols (1-pentanol, 1-hexanol, 1-octanol, 1-nonanol, 1-decanol, or 1-dodecanol) were determined at 298.15 K and atmospheric pressure. The *n*-alcohols from 1-pentanol up to 1-dodecanol can be used as extraction solvents for the separation of 1-propanol from aqueous solutions. The miscibility curves, the conode lines, and the plait points were obtained. The phase diagrams for all of these systems are of type I in according to Trayball classification. The Othmer—Tobias and Hand equations, used to verify the quality of the experimental data, give similar and generally good results for all of the systems. The experimental ternary LLE data were correlated with the universal quasichemical activity coefficient (UNIQUAC) model which represents satisfactorily the obtained experimental data. Distribution coefficients (D_i) and separation factors (S) were calculated from tie-line data to evaluate the extracting capability of the solvents, which increases with increasing alcohol chain length.

INTRODUCTION

The liquid—liquid investigations for a variety of systems are still topics of great interest. Phase equilibrium data are important and needed for simulation and the design of the efficient separation processes. Also, in scientific research, for the understanding of the properties of the multicomponent systems, liquid—liquid data (LLE) are required.

In recent years there has been an increasing interest to obtain and to study ternary systems containing water and organic compounds.[1−6] Some organic solvents have been reported in literature as extractants for 1-propanol from aqueous solution.[7]

1-Propanol is a liquid that is soluble in water and miscible with organic solvents. It has better dissolution properties than ethanol for fats and oils and dissolves polar resins. The mixture of 1-propanol and water forms a positive azeotrope, and the separation of 1-propanol from the aqueous solutions is economically infeasible by using the traditional distillation method. In this case, liquid—liquid extraction is a possible alternative method to separate such as azeotropic mixtures.

The purpose of this work is to present the liquid—liquid equilibria (LLE) data for 1-propanol + water + *n*-alcohols (1-pentanol, 1-hexanol, 1-octanol, 1-nonanol, 1-decanol, or 1-dodecanol) ternary systems to study the capability of *n*-alcohols for separating 1-propanol from aqueous solutions and to observe the effect of alkyl chain length on the efficiency of the separation process.

This study is a continuation of our works[8−11] on LLE in a ternary system with alcohols. We report in this paper the LLE data for 1-propanol + water + *n*-alcohol ternary systems: miscibility curves, tie-lines, and plait points. The LLE were studied by the cloud-point method and a modified Newsham and Ng procedure.[12,13] The consistency of the experimental tie-line data was tested using Othmer—Tobias[14] and Hand[15] equations. The LLE data were correlated with the universal quasichemical activity coefficient (UNIQUAC) solution model.[16] To determine the plait point compositions, for each ternary system, the Coolidge method[13] has been used.

After our knowledge, no data on these ternary systems have been found in literature, except for 1-pentanol.[17,18]

EXPERIMENTAL SECTION

All alcohols used in this work (mass fraction purity > 0.995) were purchased from Merck and were used without further purification. The purity of these materials was checked by gas chromatography and by refractive indices measurements. GC analysis did not detect any appreciable peaks of impurities. Bidistilled water was used throughout all of the experiments.

The refractive indices n_D of pure components were measured at 298.15 K and atmospheric pressure and compared to literature data. The refractive indices were measured using an Anton Paar (Abbemat RXA 170) refractometer. The refractive indices were measured with an accuracy of $\pm 2 \cdot 10^{-5}$, keeping the temperature constant with an accuracy of 0.03 °C. The measured refractive indices, together with literature data,[19−21] are shown in Table 1.

The equilibrium data were determined using two separate techniques: one for determination of the solubility curves and another to obtain the compositions of the conjugated points. The apparatus and the experimental procedures to obtain the miscibility curves and the tie-lines are presented in detail in previous articles.[10,11]

The solubility data for the ternary systems were determined by the cloud-point method. The data measurements were made in an installation containing an equilibrium cell equipped with isothermal fluid jacketed vessel to keep the temperature constant,

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Table 1. Refractive Index, n_D, at T/K = 298.15 and Molecular Weight, M, of the Pure Component Studied in This Work

component	n_D	
	exptl	lit.
water	1.33248	1.3324[a]
1-propanol	1.38305	1.3832[b]
1-pentanol	1.40703	1.4074[b]
1-hexanol	1.41580	1.4157[b]
1-octanol	1.42695	1.4267[b]
1-nonanol	1.43084	1.4309[b]
1-decanol	1.43436	1.4345[b]
1-dodecanol	1.44058	1.4409[c]

[a] From ref 19. [b] From ref 20. [c] From ref 21.

a thermostatically controlled bath which maintains the temperature of mixtures with an accuracy of ± 0.1 K, a magnetic stirrer, and a microburet. The inner temperature of the cell was measured by a precision thermometer with an accuracy of ± 0.1 K. The binary mixtures were prepared by weighing. An electronic balance accurate to ± 0.01 mg was used. The third component was progressively added by means of a microburet with an accuracy of ± 0.05 cm^3. The transition point between the heterogeneous and the homogeneous was determined visually. All visual experiments were repeated to acquire high reproducibility. The data for the solubility curves were therefore obtained by titrating until turbidity disappeared. The experimental uncertainty of the cloud-point method was estimated to be around ± 0.005 in mole fraction.

The experimental tie-line data were obtained by the cloud-point method using the same equilibrium cell as described above. LLE data were obtained by preparing mixtures (about 40 cm^3) of known overall composition within the heterogeneous gap for the three ternary studied systems. The period of time to ensure an intimate contact between the phases depends on n-alcohols. Each of these mixtures was filled into the equilibrium cell and intensely stirred (usually about (1 to 2) h) under isothermal conditions and set for at least (1.5 to 2) h at constant temperature until each layer appeared perfectly clear. At the end of the setting period, samples of 4 cm^3 were taken from both phases and analyzed.

The techniques for the determination of phase compositions at equilibrium are the cloud-point method and the procedure of Newsham and Ng,[12] completed with our own graphics program. The experimental uncertainty in mole fraction was estimated to be ± 0.01 in mole fraction for water-rich and alcoholic-rich phases.

RESULTS AND DISCUSSION

Experimental LLE Data. The paper presents experimental LLE data for six ternary n-alcohol systems at 298.15 K and atmospheric pressure. The miscibility curves, tie-lines, and plait points were obtained for (1-propanol + water + 1-pentanol), (1-propanol + water + 1-hexanol), (1-propanol + water + 1-octanol), (1-propanol + water + 1-nonanol), (1-propanol + water + 1-decanol), and (1-propanol + water + 1-dodecanol).

The experimental measurements for the binodal curves for the ternary systems (1-propanol + water + n-alcohol), w_i being the mass fraction of the ith component, are presented in Table 2. The

Table 2. Experimental (Liquid + Liquid) Equilibrium Mass Fractions w (Binodal Curve Data) for the System 1-Propanol (1) + Water (2) + n-Alcohol (3) at Temperature T/K = 298.15[a]

w_1	w_2	w_1	w_2	w_1	w_2
1-Propanol (1) + Water (2) + 1-Pentanol (3)					
0.000[b]	0.979[b]	0.288	0.636	0.419	0.341
0.011	0.976	0.296	0.621	0.419	0.322
0.023	0.958	0.319	0.584	0.419	0.300
0.165	0.813	0.338	0.552	0.412	0.277
0.180	0.794	0.371	0.497	0.404	0.265
0.197	0.772	0.390	0.458	0.394	0.252
0.207	0.758	0.403	0.427	0.377	0.239
0.217	0.743	0.411	0.402	0.363	0.221
0.225	0.732	0.416	0.381	0.341	0.213
0.234	0.719	0.419	0.363	0.184	0.143
0.250	0.695	0.427	0.344	0.127	0.120
0.265	0.673	0.431	0.329	0.000[b]	0.102[b]
0.273	0.657	0.419	0.357		
1-Propanol (1) + Water (2) + 1-Hexanol (3)					
0.000[b]	0.994[b]	0.325	0.610	0.443	0.238
0.127	0.867	0.337	0.592	0.443	0.220
0.181	0.808	0.348	0.575	0.404	0.193
0.201	0.783	0.373	0.538	0.396	0.180
0.220	0.759	0.393	0.506	0.372	0.170
0.230	0.745	0.422	0.456	0.350	0.157
0.242	0.729	0.443	0.418	0.319	0.143
0.256	0.711	0.467	0.337	0.277	0.127
0.264	0.699	0.466	0.324	0.221	0.107
0.271	0.688	0.468	0.307	0.089	0.088
0.283	0.673	0.468	0.289	0.052	0.084
0.298	0.650	0.463	0.270	0.000[b]	0.070[b]
0.313	0.628	0.451	0.250		
1-Propanol (1) + Water (2) + 1-Octanol (3)					
0.000[b]	0.999[b]	0.376	0.557	0.489	0.232
0.194	0.800	0.385	0.542	0.483	0.221
0.223	0.767	0.408	0.506	0.475	0.208
0.244	0.741	0.432	0.470	0.463	0.194
0.257	0.723	0.447	0.445	0.451	0.178
0.272	0.705	0.457	0.426	0.435	0.169
0.282	0.690	0.465	0.408	0.415	0.159
0.294	0.674	0.473	0.392	0.398	0.146
0.304	0.660	0.479	0.378	0.375	0.131
0.311	0.649	0.484	0.366	0.334	0.117
0.319	0.637	0.491	0.344	0.270	0.100
0.336	0.614	0.496	0.326	0.212	0.076
0.350	0.594	0.499	0.272	0.000[b]	0.047[b]
0.363	0.575	0.494	0.254		
1-Propanol (1) + Water (2) + 1-Nonanol (3)					
0.000[b]	0.999[b]	0.388	0.539	0.500	0.251
0.210	0.785	0.398	0.524	0.492	0.231
0.232	0.758	0.419	0.491	0.488	0.219
0.252	0.733	0.436	0.464	0.481	0.206
0.267	0.714	0.450	0.440	0.468	0.192
0.278	0.698	0.461	0.420	0.454	0.177

Table 2. Continued

w_1	w_2	w_1	w_2	w_1	w_2
0.290	0.682	0.470	0.402	0.442	0.167
0.300	0.668	0.476	0.388	0.428	0.155
0.310	0.655	0.483	0.374	0.412	0.142
0.319	0.642	0.487	0.362	0.389	0.128
0.326	0.631	0.494	0.341	0.351	0.114
0.335	0.619	0.497	0.329	0.255	0.072
0.340	0.610	0.498	0.317	0.143	0.043
0.356	0.589	0.503	0.302	0.000^b	0.040^b
0.367	0.572	0.502	0.287		
0.378	0.554	0.502	0.271		
1-Propanol (1) + Water (2) + 1-Decanol (3)					
0.000^b	0.999^b	0.453	0.439	0.500	0.246
0.222	0.772	0.463	0.419	0.497	0.236
0.250	0.740	0.473	0.400	0.492	0.225
0.267	0.717	0.484	0.381	0.489	0.212
0.282	0.698	0.486	0.370	0.477	0.200
0.294	0.682	0.491	0.357	0.465	0.185
0.307	0.665	0.496	0.345	0.459	0.175
0.324	0.640	0.498	0.336	0.447	0.165
0.339	0.617	0.501	0.326	0.436	0.153
0.353	0.597	0.503	0.318	0.422	0.139
0.368	0.575	0.504	0.310	0.399	0.126
0.383	0.555	0.505	0.303	0.336	0.091
0.400	0.526	0.504	0.290	0.278	0.069
0.422	0.492	0.506	0.273	0.000^b	0.030^b
0.439	0.463	0.503	0.256		
1-Propanol (1) + Water (2) + 1-Dodecanol (3)					
0.000^b	1.000^b	0.407	0.511	0.499	0.244
0.255	0.738	0.415	0.496	0.492	0.223
0.280	0.705	0.423	0.482	0.487	0.212
0.299	0.679	0.432	0.467	0.481	0.198
0.314	0.659	0.445	0.444	0.474	0.183
0.326	0.641	0.455	0.424	0.459	0.168
0.339	0.622	0.462	0.407	0.448	0.158
0.346	0.609	0.472	0.384	0.437	0.146
0.355	0.595	0.475	0.368	0.418	0.135
0.363	0.582	0.475	0.355	0.398	0.121
0.371	0.570	0.482	0.335	0.367	0.106
0.379	0.557	0.500	0.296	0.247	0.069
0.386	0.546	0.502	0.280	0.152	0.040
0.398	0.527	0.501	0.264	0.000^b	0.030^b

[a] Compositions determined with the cloud-point technique. [b] From ref 2.

mutual solubilities for water + *n*-alcohol were taken from literature.[2]

The experimental and calculated tie-line data of (1-propanol + water + *n*-alcohol) ternary systems at 298.15 K are presented in Table 5, in which x_i^{I} and x_i^{II} refer to mole fraction of the *i*th component in the water-rich phase and organic-rich phase, respectively. Comparisons with literature data for the ternary systems with 1-pentanol are also reported. As can be seen from Figure 1, our results for the ternary systems with 1-pentanol are in good agreement with those previously reported by Fernandez et al.[17] and Ghizellaoui et al.[18]

The LLE phase diagrams (the experimental miscibility curves and conodes line data) of ternary systems at 298.15 K are plotted and shown in Figure 1.

The LLE phase diagrams for (water + *n*-alcohol) mixtures show that two liquid pairs (1-propanol + water) and (1-propanol + *n*-alcohol) are completely miscible and one liquid pair is partially miscible. Consequently, all studied ternary systems exhibit type-1 of the LLE behavior, after Treyball.[22]

According to the above diagrams, the miscibility in the homologous series of water + *n*-alcohol binary and ternary systems decreases with the increase of alkyl chain in the *n*-alcohols.

One may note that the area of the two-phase region increases along the series passing from 1-pentanol to 1-decanol. The areas of the heterogeneous regions, *A*, relative to the area of the phase triangle as a function on the length of the alkyl chain, *n*, are presented in Figure 2.

Quality of Experimental Tie-Line Data. For each system, the thermodynamic consistency of the experimental tie-line data was obtained by applying Othmer−Tobias and Hand equations,[14,15] which are very sensitive to LLE data for aqueous−organic compound systems with very low solubility:

$$\ln\left(\frac{1-W_{33}}{W_{33}}\right) = a_1 + b_1 \ln\left(\frac{1-W_{22}}{W_{22}}\right) \qquad (1)$$

$$\ln\left(\frac{W_{13}}{W_{33}}\right) = a_2 + b_2 \ln\left(\frac{W_{12}}{W_{22}}\right) \qquad (2)$$

a_1 and b_1 and a_2 and b_2 are the coefficients of the Othmer−Tobias and Hand equations, respectively. W_{22} is the mass fraction of water in the water-rich phase, W_{33} the mass fraction of *n*-alcohol in the organic-rich phase, W_{13} the mass fraction of 1-propanol in the organic-rich phase, and W_{12} the mass fraction of 1-propanol in the water-rich phase.

The numerical values of (a, b) and the correlation factors (r^2) in both equations, determined by linear regression, are summarized in Table 3.

LLE Calculations. The experimental LLE data were correlated using the UNIQUAC model.[16] The UNIQUAC structural parameters *r* (the number of segments per molecule) and *q* (the relative surface area per molecule) were calculated from the Hansen's group contribution data.[23] For water, literature values were used.[24] The values of *r* and *q* used in the UNIQUAC equation are presented in Table 4.

The $a_{i,j}$ parameters in the UNIQUAC model were calculated by minimizing the residuals between experimental and calculated compositions. The objective function (OF) of the parameter determination is defined as:

$$\mathrm{OF} = \sum_k \sum_j \sum_i (x_{ijk}^{\mathrm{exp}} - x_{ijk}^{\mathrm{calc}})^2 \qquad (3)$$

where X_{ijk}^{exp} and X_{ijk}^{calc} are the experimental and calculated compositions of component *i* in phase *j* along a tie line *k*, respectively. The random search method defined by Luus and Jaakola was used for the minimization.[25,26]

The root-mean squared deviation (rmsd) was calculated from the difference between the experimental and the calculated mole

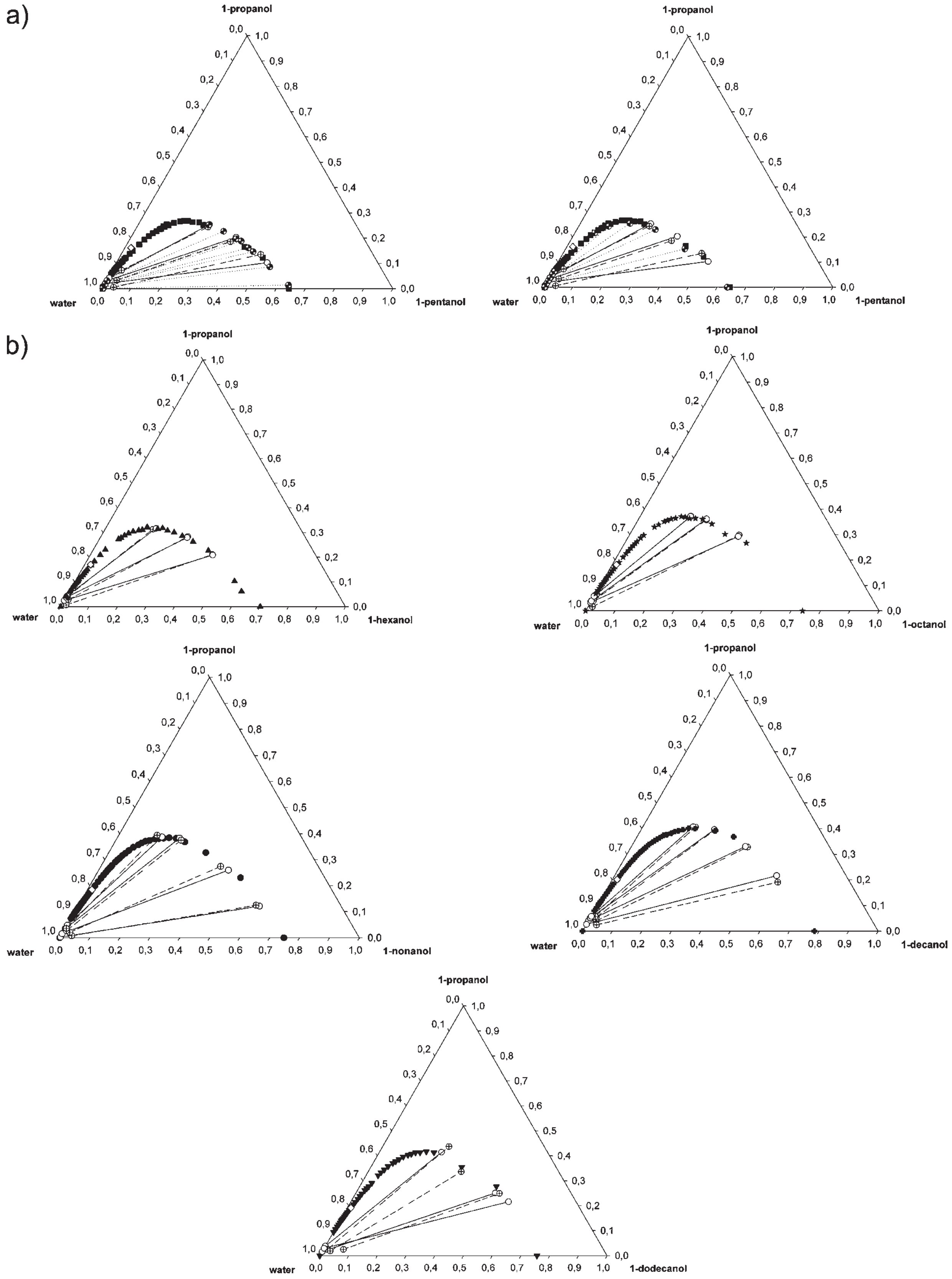

Figure 1. LLE data (molar fractions) for 1-propanol (1) + water (2) + *n*-alcohol (3) systems at 298.15 K. (a) ■, this work, 1-pentanol solubility data; ◇, this work, plait point compositions; ○ this work, experimental tie-line data; ⊕, this work, UNIQUAC tie-line data; black and white circle left side: experimental tie-line data from ref 17; black and white circle, right side: experimental tie-line data from ref 18. (b) ○, experimental tie-lines data; ◇, plait point compositions; ⊕, UNIQUAC tie-line data; solubility data: ■, 1-pentanol; ▲, 1-hexanol; ★, 1-octanol; ●, 1-nonanol; +, 1-decanol; ▼, 1-dodecanol.

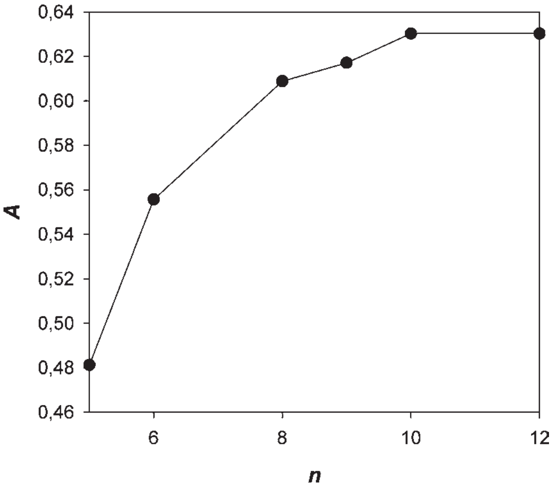

Figure 2. Heterogeneous region area, *A*, of the 1-propanol + water + *n*-alcohol systems as a function of length of the alkyl chain, *n*.

Table 3. Othmer−Tobias (a_1, b_1) and Hand Coefficients (a_2, b_2) and Correlation Factors (r^2) for the 1-Propanol (1) + Water (2) + *n*-Alcohol (3) Systems at the Temperature T/K = 298.15

a_1	b_1	r^2	a_2	b_2	r^2
1-Propanol (1) + Water (2) + 1-Pentanol (3)					
3.3459	1.8847	0.9937	3.6335	2.0764	0.9989
1-Propanol (1) + Water (2) + 1-Hexanol (3)					
3.9792	2.0526	0.8780	4.1042	2.2253	0.9001
1-Propanol (1) + Water (2) + 1-Octanol (3)					
3.0676	1.6936	0.8428	2.5796	1.5749	0.8088
1-Propanol (1) + Water (2) + 1-Nonanol (3)					
1.9885	0.9802	0.9767	1.6912	0.9656	0.9772
1-Propanol (1) + Water (2) + 1-Decanol (3)					
3.2824	2.0741	0.9772	3.2530	2.1708	0.9842
1-Propanol (1) + Water (2) + 1-Dodecanol (3)					
2.8228	1.5332	0.9970	2.4663	1.4688	0.9987

fractions according to the following equation:

$$\text{rmsd} = \left[\sum_{k=1}^{N}\left(\sum_{j=1}^{n_f}\sum_{i=1}^{n_c}\frac{(x_{ijk}^{\text{exp}} - x_{ijk}^{\text{calc}})^2}{n_c n_f N}\right)\right]^{1/2} \qquad (4)$$

where N is the number of tie-lines, $k = 1, 2, ..., N$, n_f is the number of the phases, and n_c is the number of the components.

The calculated tie-lines (dashed lines) together with the experimental data (solid line) are presented in Figure 1. For all of the investigated systems, as it is seen from Figure 1 and Table 5, good and satisfactory agreement between the calculated results from the UNIQUAC model and experimental values has been obtained. The UNIQUAC parameters, a_{ij}, obtained for the studied systems and the rmsd values are summarized in Table 6.

The UNIQUAC model was found to correlate satisfactorily the LLE data for the studied ternary systems. The parameters a_{ij} are relative to the binary system (component i + component j), and they are related to the pair interactions. In a ternary system if the coefficients for triplet interactions are omitted their contributions will be included in the pair interaction parameters. For this reason the values a_{12} and a_{21} obtained in the present work are not expected to be the same for the different ternary systems investigated. Differences in a_{12} and a_{21} parameters obtained in several runs are also due to the fact that they are regressed values and the objective function used is multimodal. Different values in a_{ij} parameter set can lead to good correlation results, a fact that also explains the differences between a_{ij} values reported in literature for the same mixtures. For practical applications the entire set of a_{ij} parameters is relevant as it can provide calculations in ternary mixtures separation problems.

Table 4. UNIQUAC Structural Parameters

component	r_i	q_i
water	0.920	1.400
1- propanol	3.2499	3.128
1-pentanol	4.5987	4.208
1-hexanol	5.2731	4.748
1-octanol	6.6219	5.828
1-nonanol	7.2963	6.368
1-decanol	7.9707	6.908
1-dodecanol	9.3195	7.988

The plait-point composition for 1-propanol + water + *n*-alcohol systems has been determined using Coolidge method,[13] and the obtained values are listed in Table 7. The plait-point positions are asymmetrical for all systems because the solubility of 1-propanol in the two phases is different.

The effectiveness of extraction of 1-propanol from aqueous solutions by superior *n*-alcohols is given by their separation factor (S), which was a measure of the solvent's ability to separate the 1-propanol from water. The separation factor is defined as the ratio of distribution coefficient of the 1-propanol (D_1) to the distribution coefficient of the water (D_2):$S = (D_1)/(D_2)$.

To indicate and compare the ability of the *n*-alcohol solvents to separate the 1-propanol from the aqueous phase, the distribution coefficient for 1-propanol and water, respectively, $D_1 = W_{13}/W_{12}$, $D_2 = W_{23}/W_{22}$, and the separation factor, S, were calculated. The W_{13} and W_{12} are the mass fractions of 1-propanol in the organic-rich phase and in the aqueous-rich phase, respectively; W_{23} and W_{22} are the mass fractions of water in the organic-rich phase and in the aqueous-rich phase.

The variation of the distribution coefficient, D_2, and separation factors, S, as a function of the mass fraction of the 1-propanol in aqueous phase, W_{12}, for the studied ternary systems are shown in Figures 3 and 4.

It is observed that the separation factor is greater than 1 for all the systems reported in this work, which means that the extraction of 1-propanol from water using these *n*-alcohols is possible. It is worth noting that increasing of the alcoholic chain increases the separation factor. Consequently, the superior alcohols are preferable solvents for the extraction of 1-propanol from water.

■ CONCLUSIONS

Liquid−liquid equilibria (LLE) data for 1-propanol + water + *n*-alcohol (1-pentanol, 1-hexanol, 1-octanol, 1-nonanol, 1-decanol, or 1-dodecanol) ternary systems were determined at

Table 5. Experimental and Calculated (Liquid + Liquid) Equilibrium Data for the System 1-Propanol (1) + Water (2) + *n*-Alcohol (3) for Mole Fractions *x* at the Temperature $T/\mathrm{K} = 298.15$[a]

water-rich phase		organic-rich phase	
x_1^{I}	x_2^{I}	x_1^{II}	x_2^{II}
1-Propanol (1) + Water (2) + 1-Pentanol (3)			
Experimental			
0.032	0.963	0.203	0.436
0.042	0.952	0.254	0.502
0.019	0.977	0.103	0.380
UNIQUAC			
0.033	0.931	0.186	0.464
0.073	0.894	0.244	0.512
0.005	0.955	0.135	0.385
1-Propanol (1) + Water (2) + 1-Hexanol (3)			
Experimental			
0.026	0.973	0.209	0.361
0.037	0.961	0.280	0.415
0.043	0.955	0.317	0.506
UNIQUAC			
0.007	0.976	0.211	0.361
0.028	0.958	0.284	0.411
0.041	0.954	0.314	0.518
1-Propanol (1) + Water (2) + 1-Octanol (3)			
Experimental			
0.033	0.033	0.033	0.033
0.039	0.039	0.039	0.039
0.057	0.057	0.057	0.057
UNIQUAC			
0.016	0.016	0.016	0.016
0.039	0.039	0.039	0.039
0.066	0.066	0.066	0.066
1-Propanol (1) + Water (2) + 1-Nonanol (3)			
Experimental			
0.004	0.996	0.122	0.272
0.016	0.984	0.260	0.307
0.036	0.964	0.383	0.408
0.049	0.950	0.387	0.465
UNIQUAC			
0.008	0.956	0.125	0.282
0.021	0.956	0.274	0.326
0.027	0.964	0.375	0.407
0.036	0.960	0.394	0.478
1-Propanol (1) + Water (2) + 1-Decanol (3)			
Experimental			
0.041	0.959	0.330	0.284
0.051	0.948	0.396	0.356
0.026	0.974	0.216	0.235
0.058	0.942	0.407	0.422
UNIQUAC			
0.039	0.935	0.328	0.278
0.054	0.927	0.394	0.356
0.024	0.941	0.191	0.244
0.057	0.929	0.406	0.415
1-Propanol (1) + Water (2) + 1-Dodecanol (3)			
Experimental			
0.016	0.984	0.251	0.264
0.038	0.962	0.415	0.369
0.030	0.970	0.216	0.235
UNIQUAC			
0.025	0.905	0.250	0.250
0.026	0.961	0.437	0.332
0.019	0.955	0.019	0.339

[a] Compositions determined with the cloud-point method and the procedure of Newsham and Ng.

Table 6. UNIQUAC Binary Interaction Parameters a_{ij} and a_{ji} (K) for the 1-Propanol (1) + Water (2) + *n*-Alcohol Systems at $T/\mathrm{K} = 298.15$

component		a_{ij}	a_{ji}	
i	*j*	K	K	rmsd
1-Propanol (1) + Water (2) + 1-Pentanol (3)				
1	2	556.996	−210.180	$2.689 \cdot 10^{-2}$
1	3	−292.849	38.540	
2	3	113.063	522.34	
1-Propanol (1) + Water (2) + 1-Hexanol (3)				
1	2	403.848	−36.204	$0.802 \cdot 10^{-2}$
1	3	−428.739	497.566	
2	3	−106.436	573.411	
1-Propanol (1) + Water (2) + 1-Octanol (3)				
1	2	466.581	−173.270	$0.725 \cdot 10^{-2}$
1	3	−30.234	−243.937	
2	3	−135.422	712.635	
1-Propanol (1) + Water (2) + 1-Nonanol (3)				
1	2	628.652	58.020	$1.427 \cdot 10^{-2}$
1	3	657.139	−332.287	
2	3	−141.851	763.352	
1-Propanol (1) + Water (2) + 1-Decanol (3)				
1	2	589.552	−8.741	$1.584 \cdot 10^{-2}$
1	3	192.183	−113.392	
2	3	−132.136	796.055	
1-Propanol (1) + Water (2) + 1-Dodecanol (3)				
1	2	326.021	6.031	$3.1280 \cdot 10^{-2}$
1	3	138.929	−234.674	
2	3	−119.421	936.184	

Table 7. Plait-Point Compositions, *P*, in Mass Fraction for the 1-Propanol (1) + Water (2) + *n*-Alcohol (3) Systems at the Temperature *T*/K = 298.15

ternary systems	*P*		
	W_1	W_2	W_3
1-propanol (1) + water (2) + 1-pentanol (3)	0.37	0.56	0.07
1-propanol (1) + water (2) + 1-hexanol (3)	0.38	0.54	0.08
1-propanol (1) + water (2) + 1-octanol (3)	0.40	0.53	0.07
1-propanol (1) + water (2) + 1-nonanol (3)	0.40	0.52	0.08
1-propanol (1) + water (2) + 1-decanol (3)	0.42	0.49	0.09
1-propanol (1) + water (2) + 1-dodecanol (3)	0.41	0.51	0.08

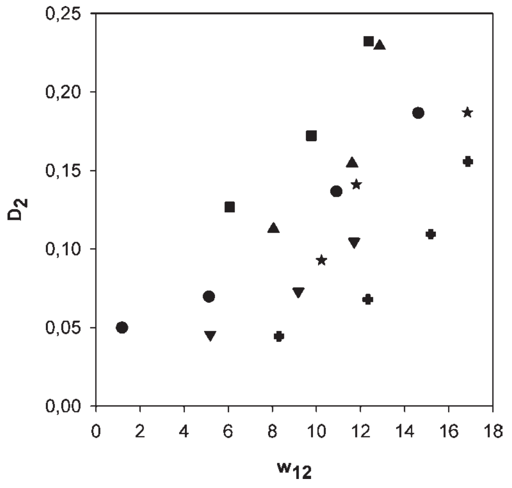

Figure 3. Distribution coefficient of water vs mass fraction percent of 1-propanol in the water-rich phase at 298.15 K: ■, 1-pentanol; ▲, 1-hexanol; ★, 1-octanol; ●, 1-nonanol; +, 1-decanol; ▼, dodecanol.

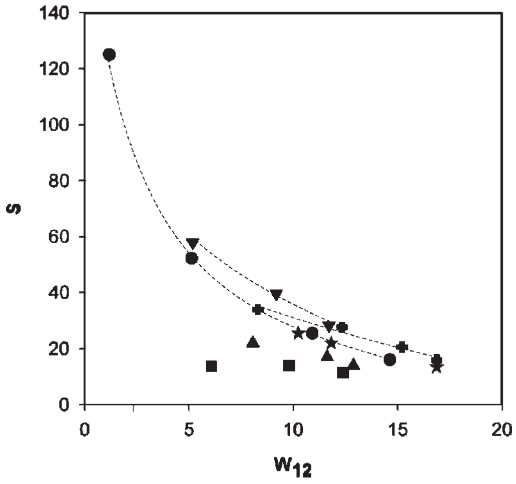

Figure 4. - Separation factor vs mass fraction percent of 1-propanol in the water-rich phase at 298.15 K: ■, 1-pentanol; ▲, 1-hexanol; ★, 1-octanol; ●, 1-nonanol; +, 1-decanol; ▼, dodecanol.

atmospheric pressure and 298.15 K. All of the investigated systems form a type-1 phase diagram of LLE. The two-phase region increases in the order 1-pentanol until 1-dodecanol, with a significant difference between 1-pentanol and 1-octanol.

The UNIQUAC model was found to correlate satisfactorily the LLE data for the studied ternary systems.

In all of the cases the plait-points, determined by Coolidge method, are located asymmetrically on the binodal curve because the solubility of 1-propanol in aqueous and alcoholic phase is very different; see Figure 1.

The separation capacity of *n*-alcohols for aqueous solutions of 1-propanol was assessed by determining the distribution coefficients and separation factors. All of the *n*-alcohols can serve as possible suitable solvents to extract 1-propanol from its aqueous solution; among these solvents 1-nonanol, 1-decanol, and 1-dodecanol are the most selective, having the highest distribution coefficients and separation factors.

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