

# Liquid–Liquid Equilibria of Water + 2,3-Butanediol + Butyl Acetate at $T = 298.15$ K, $T = 308.15$ K, and $T = 318.15$ K

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Liquid–liquid equilibrium (LLE) data of the solubility curves and tie-line compositions have been determined for mixtures of (water + 2,3-butanediol + butyl acetate) at (298.15, 308.15, and 318.15) K and atmospheric pressure. Distribution coefficients and separation factors have been evaluated for the immiscibility region. The Othmer–Tobias correlation provides the coefficients of the log–log plot that is not a sensitive criterion. The LLE data of the ternary systems have been predicted by UNIFAC methods.

## Introduction

The production of 2,3-butanediol by fermentation has been considered as a potential source of fuels<sup>1,2</sup> or chemical feedstock.<sup>3</sup> Its microbial preparation has been observed in several yeasts and bacteria from various genera such as *Klebsiella*, *Bacillus*, *Serratia*, and *Pseudomonas*.<sup>4–10</sup> The separation and purification of 2,3-butanediol from fermentation broth is essential to realize the industrial production for 2,3-butanediol.

Since the fermented liquors contain only a few percent of 2,3-butanediol along with various other materials which cause difficulty in separation and since 2,3-butanediol has a much higher boiling point than that of water and may not be distilled out directly, extraction from the fermentation liquors by a suitable solvent seems to be a feasible method. Various organic solvents have been investigated and reported for 2,3-butanediol extraction.<sup>11</sup> Butyl acetate used in this study may be a suitable solvent for extraction of 2,3-butanediol from water, being capable of forming azeotropic mixtures with water to take it from 2,3-butanediol.

The aim of this work is to present the phase behavior of LLE for the (water + 2,3-butanediol + butyl acetate) ternary system at (298.15, 308.15, and 318.15) K and atmospheric pressure. The tie lines have also been predicted using the UNIFAC method (a group contribution method) developed by Fredenslund et al.<sup>12</sup> and compared with the experimental data.

## Experimental

**Chemicals.** All the chemicals used in this study were purchased from commercial sources. 2,3-Butanediol was supplied by Sino-pharm Chemical Reagent Co., Ltd., with a minimum mass fraction purity of 99.2 %. Butyl acetate was provided by Shanghai Lingfeng Chemical Reagent Co., Ltd., and had a minimum mass fraction purity of 99.5 %. They were used directly without further treatment in this study. Water was distilled twice before utilization. The purity of these materials was checked and assured by gas chromatography. The normal boiling point and refractive index values were measured in this study and reported in Table 1 in comparison with the literature data to demonstrate the purity of the compounds. The boiling

**Table 1. Refractive Indexes ( $n_D$ ) at  $T = 293.15$  K and Boiling Points ( $T_b$ ) at 101.3 kPa, of the Compounds**

component	$n_D$		$T_b$ /K	
	exptl	lit. <sup>a</sup>	exptl	lit. <sup>a</sup>
2,3-butanediol <sup>b</sup>	1.4375	1.4366	454.21	454.20
butyl acetate	1.3941	1.3942	399.11	399.15
water	1.3325	1.3325	373.30	373.26

<sup>a</sup> Taken from ref 13. <sup>b</sup> Taken from ref 14.

points were determined by an Ebuillometer (DZBW model, made in Nanjing, China), with an accuracy of  $\pm 0.01$  K.

**Equilibrium Measurements.** Three different temperatures [(298.15, 308.15, and 318.15) K] at atmospheric pressure were selected to study the ternary equilibrium system to observe the evaluation of the binodal curves and tie-lines.

The binodal (solubility) curves were determined by the cloud point method in an equilibrium glass cell with a water jacket to maintain isothermal conditions. The temperature in the cell was kept constant by circulating water from a water bath (SUPER-CONSTANTTEP BATH, Shanghai precision science instrument Co., Ltd.), which is equipped with a temperature controller capable of maintaining the temperature within  $\pm 0.1$  K. The major central part of the solubility curves was obtained by titrating heterogeneous mixtures of water + butyl acetate with 2,3-butanediol until the turbidity had disappeared. For the water-side and solvent-side regions in which the curve and the sides of the triangle are close and exhibit similar slopes, binary mixtures of either (water + 2,3-butanediol) or (butyl acetate + 2,3-butanediol) were titrated against the third component until the transition from homogeneity to heterogeneity was observed.

All mixtures were prepared by weighing with a Sartorius scale accurate to within  $\pm 10^{-4}$  g. Mutual solubility values of the (water + butyl acetate) binary were measured using the method based on the detection of the cloud point.<sup>15–17</sup> The transition point between the homogeneous and heterogeneous zones was determined visually. The reliability of the method depends on the precision of the microburette with an accuracy of  $\pm 0.01$  cm<sup>3</sup> and is limited by the visual inspection of the transition across the apparatus. The accuracy of the visual inspection of the transition is achieved by waiting approximately 5 min in the transition point and observing the heterogeneity. All visual experiments were repeated at least three times to acquire high accuracy.

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**Table 2. Experimental Binodal Curve Data (Mass Fraction  $W_i$ ) of {Water (1) + 2,3-Butanediol (2) + Butyl Acetate (3)} at Different Temperatures**

$T/K$	$W_1$	$W_2$	$W_3$	$W_1$	$W_2$	$W_3$	$W_1$	$W_2$	$W_3$
298.15	0.0108	0.0000	0.9892	0.1605	0.3980	0.4415	0.3392	0.5297	0.1311
	0.0182	0.0370	0.9448	0.1763	0.4236	0.4000	0.3575	0.5277	0.1149
	0.0271	0.0753	0.8977	0.1966	0.4537	0.3497	0.4360	0.4975	0.0665
	0.0401	0.1198	0.8401	0.2102	0.4696	0.3202	0.5000	0.4595	0.0405
	0.0598	0.1752	0.7650	0.2236	0.4842	0.2922	0.5299	0.4407	0.0295
	0.0900	0.2500	0.6600	0.2392	0.4983	0.2626	0.5834	0.3954	0.0212
	0.1272	0.3437	0.5290	0.2487	0.5054	0.2459	0.6750	0.3117	0.0133
	0.1334	0.3519	0.5147	0.2764	0.5191	0.2045	0.7321	0.2570	0.0109
	0.1490	0.3784	0.4727	0.3037	0.5279	0.1684	0.9876	0.0000	0.0124
	308.15	0.0243	0.0000	0.9757	0.2041	0.4150	0.3809	0.4942	0.4577
0.0333		0.0591	0.9076	0.2144	0.4280	0.3577	0.5186	0.4391	0.0423
0.0419		0.0856	0.8726	0.2234	0.4378	0.3389	0.5521	0.4141	0.0338
0.0501		0.1098	0.8401	0.2352	0.4511	0.3138	0.6246	0.3557	0.0197
0.0686		0.1664	0.7650	0.2514	0.4675	0.2811	0.6696	0.3125	0.0180
0.1050		0.2350	0.6600	0.2659	0.4792	0.2549	0.7034	0.2812	0.0155
0.1330		0.2980	0.5640	0.3037	0.4879	0.1684	0.7536	0.2332	0.0133
0.1717		0.3679	0.4604	0.3392	0.4997	0.1311	0.7934	0.1944	0.0122
0.1817		0.3832	0.4352	0.4150	0.4940	0.0915	0.8583	0.1317	0.0101
0.1952		0.4039	0.4009	0.4760	0.4645	0.0595	0.9919	0.0000	0.0081
318.15	0.0243	0.0000	0.9757	0.2390	0.4230	0.3480	0.6105	0.3670	0.0325
	0.0386	0.0652	0.8980	0.2859	0.4592	0.2549	0.6260	0.3457	0.0283
	0.0588	0.1180	0.8230	0.3037	0.4609	0.1954	0.7260	0.2550	0.0160
	0.0786	0.1564	0.7650	0.3610	0.4980	0.1515	0.7755	0.2107	0.0138
	0.1070	0.2040	0.6900	0.4010	0.4930	0.1165	0.8230	0.1660	0.0107
	0.1190	0.2160	0.6650	0.4630	0.4660	0.0706	0.9128	0.0782	0.0090
	0.1480	0.2830	0.5640	0.5090	0.4370	0.0530	0.9450	0.0476	0.0082
	0.1845	0.3490	0.4690	0.5630	0.3970	0.0385	0.9930	0.0000	0.0069

End-point determinations of the tie-lines were based upon the independent analysis of the conjugate phases that were regarded as being in equilibrium. For this purpose, mixtures of known masses of water, 2,3-butanediol, and butyl acetate lying within the heterogeneous zone were introduced into the equilibrium cell and were agitated for 3 h with a magnetic stirrer vigorously and then left for 4 h to settle down into raffinate (aqueous) and extract (solvent) layers. The compositions of liquid samples withdrawn from conjugate phases were analyzed by a gas chromatograph (GC112A) with a thermal conductivity detector (TCD), after calibration with gravimetrically prepared standard solutions. A GDX-102 packed column (3 m  $\times$   $\Phi$ 3 mm  $\times$  0.5 mm) was used to separate components. They were all produced by Shanghai Hengping Scientific Instrument Co., Ltd. The oven, injector, and detector temperatures were (453.15, 473.15, and 493.15) K, respectively. High-purity hydrogen (99.9999 % purity) was used as the carrier gas at a constant flow rate of 30 mL  $\cdot$  min $^{-1}$ . The detector was connected to a FJ-2003B integrator. Each sample was analyzed at least thrice to ensure accuracy. The uncertainty in mass fractions was within  $\pm$  0.0001.

## Results and Discussion

The LLE measurements were made for the ternary system of (water + 2,3-butanediol + butyl acetate) at (298.15, 308.15, and 318.15) K and atmospheric pressure. The experimental binodal curves for this ternary system at each temperature are listed in Table 2, for which  $W_i$  refers to the mass fraction of  $i$ th component. The experimental tie-line compositions of the equilibrium phases are shown in Table 3, for which  $W_{i1}$  and  $W_{i3}$  refer to the mass fractions of the  $i$ th component in the aqueous and solvent phases, respectively.

The experimental and predicted equilibrium data through the UNIFAC model of the ternary system at  $T = 298.15$  K are plotted in Figure 1. As can be seen from Figure 1, the system exhibited type 1 phase behavior,<sup>18,19</sup> having only one liquid pair of partially miscible (butyl acetate + water) and two pairs of completely miscible (water + 2,3-butanediol) and (2,3-butane-

**Table 3. Experimental Tie-Line Data in Mass Fractions for the Water (1) + 2,3-Butanediol (2) + Butyl Acetate (3) Ternary System**

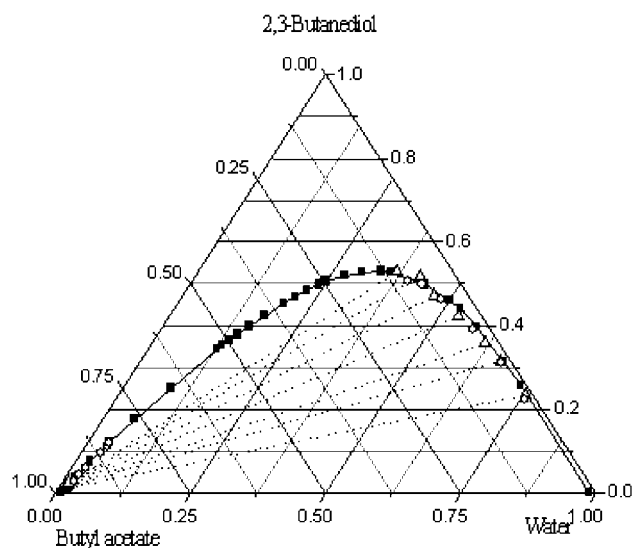
$T/K$	organic phase			aqueous phase		
	$W_{13}$	$W_{23}$	$W_{33}$	$W_{11}$	$W_{21}$	$W_{31}$
298.15	0.7574	0.2224	0.0201	0.0216	0.0270	0.9514
	0.6689	0.3110	0.0201	0.0231	0.0440	0.9330
	0.4291	0.4996	0.0713	0.0408	0.1121	0.8471
	0.4839	0.4622	0.0539	0.0396	0.0931	0.8674
	0.5799	0.3891	0.0309	0.0264	0.0604	0.9132
308.15	0.4001	0.5057	0.0942	0.0405	0.1186	0.8409
	0.4144	0.5034	0.0822	0.0520	0.1137	0.8344
	0.4794	0.4607	0.0599	0.0479	0.0960	0.8561
	0.5714	0.3930	0.0356	0.0383	0.0634	0.8983
	0.3901	0.4991	0.1108	0.0559	0.1319	0.8122
318.15	0.6703	0.3112	0.0184	0.0299	0.0419	0.9282
	0.7333	0.2432	0.0235	0.0300	0.0314	0.9387
	0.6230	0.3452	0.0319	0.0373	0.0518	0.9109
	0.6628	0.3137	0.0235	0.0309	0.0348	0.9343
	0.7173	0.2588	0.0239	0.0268	0.0273	0.9459
	0.6128	0.3506	0.0366	0.0340	0.0417	0.9242
	0.4069	0.4977	0.0954	0.0672	0.1264	0.8064
	0.4711	0.4574	0.0715	0.0568	0.1082	0.8350
	0.5560	0.3986	0.0453	0.0438	0.0675	0.8886
	0.3809	0.4895	0.1296	0.0736	0.1509	0.7755

diol + butyl acetate). Also, similar results are observed at  $T = 308.15$  K and  $T = 318.15$  K in Figures 2 and 3.

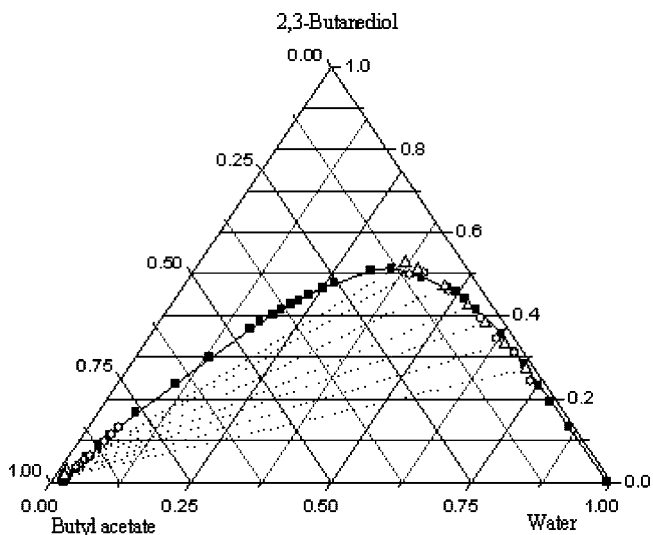
The effectiveness of 2,3-butanediol extraction by butyl acetate is given by its separation factor, which is a measure of the ability of butyl acetate to separate the 2,3-butanediol from water. To show the selectivity and extraction strength of the solvent to extract 2,3-butanediol, the distribution coefficients,  $D_i$ , for water ( $i = 1$ ) and 2,3-butanediol ( $i = 2$ ) and the separation factors,  $S$ , are calculated according to the following equations

$$D_i = \frac{W_{i3}}{W_{i1}} \quad (1)$$

$$S = \frac{\text{distribution coefficient of 2,3-butanediol}}{\text{distribution coefficient of water}} = \frac{D_2}{D_1} \quad (2)$$



**Figure 1.** Ternary diagram for LLE of (water + 2,3-butanediol + butyl acetate) at 298.15 K: ■, experimental solubility; —, experimental solubility curve; ○, experimental tie-line data; △, calculated (UNIFAC) tie-line data; . . ., calculated tie-lines.



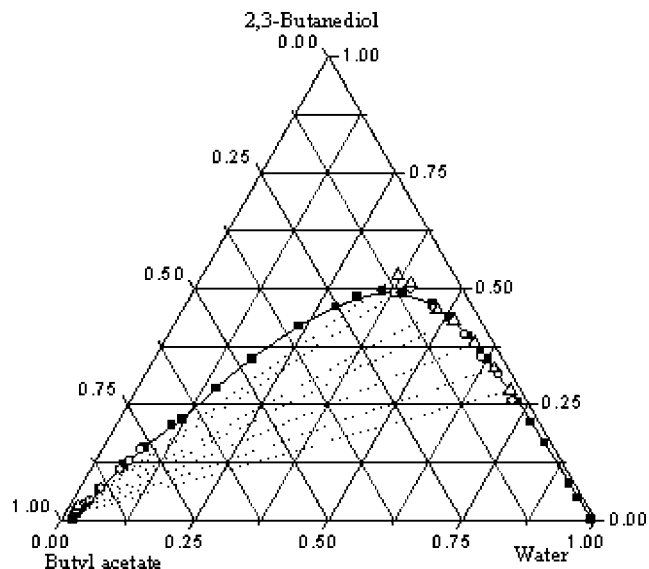
**Figure 2.** Ternary diagram for LLE of (water + 2,3-butanediol + butyl acetate) at 308.15 K: ■, experimental solubility; —, experimental solubility curve; ○, experimental tie-line data; △, calculated (UNIFAC) tie-line data; . . ., calculated tie-lines.

where  $W_{i3}$  and  $W_{i1}$  are the mass concentrations of component  $i$  in solvent-rich and water-rich phases, and  $D_1$  and  $D_2$  are the distribution coefficients of water and 2,3-butanediol, respectively.

The distribution coefficients and separation factors for each temperature are given in Table 4. Separation factors was found to be greater than 1, for the systems reported here, which means that the extraction of 2,3-butanediol by butyl acetate is possible. The separation factor is not constant over the whole two-phase region. The extracting power of the solvent at each temperature, plots of  $D_2$  versus  $W_{21}$  and  $S$  versus  $W_{21}$ , is shown in Figures 4 and 5, respectively.

The reliability of experimentally measured tie-line data can be ascertained by applying the Othmer–Tobias correlation<sup>20</sup> at each temperature as below

$$\ln\left(\frac{1 - W_{11}}{W_{11}}\right) = a + b \ln\left(\frac{1 - W_{33}}{W_{33}}\right) \quad (3)$$



**Figure 3.** Ternary diagram for LLE of (water + 2,3-butanediol + butyl acetate) at 318.15 K: ■, experimental solubility; —, experimental solubility curve; ○, experimental tie-line data; △, calculated (UNIFAC) tie-line data; . . ., calculated tie-lines.

**Table 4.** Distribution Coefficients ( $D_i$ ) of Water ( $i = 1$ ) and 2,3-Butanediol ( $i = 2$ ) and Separation Factors ( $S$ )

$T/K$	$D_1$	$D_2$	$S$
298.15	0.0285	0.1215	4.2595
	0.0345	0.1414	4.1024
	0.0950	0.2244	2.3618
	0.0818	0.2014	2.4628
	0.0456	0.1552	3.4062
308.15	0.1012	0.2346	2.3181
	0.1254	0.2258	1.8008
	0.0999	0.2083	2.0859
	0.0671	0.1613	2.4060
	0.1433	0.2642	1.8441
318.15	0.0446	0.1347	3.0224
	0.0409	0.1290	3.1569
	0.0598	0.1501	2.5096
	0.0466	0.1109	2.3779
	0.0374	0.1056	2.8247
	0.0555	0.1190	2.1431
	0.1651	0.2540	1.5383
0.1205	0.2366	1.9637	
0.0788	0.1694	2.1490	
0.1932	0.3083	1.5957	

where  $W_{11}$  is the mass fraction of water in the water-rich phase;  $W_{33}$  is the mass fraction of butyl acetate in the solvent-rich phase; and  $a$  and  $b$  are the constants.

The parameters of this correlation are listed in Table 5, and the correlation is shown in Figure 6 for the temperatures studied. The correlation factor ( $R^2$ ) being approximately unity indicates the degree of consistency of the related data.

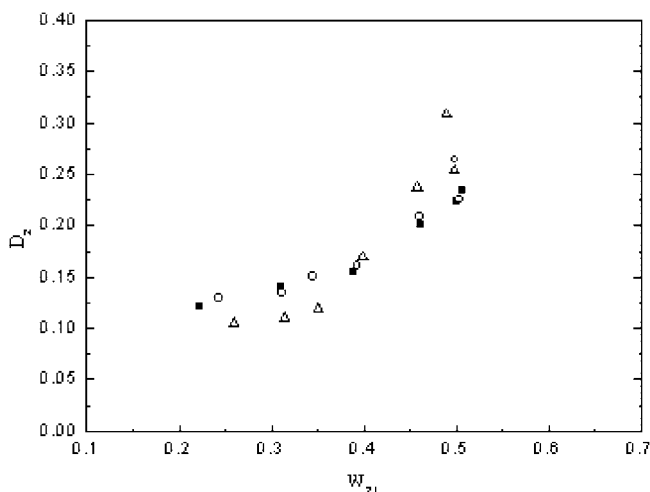
The experimental equilibrium data have been compared with predicted values by UNIFAC using the interaction parameters between  $\text{CH}_3$ ,  $\text{CH}_2$ ,  $\text{CH}$ ,  $\text{OH}$ ,  $\text{CH}_3\text{COO}$ , and  $\text{H}_2\text{O}$  functional groups obtained by Magnussen et al.<sup>21</sup> As shown in Figure 1, LLE data predicted by the UNIFAC method cannot be adequately fitted with the experimental LLE data at  $T = 298.2$  K. A similar lack of fits is observed at  $T = 308.2$  K and  $T = 318.2$  K.

The root-mean-square deviations (RMSDs) are calculated from the difference between the experimental data and the predictions of the UNIFAC model at each temperature according to the following formula

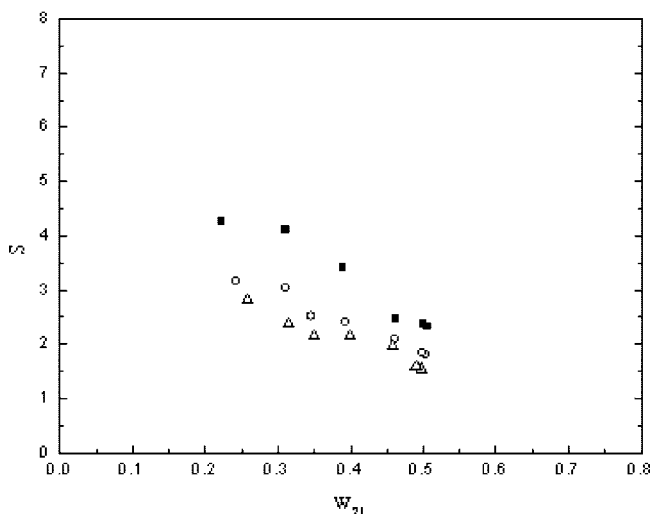
$$\text{RSMD} = \left[ \frac{\sum_k^N \sum_j \sum_i (W_{ijk}^{\text{exp}} - W_{ijk}^{\text{cal}})^2}{6N} \right]^{1/2} \quad (4)$$

where  $W_{ijk}$  is the composition of component  $i$  in phase  $j$  on tie-line  $k$ .  $N$  is the number of the tie-lines. The UNIFAC model predicts the LLE data for (298.15, 308.15, and 318.15) K with a root-mean-square deviation of (4.77, 4.95, and 5.55) %, respectively, between the observed and calculated mass concentrations. This value indicates that the LLE data of this ternary system were not predicted well with this equilibrium model. As can be seen from Figures 1 to 3, the predicted tie lines (dashed lines) are relatively in poor agreement with the experimental data (solid lines). However, in the lack of experimental data, this model can be used for correlation.

Selectivity diagrams on a solvent-free basis are obtained by plotting  $W_{23}/(W_{23} + W_{13})$  versus  $W_{21}/(W_{21} + W_{11})$  for each



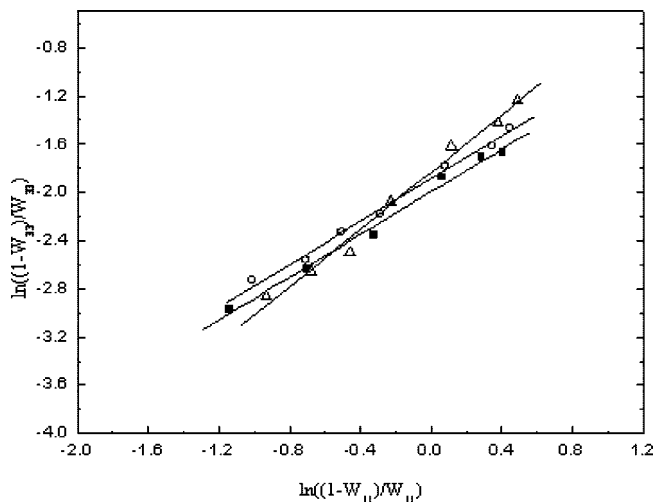
**Figure 4.** Distribution coefficient  $D_2$  of 2,3-butanediol as a function of the mass fraction  $W_{21}$  of 2,3-butanediol in the aqueous phase: ■, 298.15 K; ○, 308.15 K; △, 318.15 K.



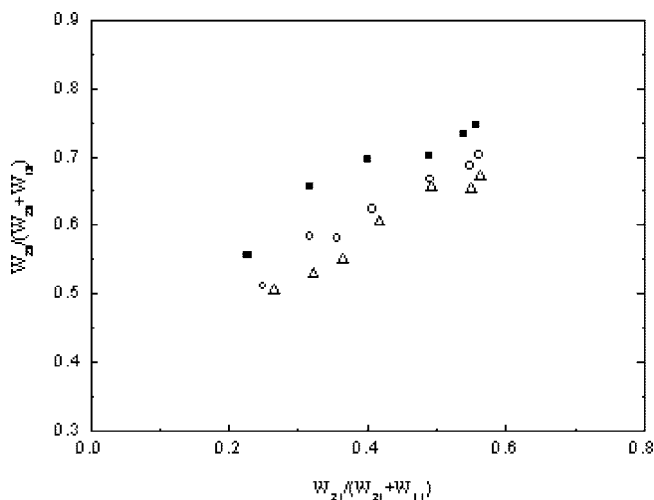
**Figure 5.** Separation factor,  $S$ , as a function of the mass fraction of 2,3-butanediol in the aqueous phase,  $W_{21}$ : ■, 298.15 K; ○, 308.15 K; △, 318.15 K.

**Table 5.** Constants of the Othmer–Tobias Equation for the Water + 2,3-Butanediol + Butyl Acetate Ternary System ( $R^2$ : Regression Coefficient)

$T/K$	$a$	$b$	$R^2$
298.15	0.8868	-1.9941	0.9918
308.15	0.8778	-1.8886	0.9935
318.15	1.1843	-1.8325	0.9879



**Figure 6.** Othmer–Tobias plots of the (water + 2,3-butanediol + butyl acetate) ternary systems: ■, 298.15 K; ○, 308.15 K; △, 318.15 K; —, eq 3.



**Figure 7.** Selectivity diagram at investigated temperature values (solvent-free basis): ■, 298.15 K; ○, 308.15 K; △, 318.15 K.

temperature in Figure 7. The selectivity diagram indicated that the performance of the solvent decreases with increasing temperature.

## Conclusion

The LLE data of the ternary mixtures water + 2,3-butanediol + butyl acetate have been presented at (298.15, 308.15, and 318.15) K. The UNIFAC model has been used to predict the LLE data. It has been observed that the UNIFAC predictions do not fit the experimental results quantitatively, but it agrees qualitatively. The separation factor is found to be greater than 1, and it is not constant over the whole two-phase region. It is concluded that butyl acetate may serve as a feasible solvent to 2,3-butanediol from its aqueous solutions.

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