Isobaric Vapor−Liquid Equilibria for Binary and Ternary Mixtures of Diisopropyl Ether, 2-Propyl Alcohol, and *n*-Butyl Propionate at 101.3 kPa

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Consistent vapor−liquid equilibrium data at 101.3 kPa have been determined for the ternary system diisopropyl ether (1) + 2-propyl alcohol (2) + *n*-butyl propionate (3) and two constituent binary systems: diisopropyl ether (1) + *n*-butyl propionate (3) and 2-propyl alcohol (2) + *n*-butyl propionate (3). The diisopropyl ether (1) + *n*-butyl propionate (3) system does not present deviation from ideal behavior, and the 2-propyl alcohol (2) + *n*-butyl propionate (3) system shows light positive deviation from Raoult's law. The activity coefficients of the solutions were correlated with their compositions by the Wilson, NRTL, and UNIQUAC models. Wisniak−Tamir equations were used to correlate the boiling points of the solutions with its composition. The binary VLE data measured in the present study passed the thermodynamic consistency test of Fredeslund et al. The ternary system is very well predicted from binary interaction parameters and passed both the Wisniak *L*−*W* and McDermott−Ellis consistency tests. The change of phase equilibria behavior due to solvent is insignificant; therefore, this solvent seems not to be an effective agent for the separation of the azeotropic mixture by extractive distillation.

Introduction

The most common method of manufacturing 2-propyl alcohol is by dehydration of propylene using sulfuric acid as the catalyst.[1] However, before the 2-propyl alcohol can be removed from the reaction mixture, some of it reacts with sulfuric acid to form diisopropyl ether. 2-Propyl alcohol and diisopropyl ether form a binary homogeneous azeotrope. Normally a mixture of several solvents is separated and recovered by fractionation in a rectification column, and the ease of separation depends upon the difference in boiling points of the components to be separated. However, the separation of a homogeneous azeotrope mixture, which is a common task in the chemical industry, cannot be carried out by conventional distillation. The separation can be improved by adding an agent that alters the relative volatility of the components (extractive distillation[2,3]) or making a simple change in pressure, provided that the azeotropic composition is sensitive to pressure (pressure swing distillation[4]).

It is evident that the selection of a suitable solvent is very important to ensure an effective and economical design of extractive distillation. The thermodynamic analysis prediction and computer simulation of phase equilibrium help to understand the separation process. However, when dealing with complex mixtures, experimental data are still needed for reliable design.

The study of the separation of the azeotropic system diisopropyl ether (1) and 2-propyl alcohol (2) by extractive distillation requires a previous selection of possible solvents. In general, qualitative indicators[5] show that the homologous series of ethers or alcohols look promising.

This work was undertaken as a part of the thermodynamic research on the separation of diisopropyl ether (1) and 2-propyl alcohol (2) using different solvents. The influence of the solvent is usually quantified in terms of the so-called selectivity, S_{ij}, which is defined as the ratio of the activity coefficients of the two key components, diisopropyl ether (1) and 2-propyl alcohol (2), in the presence of the solvent

$$S_{ij} = \frac{\gamma_i^{\mathrm{S}}}{\gamma_j^{\mathrm{S}}} \qquad (1)$$

As the activity coefficients depend on the phase composition and the solvent effect tends to increase as its concentration increases, it is a common practice to consider, at least in a preliminary solvent selection, the situation at infinite dilution. The selectivity at infinite dilution is defined as the ratio of the activity coefficients of both key components at infinite dilution in the solvent

$$S_{ij}^{\infty} = \frac{\gamma_i^{\mathrm{S}\infty}}{\gamma_j^{\mathrm{S}\infty}} \qquad (2)$$

where $\gamma_i^{\mathrm{S}\infty}$ and $\gamma_j^{\mathrm{S}\infty}$ are the activity coefficients at infinite dilution of components *i* and *j* in the respective binary systems with the solvent.

In previous works,[6,7] we chose 2-methoxyethanol and 3-methyl-1-butanol as entrainers for the extractive distillation to separate the azeotropic mixture. In the present paper, the behavior of *n*-butyl propionate (3) as a possible entrainer is investigated. The selectivity at infinite dilution of this solvent is 0.64 (predicted using the UNIFAC group-contribution method). Moreover the *n*-butyl propionate has a higher boiling point than the components of the binary mixture, and no additional azeotropes are present (estimated by UNIFAC).

We measured isobaric vapor−liquid equilibrium (VLE) data for the ternary system diisopropyl ether (1) + 2-propyl alcohol (2) + *n*-butyl propionate (3) and two constituent binary systems diisopropyl ether (1) + *n*-butyl propionate (3) and 2-propyl alcohol (2) + *n*-butyl propionate (3) at 101.3 kPa. In a previous

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Table 1. Density *d*, Refractive Index n_D, and Normal Boiling Point T_b of Pure Components

	d(298.15 K)/kg·m^{-3}		n_D(298.15 K)		T_b(101.3 kPa)/K	
component	exptl	lit.[a]	exptl	lit.[a]	exptl	lit.[b]
diisopropyl ether (1)	718.32	718.20	1.3652	1.3655	341.49	341.45
2-propyl alcohol (2)	782.69	781.26	1.3754	1.3752	355.35	355.41
n-butyl propionate (3)	870.88	871.40	1.3992	1.4000	418.69	419.75

[a] Ref 17. [b] Ref 18.

Table 2. Experimental Vapor−Liquid Equilibrium Data for the Binary System Diisopropyl Ether (1) + *n*-Butyl Propionate (3) at 101.3 kPa

T/K	x_1	y_1	γ_1	γ_3
418.69	0.000	0.000		1.000
410.65	0.041	0.252	0.999	0.981
402.95	0.082	0.424	0.994	0.993
395.60	0.130	0.568	0.992	0.987
388.73	0.181	0.672	0.995	0.996
383.55	0.227	0.738	0.989	1.005
378.16	0.279	0.797	0.996	1.009
373.79	0.324	0.840	1.013	0.992
368.97	0.383	0.878	1.018	0.992
365.89	0.433	0.900	1.006	0.987
362.25	0.484	0.918	1.015	1.026
357.99	0.561	0.941	1.015	1.038
354.63	0.633	0.958	1.011	1.003
351.70	0.699	0.969	1.012	1.026
349.23	0.762	0.978	1.009	1.026
347.16	0.818	0.984	1.008	1.069
345.18	0.872	0.990	1.013	1.031
343.88	0.913	0.994	1.012	1.047
342.69	0.952	0.996	1.010	1.241
341.49	1.000	1.000	1.000	

work,[6] we reported VLE data for the binary system diisopropyl ether (1) + 2-propyl alcohol (2) at (30 and 101.3) kPa.

VLE data of binary and ternary systems were found to be thermodynamically consistent. Data reduction was carried out using the Wilson,[8] NRTL,[9] and UNIQUAC[10] equations to relate activity coefficients with compositions, and the Wisniak−Tamir equation was used to correlate the boiling points of the solutions with its composition.

Experimental Section

Chemicals. Diisoproyl ether ($w = 99.0$ %, analytical grade) was purchased from Fluka, and 2-propyl alcohol ($w > 99.8$ %, analytical grade) and *n*-butyl propionate ($w > 99.0$ %, grade GC) were supplied from Aldrich Ltd. The reagents were used without further purification after chromatography failed to show any significant impurities. The water content, determined using a Karl Fischer volumetric automatic titrator (Metrohm, 701 KF Titrino), was small in all chemicals ($w < 0.05$ %). Appropriate precautions were taken when handling the reagents to avoid hydration. Before measurements, the liquids were degassed and subsequently dried over molecular sieves (Union Carbide, type 4 Å, 1/16 in. pellets). Moreover, once the experiment was over, the equipment was kept under an inert nitrogen atmosphere. The refractive indexes of the pure components were measured at 298.15 K using an Abbe refractometer Atago 3T, and the densities were measured at 298.15 K using an Anton Paar DMA 58 densimeter. Temperature was controlled to ± 0.01 K with a thermostatted bath. The uncertainties in refractive index and density measurements are ± 0.0002 and ± 0.01 kg·m^{-3}, respectively. The experimental values of these properties and the boiling points are given in Table 1 together with those given in the literature.

Table 3. Experimental Vapor−Liquid Equilibrium Data for the Binary System 2-Propyl Alcohol (2) + *n*-Butyl Propionate (3) at 101.3 kPa

T/K	x_2	y_2	γ_2	γ_3
418.69	0.000	0.000		1.000
411.37	0.027	0.229	1.365	0.976
402.72	0.066	0.430	1.336	0.972
394.81	0.110	0.572	1.346	0.981
388.02	0.161	0.671	1.331	0.998
383.70	0.202	0.726	1.318	1.012
378.51	0.265	0.788	1.294	1.018
374.35	0.326	0.828	1.274	1.046
370.96	0.389	0.861	1.249	1.056
368.10	0.454	0.886	1.220	1.079
366.24	0.506	0.900	1.190	1.123
364.20	0.574	0.916	1.150	1.184
362.59	0.637	0.931	1.119	1.216
361.23	0.696	0.941	1.089	1.310
360.07	0.750	0.951	1.067	1.385
359.04	0.801	0.959	1.048	1.518
358.10	0.849	0.968	1.035	1.621
357.24	0.894	0.977	1.026	1.719
356.48	0.935	0.984	1.018	2.012
355.79	0.972	0.992	1.014	2.402
355.35	1.000	1.000	1.000	

Apparatus and Procedure. The equilibrium vessel used in the measurements (Labodest VLE 602/D) was an all-glass dynamic-recirculating still equipped with a Cottrell circulation pump, manufactured by Fischer Labor and Verfahrenstechnik (Germany). The apparatus is capable of handling pressures from (0.25 to 130) kPa and temperatures up to 523.15 K. The Cottrell pump ensures that both liquid and vapor phases are in intimate contact during boiling and also in contact with the temperature sensing element. The equilibrium temperature was measured with a digital Hart Scientific thermometer model 1502A and a Pt100 probe Hart Scientific model 5622 calibrated at the ENAC-Spanish Instituto Nacional de Técnica Aeroespacial. The uncertainty is estimated to be ± 0.01 K. To guarantee the correct operation of the temperature probe, the boiling and the ice points of distillate water were measured. A Fisher M101 pressure control system was used to measure and control the pressure and the heating power. The measured pressure in the still was

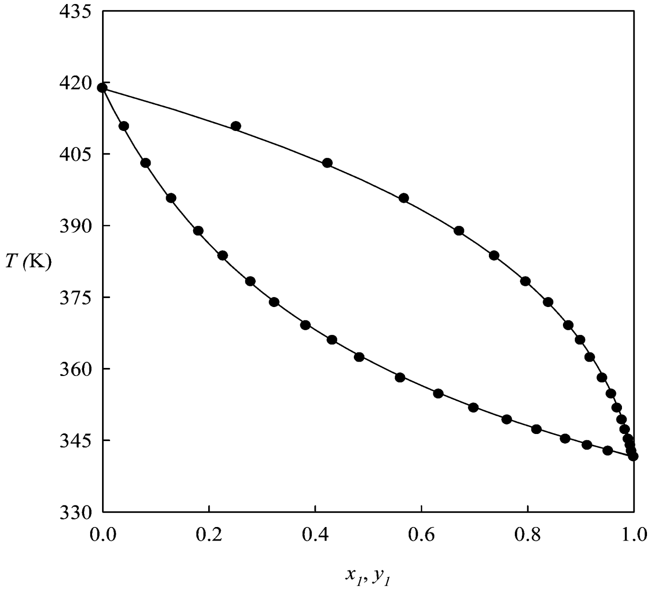

Figure 1. Experimental VLE data for the system diisopropyl ether (1) + *n*-butyl propionate (3) at 101.3 kPa: ●, experimental data. Smoothed data using the Wilson model with the parameters given in Table 5.

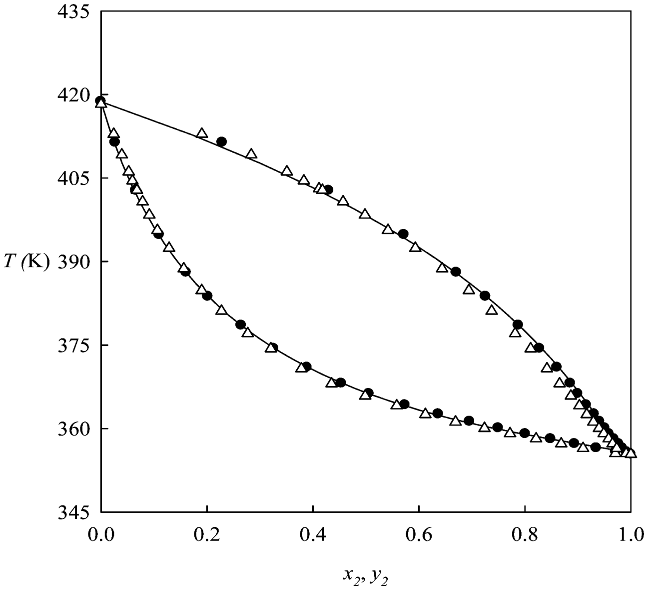

Figure 2. Experimental VLE data for the system 2-propyl alcohol (2) + *n*-butyl propionate (3) at 101.3 kPa: ●, experimental data; Δ, Gonzalez el al.[16] data. Smoothed data using the Wilson model with the parameters given in Table 5.

Table 4. Consistency Test for the Binary Systems Considered in VLE Measurement

system $i + j$	A_1[a]	A_2[a]	A_3[a]	AADy_i[b]	AADPy_i[c] kPa
diisopropyl ether (1) + *n*-butyl propionate (3)	0.0056	0.0708	0.0076	0.0026	0.46
2-propyl alcohol (2) + *n*-butyl propionate (3)	0.4930	0.2580	0.0194	0.0044	0.46

[a] Legendre polynomial parameters [b] Average absolute deviation in vapor phase composition. [c] Average absolute deviation in pressure.

(101.3 ± 0.1) kPa. The manometer was calibrated using the vapor pressure of ultrapure water.

In each experiment, the pressure was fixed, and the heating and stirring system of the liquid mixture was turned on. The still was operated at constant pressure until equilibrium was reached. Equilibrium conditions were assumed when constant temperature and pressure remained for 30 min or longer, and moreover, to verify the equilibrium conditions, we analyze the vapor until the variation of the mole fraction of the vapor phase composition is less than 0.001. Then, samples of liquid and condensate were taken for analysis. The sampling was carried out with special syringes that allowed withdrawal of small volume samples.

Analysis. The composition of the sampled liquid and condensed vapor phase was determined using a CE Instruments GC 8000 Top gas chromatograph (GC), after calibration with gravimetrically prepared standard solutions. A flame ionization detector was used together with a 30 m, 0.454 mm i.d., capillary column (DB-MTBE, J & Scientific). The GC response peaks were treated with Chrom-Card for Windows. Column, injector, and detector temperatures were (453, 473, and 498) K, respectively, for all systems. Very good peak separation was achieved under these conditions, and calibration analyses were carried out to convert the peak area ratio to the mass composition of the sample. At least two analyses were made of each liquid and vapor composition. The standard deviation in the mole fraction was usually less than 0.001.

Results and Discussion

Binary Systems. The temperature T and the liquid-phase x_i and vapor-phase y_i mole fractions at 101.3 kPa for the systems diisopropyl ether (1) + *n*-butyl propionate (3) and 2-propyl alcohol (2) + *n*-butyl propionate (3) are reported in Tables 2 and 3 and plotted in Figures 1 and 2. The activity coefficients γ_i for these systems were calculated from the following equation

$$\gamma_i = \frac{y_i P}{x_i P_i^\circ} \qquad (3)$$

where y_i is the mole fraction of component i in the vapor phase; x_i is the mole fraction of component i in the liquid phase; γ_i is the activity coefficient of the component i in the liquid phase; P is the total pressure; and P_i° is the saturation vapor pressure for the pure liquid i. The vapor phase is assumed to be an ideal gas, and the pressure dependence of the liquid phase fugacity is neglected.

The activity coefficients presented in Tables 2 and 3 indicate that the diisopropyl ether (1) + *n*-butyl propionate (3) system shows no deviation from ideal behavior and that the 2-propyl alcohol (2) + *n*-butyl propionate (3) system exhibits light positive deviation from Raoult's law and no additional azeotropes are present.

The test of Fredenslund[11] was applied to the binary experimental data to test thermodynamic consistency. In Table 4, the parameters of the Legendre polynomial together with the pertinent statistics required by the Fredenslund test are given. The residuals for both systems at 101.3 kPa show a reasonable random distribution.

Table 5. Parameters and Deviations Between Experimental and Calculated Values for Different G^E Models for the System Diisopropyl Ether (1) + 2-Propyl Alcohol (2) + *n*-Butyl Propionate (3)

		A_{ij}	A_{ji}		bubble point		
model	system $i + j$	J·mol^{-1}	J·mol^{-1}	α_{ij}	AADT[a]	AADy_1[b]	AADy_2[b]
Wilson[c]	1 + 2[d]	−476.15	4397.34		0.07	0.0064	
	1 + 3	−1000.07	1287.71		0.31	0.0016	
	2 + 3	783.98	2261.08		0.15		0.0028
	1 + 2 + 3[e]				0.31	0.0056	0.0076
NRTL	1 + 2[d]	2733.36	898.07	0.30	0.11	0.0066	
	1 + 3	2000.75	−1650.64	0.30	0.30	0.0016	
	2 + 3	5362.53	−2260.07	0.30	0.17		0.0029
	1 + 2 + 3[e]				0.35	0.0049	0.0077
UNIQUAC[f]	1 + 2[d]	2561.80	−877.48		0.11	0.0071	
	1 + 3	−88.92	94.51		0.31	0.0016	
	2 + 3	200.49	489.37		0.27		0.0014
	1 + 2 + 3[e]				0.50	0.0060	0.0067

[a] Average absolute deviation in temperature. [b] Average absolute deviation in vapor phase composition. [c] Molar liquid volumes of pure components from ref 19. [d] Ref 6. [e] Ternary prediction from binary parameters. [f] Volume and surface parameters from ref 19.

Table 6. Coefficients in Correlation of Boiling Points, Equations 5 and 6, Average Deviation, and Root Mean Square Deviation in Temperature

system $i + j$	C_0	C_1	C_2	C_3	AADT^a/K	rmsd^b/K
$1 + 2^c$	−31.45	10.04	−18.11	1.53	0.07	0.06
$1 + 3$	−74.51	39.57	−17.73	0.85	0.10	0.07
$2 + 3$	−81.54	59.04	−46.53	27.80	0.14	0.09

system $i + j + k$	A	B	C	D	AADT^a/K	rmsd^b/K
$1 + 2 + 3$	27.73	−48.74	24.08	3.57	0.20	0.04

[a] Average absolute deviation in temperature. [b] Root mean square deviation: $1/N\cdot(\Sigma(T_{\text{exptl}} - T_{\text{calc}})^2)^{0.5}$. [c] Ref 6.

The activity coefficients were correlated with the Wilson, NRTL, and UNIQUAC equations. The parameters of these equations were obtained by minimizing the following objective function (OF)

$$\mathrm{OF} = \sum_{i=1}^{N}\left(\left|\frac{T_{\mathrm{i}}^{\mathrm{exptl}} - T_i^{\mathrm{calc}}}{T_{\mathrm{i}}^{\mathrm{exptl}}}\right| + |y_i^{\mathrm{exptl}} - y_i^{\mathrm{calc}}|\right) \qquad (4)$$

and are reported in Table 5, together with the pertinent statistics of each VLE correlation.

The boiling point temperatures of each binary system at 101.3 kPa were well correlated with mole fractions by the equation proposed by Wisniak and Tamir[12]

$$T = x_iT_i^0 + x_jT_j^0 + x_ix_j\sum_{k=0}^{m} C_k(x_i - x_j)^k \qquad (5)$$

In this equation, T_i^0 is the boiling point of the pure components i and m is the number of terms used in the series expansion of $(x_i - x_j)$. The various constants of eq 5 are reported in Table 6, with information indicating the goodness of the correlation fit.

Ternary System. VLE data for the ternary system diisopropyl ether (1) + 2-propyl alcohol (2) + *n*-butyl propionate (3) are reported in Table 7. Figure 3 shows the plot of the vapor-phase mole fraction calculated with the Wilson model with the parameters given in Table 5 against the experimental vapor phase composition. The ternary data were found to be thermodynamically consistent by the Wisniak and Tamir[13] modification of the McDermott−Ellis[14] test ($D < D_{\max}$ at all data points) and the Wisniak $L-W$ test[15] ($0.92 < L_i/W_i < 1.10$).

VLE data for the ternary system have been predicted using the Wilson, NRTL, and UNIQUAC equations with the binary interaction parameters obtained from the regression of binary data. Table 5 lists the mean absolute deviations between experimental and calculated temperature and vapor-phase mole fractions. From these results, it can be concluded that the binary contributions allow a good prediction of the ternary system, representing the data successfully. Thus, the models can be used to calculate boiling points from liquid-phase compositions at the system pressure.

The boiling points of the ternary system were correlated by the equation proposed by Wisniak and Tamir.[13]

$$T = \sum_{i=1}^{3} x_iT_i^0 + \sum_{j>i=1}^{3}\left[x_ix_j\sum_{k=0}^{m} C_k(x_i - x_j)^k\right] + x_1x_2x_3[A + B(x_1 - x_2) + C(x_1 - x_3) + D(x_2 - x_3)] \qquad (6)$$

Table 7. Experimental Vapor−Liquid Equilibrium Data for Diisopropyl Ether (1) + 2-Propyl Alcohol (2) + *n*-Butyl Propionate (3) at 101.3 kPa

T/K	x_1	x_2	y_1	y_2	γ_1	γ_2	γ_3
340.70	0.688	0.269	0.750	0.248	1.122	1.706	1.029
341.71	0.895	0.056	0.914	0.083	1.017	2.635	1.111
341.73	0.465	0.510	0.639	0.359	1.370	1.248	1.096
342.56	0.590	0.318	0.706	0.287	1.160	1.548	1.047
342.78	0.793	0.106	0.850	0.143	1.032	2.291	1.079
344.56	0.367	0.549	0.578	0.415	1.435	1.188	1.102
344.83	0.266	0.703	0.512	0.485	1.738	1.073	1.244
345.51	0.481	0.350	0.651	0.336	1.195	1.448	1.047
346.24	0.702	0.100	0.839	0.144	1.032	2.118	1.062
346.41	0.586	0.198	0.741	0.242	1.084	1.771	1.019
347.13	0.374	0.441	0.577	0.408	1.296	1.303	1.002
348.35	0.274	0.559	0.493	0.491	1.452	1.178	1.059
348.96	0.162	0.754	0.383	0.608	1.878	1.053	1.302
349.48	0.474	0.234	0.676	0.298	1.114	1.628	0.973
350.30	0.376	0.326	0.590	0.383	1.193	1.455	0.968
351.50	0.272	0.440	0.481	0.492	1.295	1.316	0.971
351.78	0.173	0.623	0.370	0.607	1.558	1.136	1.115
352.32	0.076	0.844	0.222	0.765	2.080	1.034	1.499
354.00	0.033	0.919	0.111	0.880	2.271	1.020	1.727
354.28	0.374	0.216	0.628	0.328	1.133	1.605	0.945
354.58	0.180	0.501	0.369	0.596	1.372	1.237	0.987
354.73	0.277	0.326	0.506	0.453	1.218	1.437	0.911
354.77	0.478	0.109	0.762	0.192	1.059	1.817	0.991
354.87	0.073	0.751	0.193	0.782	1.762	1.072	1.259
355.06	0.566	0.041	0.879	0.077	1.023	1.948	0.968
357.60	0.071	0.638	0.176	0.784	1.526	1.138	1.059
357.70	0.183	0.390	0.383	0.569	1.277	1.343	0.888
358.34	0.036	0.718	0.100	0.864	1.672	1.082	1.105
359.85	0.276	0.208	0.549	0.385	1.140	1.568	0.915
360.69	0.070	0.517	0.171	0.774	1.363	1.230	0.916
362.07	0.180	0.284	0.398	0.531	1.191	1.458	0.873
363.59	0.037	0.506	0.095	0.839	1.316	1.224	0.882
364.27	0.367	0.061	0.768	0.143	1.058	1.690	0.937
364.52	0.070	0.400	0.170	0.752	1.218	1.338	0.872
367.38	0.270	0.102	0.639	0.254	1.096	1.596	0.905
368.80	0.073	0.303	0.189	0.705	1.160	1.419	0.855
371.51	0.040	0.309	0.107	0.777	1.118	1.392	0.808
372.99	0.173	0.132	0.452	0.380	1.042	1.514	1.044
381.69	0.173	0.050	0.577	0.192	1.061	1.507	0.942
385.18	0.073	0.110	0.263	0.462	1.052	1.462	0.942
395.78	0.038	0.068	0.178	0.397	1.075	1.471	0.937

where T_i^0 is the boiling point of the pure components i; m is the number of terms considered in the series expansion of $(x_i - x_j)$; and C_k is the binary constant; whereas A, B, C, and D are ternary constants. The constants of eq 6 are reported in Table 6, with information indicating the quality of the correlation.

Solvent Effects. To carry out the separation of the azeotropic mixture of diisopropyl ether (1) + 2-propyl alcohol (2) by extractive distillation, we study the influence on the phase

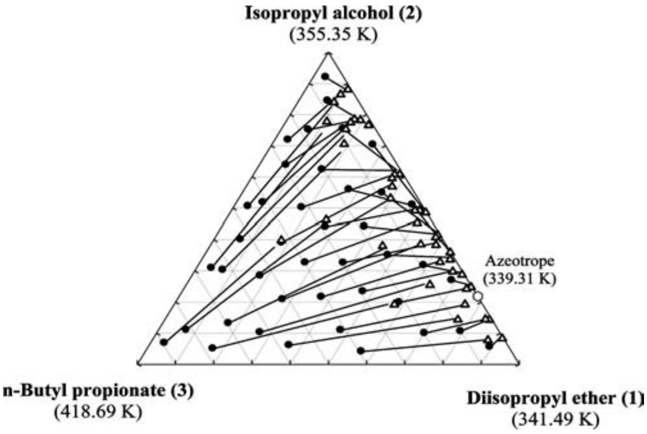

Figure 3. Diagram of VLE for the ternary system diisopropyl ether (1) + 2-propyl alcohol (2) + *n*-butyl propionate (3) at 101.3 kPa: ●, liquid-phase mole fraction; Δ, vapor-phase mole fraction; ○, azeotrope.[6] Smoothed lines calculated with the Wilson equation with the parameters given in Table 5.

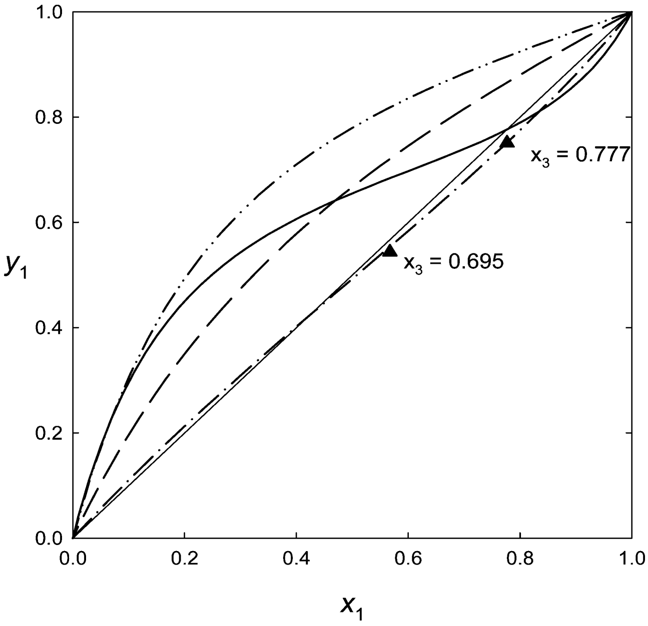

Figure 4. VLE data plotted on a solvent-free basis for the system diisopropyl ether (1) + 2-propyl alcohol (2) + solvent (3) at 101.3 kPa. Continuous line[6] for $x_3 = 0.00$; dashed line calculated using the Wilson equation with the parameters given in Table 5 for $x_3 = 0.7$; -••-, with 2-methoxyethanol;[6] - -, with 3-methyl-1-butanol;[7] and — • —, with *n*-butyl propionate (in this work). Experimental points for $x_3 \approx 0.70$: ▲, with *n*-butyl propionate.

equilibrium behavior of the azeotropic mixture of the three different solvents: 2-methoxyethanol, 3-methyl-1-butanol (studied in previous papers[6,7]), and *n*-butyl propionate (in this work). In Figure 4, the VLE of the ternary mixtures, on a solvent-free basis, was plotted. As can be seen in this figure, two solvents eliminate the diisopropyl ether-2-propyl alcohol azeotrope, allowing the separation of pure diisopropyl ether from 2-propyl alcohol by rectification when they are employed as solvents in extractive distillation. The 2-methoxyethanol and 3-methyl-1-butanol enhance the relative volatility of diisopropyl ether to 2-propyl alcohol, but 2-methoxyethanol brings about a larger enhancement of the relative volatility ($\alpha_{12}^S = 3.48$ with 2-methoxyethanol and $\alpha_{12}^S = 2.00$ with 3-methyl-1-butanol; α_{ij}^S is relative volatility in the presence of the solvent). However, the *n*-butyl propionate reverses the volatility of the original mixture, although it does not reach to break the azeotrope.

Conclusions

Consistent VLE data at 101.3 kPa have been determined for the binary systems diisopropyl ether (1) + *n*-butyl propionate (3) and 2-propyl alcohol (2) + *n*-butyl propionate (3) and the ternary system diisopropyl ether (1) + 2-propyl alcohol (2) + *n*-butyl propionate (3). The Wilson, NRTL, and UNIQUAC models were capable of correlating all the binary systems and yielded reasonable predictions for the ternary system.

The experimental results revealed that the presence of *n*-butyl propionate does not enhance the relative volatility of diisopropyl ether (1) to 2-propyl alcohol (2); the relative volatility on a solvent-free basis ($\alpha_{12}^S = 0.97$) confirms that *n*-butyl propionate (3) does not break the azeotropic mixture and therefore is not a good entrainer.

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