

Liquid–Liquid Equilibria for the Ternary System Water (1) + Acetic Acid (2) + Diisopropyl Ether (3) at (293.15, 303.15, and 313.15) K

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Liquid–liquid equilibria (LLE) data for the ternary system water + acetic acid + diisopropyl ether (DIPE) at (293.15, 303.15, and 313.15) K have been measured under atmospheric pressure. The reliability of the experimental LLE data was ascertained through the Othmer–Tobias and Bachman correlations. The LLE data were correlated using the nonrandom two-liquid (NRTL) and universal quasichemical activity coefficient (UNIQUAC) models. The interaction parameters of those two models were regressed. The calculated values from both models agree well with the experimental values.

Introduction

The recovery of acetic acid from aqueous solutions is industrially and environmentally significant. Although acetic acid and water do not form an azeotrope, conventional distillation is highly uneconomical to separate these two components. The reason is because the system has a tangent pinch on the water end, which indicates a high number of column stages or high reflux ratio to get pure products.^{1–4} Among many methods to separate acetic acid from aqueous solution, the integration of extraction and heterogeneous azeotropic distillation is considered to be a comparatively effective method because of its lower energy cost.^{5–9} The key of this method is to find a kind of appropriate solvent which is used as both extractant and entrainer. In a previous work,^{10,11} we have reported the liquid–liquid equilibria (LLE) data of the ternary system of water + acetic acid + methyl *tert*-butyl ether (MTBE) and the quaternary system of water + acetic acid + MTBE + NaCl. Compared to MTBE, diisopropyl ether (DIPE) has a lower latent heat of vaporization, density, viscosity, and solubility. More importantly, the azeotrope of DIPE and water has the azeotropic composition containing more water. This means that this entrainer is more capable of carrying water to the top of the column and thus less entrainer is needed in the azeotropic distillation process. In addition, being soluble in water and recalcitrant to biodegradation, MTBE was a potential pollutant of water in aquifers contaminated.^{12,13} DIPE may be a promising solvent for the integration of extraction and heterogeneous azeotropic distillation. As basic research, we measured the LLE data of the ternary system of water + acetic acid + DIPE at (293.15, 303.15, and 313.15) K in this work.

Experimental Section

Chemicals. DIPE ($w \geq 99.9\%$) and acetic acid ($w \geq 99.5\%$) were purchased from Shanghai Chemical Reagent Co., Ltd. Double-distilled water was prepared in our laboratory. All of the liquid chemicals were checked with chromatographic analysis and used without further purification.

Apparatus and Procedure. The LLE data for the system of interest were measured under atmospheric pressure. The experimental apparatus included a jacketed glass cell (internal volume about 50 cm³), a thermostatically controlled bath, and a magnetic agitator. The circulating water from the thermostati-

cally controlled bath was introduced into the jacket to keep the temperature of the liquid mixture essentially constant. The temperature fluctuation was controlled within ± 0.05 K. At the beginning of the experiments, water, acetic acid, and DIPE were added into the cell by mass at known ratios. The weights of these reagents were determined by an electronic balance (BS110S, ± 0.1 mg). The heterogeneous mixtures were stirred for 2 h with a magnetic stirrer and allowed to settle for more than 4 h for complete phase separation. Samples were carefully taken from each phase and analyzed. The upper solvent-rich phase and the lower water-rich phase were sampled using different syringes.

Sample Analysis. A gas chromatograph (model: GC-122, Shanghai Precision Instrument Co. Ltd., China), equipped with a thermal conductivity detector (TCD), was used to analyze the compositions. A 2 m \times 2 mm inner diameter (i.d.) stainless steel column packed with a Porapak Q-S 80/100 was used for chromatographic analysis. The temperatures of the oven, injection port, and detector were all held at 478.15 K. The injection volume was 1 μ L. The bridge current of the TCD was 150 mA. The flow rate of the carrier gas, hydrogen, was kept at 34 mL \cdot min⁻¹. Very good peak separation was achieved under above-mentioned chromatographic conditions. The external standard method was used to analyze the content of the three components.

Results and Discussion

Experimental Results. The LLE data of the ternary system of water + acetic acid + DIPE at (293.15, 303.15, and 313.15) K have been measured and listed in Table 1. All concentrations are expressed in mass fraction.

To inspect the reliability of the experimental data, the Othmer–Tobias equation or Bachman equation were used to correlate the experimental tie-line data.^{14–19} The equations above are represented as follows, respectively:

$$\ln\left(\frac{1 - w_3^I}{w_3^I}\right) = a + b \ln\left(\frac{1 - w_1^{II}}{w_1^{II}}\right) \quad (1)$$

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Table 1. Comparison of Experimental and Predicted LLE Data (Mass Fraction) for the Water (1) + Acetic Acid (2) + DIPE (3) System at (293.15, 303.15, and 313.15) K

| experimental data | | | | NRTL | | | | UNIQUAC | | | |
|--------------------|---------|------------------|------------|--------------------|---------|------------------|------------|--------------------|---------|------------------|------------|
| solvent-rich phase | | water-rich phase | | solvent-rich phase | | water-rich phase | | solvent-rich phase | | water-rich phase | |
| w_1^I | w_2^I | w_1^{II} | w_2^{II} | w_1^I | w_2^I | w_1^{II} | w_2^{II} | w_1^I | w_2^I | w_1^{II} | w_2^{II} |
| T/K = 293.15 | | | | | | | | | | | |
| 0.0054 | 0.0000 | 0.9890 | 0.0000 | 0.0056 | 0.0000 | 0.9883 | 0.0000 | 0.0056 | 0.0000 | 0.9890 | 0.0000 |
| 0.0095 | 0.0425 | 0.8620 | 0.1205 | 0.0091 | 0.0412 | 0.8598 | 0.1232 | 0.0094 | 0.0434 | 0.8609 | 0.1229 |
| 0.0144 | 0.0849 | 0.7682 | 0.2102 | 0.0137 | 0.0815 | 0.7639 | 0.2137 | 0.0138 | 0.0858 | 0.7670 | 0.2111 |
| 0.0195 | 0.1306 | 0.6871 | 0.2836 | 0.0197 | 0.1249 | 0.6832 | 0.2881 | 0.0194 | 0.1318 | 0.6861 | 0.2849 |
| 0.0252 | 0.1732 | 0.6227 | 0.3406 | 0.0261 | 0.1661 | 0.6172 | 0.3475 | 0.0256 | 0.1740 | 0.6242 | 0.3393 |
| 0.0282 | 0.1923 | 0.5899 | 0.3703 | 0.0281 | 0.1786 | 0.5853 | 0.3756 | 0.0288 | 0.1939 | 0.5979 | 0.3617 |
| 0.0373 | 0.2385 | 0.5415 | 0.4109 | 0.0414 | 0.2566 | 0.5372 | 0.4169 | 0.0364 | 0.2355 | 0.5471 | 0.4035 |
| 0.0468 | 0.2805 | 0.4910 | 0.4523 | 0.0509 | 0.3092 | 0.4831 | 0.4616 | 0.0451 | 0.2765 | 0.5012 | 0.4390 |
| 0.0535 | 0.3115 | 0.4668 | 0.4637 | 0.0572 | 0.3415 | 0.4529 | 0.4854 | 0.0533 | 0.3096 | 0.4662 | 0.4642 |
| 0.0565 | 0.3189 | 0.4522 | 0.4787 | 0.0609 | 0.3591 | 0.4369 | 0.4976 | 0.0550 | 0.3159 | 0.4597 | 0.4687 |
| T/K = 303.15 | | | | | | | | | | | |
| 0.0060 | 0.0000 | 0.9722 | 0.0000 | 0.0062 | 0.0000 | 0.9710 | 0.0000 | 0.0067 | 0.0000 | 0.9731 | 0.0000 |
| 0.0111 | 0.0293 | 0.8484 | 0.1148 | 0.0110 | 0.0297 | 0.8511 | 0.1117 | 0.0102 | 0.0296 | 0.8472 | 0.1155 |
| 0.0134 | 0.0441 | 0.7898 | 0.1672 | 0.0133 | 0.0443 | 0.7963 | 0.1605 | 0.0124 | 0.0463 | 0.7924 | 0.1641 |
| 0.0176 | 0.0712 | 0.7112 | 0.2335 | 0.0174 | 0.0713 | 0.7203 | 0.2247 | 0.0168 | 0.0753 | 0.7145 | 0.2310 |
| 0.0193 | 0.0957 | 0.6711 | 0.2636 | 0.0195 | 0.0933 | 0.6653 | 0.2708 | 0.0202 | 0.0954 | 0.6697 | 0.2680 |
| 0.0270 | 0.1251 | 0.6055 | 0.3156 | 0.0271 | 0.1259 | 0.6122 | 0.3120 | 0.0267 | 0.1300 | 0.6044 | 0.3190 |
| 0.0326 | 0.1767 | 0.5570 | 0.3530 | 0.0331 | 0.1759 | 0.5635 | 0.3499 | 0.0338 | 0.1622 | 0.5525 | 0.3566 |
| 0.0407 | 0.2024 | 0.5094 | 0.3890 | 0.0404 | 0.1993 | 0.5172 | 0.3805 | 0.0410 | 0.1911 | 0.5110 | 0.3843 |
| 0.0549 | 0.2499 | 0.4536 | 0.4257 | 0.0535 | 0.2376 | 0.4578 | 0.4175 | 0.0532 | 0.2331 | 0.4564 | 0.4165 |
| 0.0658 | 0.2728 | 0.4181 | 0.4380 | 0.0649 | 0.2703 | 0.4129 | 0.4423 | 0.0642 | 0.2653 | 0.4176 | 0.4358 |
| T/K = 313.15 | | | | | | | | | | | |
| 0.0104 | 0.0000 | 0.9692 | 0.0000 | 0.0109 | 0.0000 | 0.9696 | 0.0000 | 0.0116 | 0.0000 | 0.9737 | 0.0000 |
| 0.0193 | 0.0542 | 0.8017 | 0.1532 | 0.0185 | 0.0546 | 0.8020 | 0.1511 | 0.0192 | 0.0563 | 0.8030 | 0.1557 |
| 0.0239 | 0.0821 | 0.7338 | 0.2086 | 0.0235 | 0.0832 | 0.7330 | 0.2104 | 0.0239 | 0.0851 | 0.7366 | 0.2134 |
| 0.0325 | 0.1149 | 0.6690 | 0.2631 | 0.0301 | 0.1164 | 0.6646 | 0.2671 | 0.0301 | 0.1193 | 0.6697 | 0.2691 |
| 0.0350 | 0.1434 | 0.6118 | 0.3109 | 0.0360 | 0.1429 | 0.6168 | 0.3048 | 0.0350 | 0.1434 | 0.6281 | 0.3022 |
| 0.0428 | 0.1779 | 0.5598 | 0.3481 | 0.0442 | 0.1768 | 0.5626 | 0.3455 | 0.0428 | 0.1779 | 0.5746 | 0.3425 |
| 0.0484 | 0.2001 | 0.5316 | 0.3647 | 0.0501 | 0.1990 | 0.5301 | 0.3685 | 0.0485 | 0.1999 | 0.5431 | 0.3647 |
| 0.0640 | 0.2522 | 0.4653 | 0.4084 | 0.0648 | 0.2497 | 0.4632 | 0.4117 | 0.0641 | 0.2522 | 0.4744 | 0.4084 |
| 0.0701 | 0.2697 | 0.4481 | 0.4206 | 0.0693 | 0.2636 | 0.4462 | 0.4217 | 0.0701 | 0.2697 | 0.4527 | 0.4206 |
| 0.0850 | 0.3073 | 0.3993 | 0.4428 | 0.0848 | 0.3070 | 0.3959 | 0.4478 | 0.0850 | 0.3073 | 0.4074 | 0.4428 |

Table 2. Constants of the Othmer–Tobias and Bachman Equations for the Water (1) + Acetic Acid (2) + DIPE (3) System at (293.15, 303.15, and 313.15) K

| T/K | Othmer–Tobias | | | | Bachman | | | |
|--------|---------------|--------|--------|--------|---------|---------|--------|--------|
| | a | b | R^a | SD^a | m | N | R^a | SD^a |
| 293.15 | -0.9468 | 0.9703 | 0.9966 | 0.0860 | 1.6716 | -0.6680 | 0.9907 | 0.0121 |
| 303.15 | -1.2270 | 1.1148 | 0.9979 | 0.0638 | 1.5216 | -0.4918 | 0.9831 | 0.0149 |
| 313.15 | -1.0145 | 1.0427 | 0.9988 | 0.0444 | 1.6577 | -0.6354 | 0.9909 | 0.0121 |

^a R is the linear correlation coefficient, and SD is the standard deviation.

$$w_3^I = m + n \left(\frac{w_3^I}{w_1^{II}} \right) \quad (2)$$

where w_3^I is the mass fraction of DIPE in the solvent-rich phase; w_1^{II} is the mass fraction of water in the water-rich phase; the letters a and b and m and n are constants of the equations of Othmer–Tobias and Bachman, respectively.

The parameters of Othmer–Tobias and Bachman equations are listed in Table 2. All of the linear correlation coefficients (R) are greater than 0.9907. The standard deviations (SD s) are less than 0.086. These results suggest that it is reasonable to accept the LLE data of the considered systems as reliable.

LLE Calculations. The relationship of liquid–liquid equilibrium can be represented with activity coefficient model. In

this model, the basic relationships for every component i in two coexistent liquid phases of a system at equilibrium are

$$x_i^I r_i^I = x_i^{II} r_i^{II} \quad (3)$$

$$\sum x_i^I = 1 \quad (4)$$

$$\sum x_i^{II} = 1 \quad (5)$$

where x_i^I and x_i^{II} are the mole fractions of component i in phases I and II and r_i^I and r_i^{II} are the activity coefficients of component i in phases I and II.

The experimental data were correlated with the nonrandom two-liquid (NRTL) and universal quasichemical activity coefficient (UNIQUAC) models. The adjustable parameter of those two models is defined as follows, respectively

$$\tau_{ij} = a_{ij} + b_{ij}/T \quad (6)$$

Table 3. UNIQUAC Structural Parameters of the Used Pure Component

| component | r_i | q_i |
|-------------|--------|--------|
| water | 0.9200 | 1.4000 |
| acetic acid | 2.2024 | 2.0720 |
| DIPE | 4.7423 | 4.0880 |

Table 4. Values of the NRTL and UNIQUAC Binary Parameters Regressed from LLE Data and rmsd for the Water (1) + Acetic Acid (2) + DIPE (3) System at (293.15, 303.15, and 313.15) K

| T/K | component | | NRTL | | | UNIQUAC | | |
|--------|------------|-------------------------|-------------------------|-----------------|--------|-------------------------|-------------------------|--------|
| | <i>i-j</i> | <i>b_{ij}/K</i> | <i>b_{ij}/K</i> | α_{ij}^a | rmsd | <i>b_{ij}/K</i> | <i>b_{ij}/K</i> | rmsd |
| 293.15 | 1-2 | 497.99 | 234.77 | 0.35 | 0.0040 | 291.1 | 27.10 | 0.0065 |
| | 1-3 | 1552.40 | 940.09 | 0.35 | | -76.78 | -693.08 | |
| | 2-3 | 501.75 | 279.47 | 0.37 | | -157.7 | 345.87 | |
| 303.15 | 1-2 | 613.58 | 122.337 | 0.35 | 0.0038 | 605.9 | 37.93 | 0.0039 |
| | 1-3 | 1350.33 | 876.64 | 0.35 | | -14.04 | -752.92 | |
| | 2-3 | 349.45 | 458.56 | 0.37 | | -161.7 | 601.66 | |
| 313.15 | 1-2 | 493.82 | 118.437 | 0.35 | 0.0021 | 673.9 | 13.49 | 0.0041 |
| | 1-3 | 1356.11 | 793.12 | 0.35 | | -16.83 | -676.68 | |
| | 2-3 | 363.45 | 263.48 | 0.37 | | -141.1 | 672.97 | |

^a α_{ij} is the nonrandomness factor of the NRTL model.

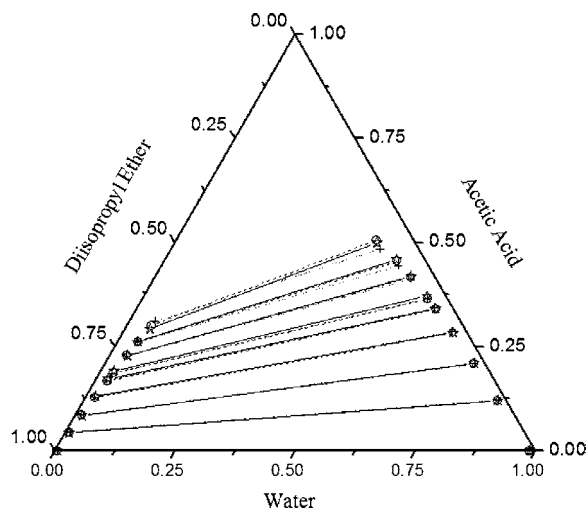


Figure 1. LLE phase diagram for the water (1) + acetic acid (2) + DIPE (3) system at 293.15 K: ☆, solid lines, experimental data tie lines; ○, dashed lines, tie lines calculated from NRTL; +, dotted lines, tie lines calculated from UNIQUAC.

$$\tau_{ij} = \exp(a_{ij} + b_{ij}/T) \quad (7)$$

where a_{ij} and b_{ij} are the binary parameters and T is temperature. These parameters were determined by minimizing the deviation between the experimental data and the model calculated values.

The binary interaction parameters of NRTL and UNIQUAC models were calculated using Aspen Plus software. In the process of regression calculations, the parameter of those two models in eqs 6 and 7, a_{ij} , was set to zero. For the NRTL model, the value of the nonrandomness parameter, α , is adjustable for a different pair of compounds. For the UNIQUAC model, the pure component structural parameters (r , q) are listed in Table 3.^{20,21} The values of binary parameter b_{ij} and α were listed in Table 4. The regression method used in the Aspen Plus was the least-squares method based on the maximum likelihood principles. The Britt-Luecke algorithm was employed to obtain the model parameters with the Deming initialization method.

The calculated values from both models and experimental results were all listed in Table 1. Table 4 lists the values of the root-mean-square deviations (rmsd's) of both models at each temperature. The rmsd is defined as

$$\text{rmsd} = \left(\sum_{k=1}^n \sum_{j=1}^2 \sum_{i=1}^3 \left(\frac{(w_{ijk}^{\text{calcd}} - w_{ijk}^{\text{exptl}})^2}{6n} \right) \right)^{1/2} \quad (8)$$

where w_{ijk}^{calcd} and w_{ijk}^{exptl} are the calculated and the experimental mass fractions of component i in phase j on tie-line k , and n is the number of tie-lines, respectively.

The LLE diagrams for the water + acetic acid + DIPE system at (293.15, 303.15, and 313.15) K are shown in Figures 1 to 3,

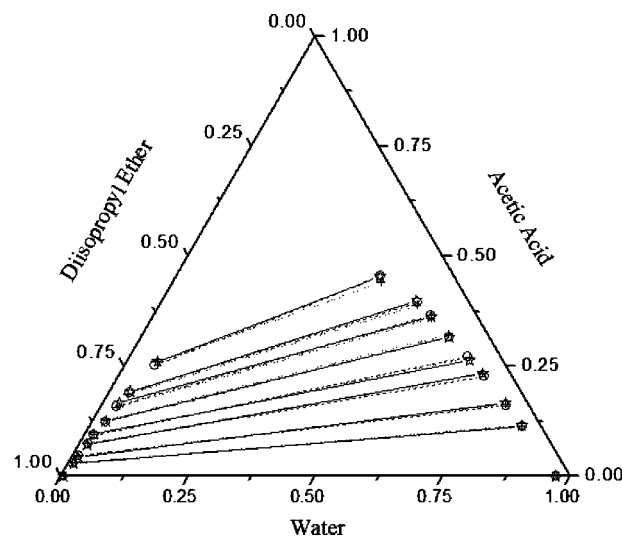


Figure 2. LLE phase diagram for the water (1) + acetic acid (2) + DIPE (3) system at 303.15 K: ☆, solid lines, experimental data tie lines; ○, dashed lines, tie lines calculated from NRTL; +, dotted lines, tie lines calculated from UNIQUAC.

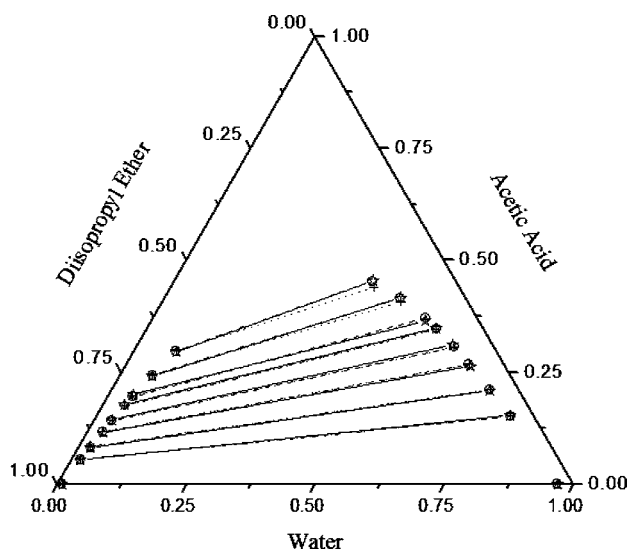


Figure 3. LLE phase diagram for the water (1) + acetic acid (2) + DIPE (3) system at 313.15 K: ☆, solid lines, experimental data tie lines; ○, dashed lines, tie lines calculated from NRTL; +, dotted lines, tie lines calculated from UNIQUAC.

Table 5. Distribution Coefficients for Water (D_1) and Acetic Acid (D_2) and Separation Factors (S) at (293.15, 303.15, and 313.15) K

| D_1 | D_2 | S | D_1 | D_2 | S | D_1 | D_2 | S | |
|--------|----------------|---------|--------|----------------|---------|--------|----------------|---------|--|
| | $T = 293.15$ K | | | $T = 303.15$ K | | | $T = 313.15$ K | | |
| 0.0110 | 0.3528 | 32.0087 | 0.0130 | 0.2553 | 19.5697 | 0.0240 | 0.3540 | 14.7265 | |
| 0.0187 | 0.4039 | 21.5478 | 0.0170 | 0.2639 | 15.5438 | 0.0326 | 0.3936 | 12.0838 | |
| 0.0283 | 0.4605 | 16.2505 | 0.0247 | 0.3050 | 12.3466 | 0.0486 | 0.4369 | 8.9982 | |
| 0.0405 | 0.5086 | 12.5623 | 0.0288 | 0.3631 | 12.6134 | 0.0573 | 0.4612 | 8.0537 | |
| 0.0478 | 0.5193 | 10.8536 | 0.0447 | 0.3965 | 8.8775 | 0.0764 | 0.5111 | 6.6862 | |
| 0.0702 | 0.5455 | 7.7696 | 0.0587 | 0.4604 | 7.8446 | 0.0911 | 0.5487 | 6.0260 | |
| 0.0890 | 0.5682 | 6.3851 | 0.0815 | 0.4823 | 5.9179 | 0.1400 | 0.5817 | 4.1561 | |
| 0.1086 | 0.5859 | 5.3974 | 0.1229 | 0.5477 | 4.4569 | 0.1637 | 0.6019 | 3.6757 | |
| 0.1243 | 0.5860 | 4.7128 | 0.1530 | 0.5733 | 3.7483 | 0.2188 | 0.6508 | 2.9747 | |

respectively. These LLE diagrams compare the experimental results with the calculated binodal locus and tie-lines from the NRTL and UNIQUAC models.

The rmsd is a measure of agreement between experimental and calculated data. As seen from Table 4 and Figures 1 to 3, good agreements between the calculated values and experimental results have been obtained for the system of water + acetic acid + DIPE.

To estimate the capability of solvent to separate acetic acid from water, the distribution ratio, D_1 for water and D_2 for acetic

acid, and the separation factor, S , at investigated temperatures were calculated and listed in Table 5. The D_i and S were determined as follows:

$$D_i = \frac{w_i^I}{w_i^{II}} \quad (9)$$

$$S = \frac{D_2}{D_1} \quad (10)$$

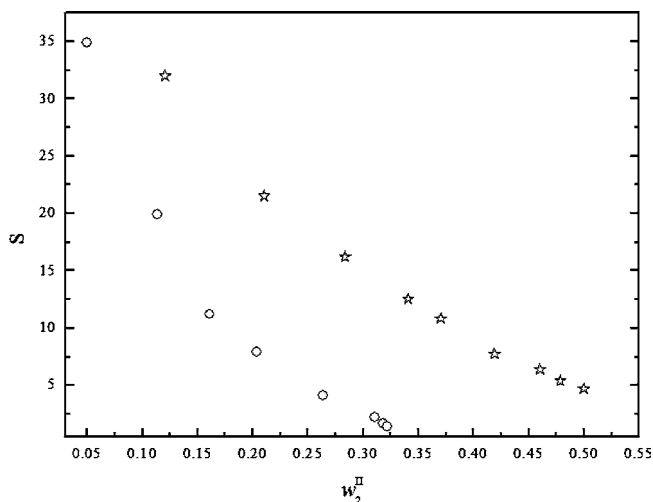


Figure 4. Separation factor, S , plotted against the mass fraction of acetic acid in the aqueous phase, w_2^{II} , at 293.15 K: ☆, DIPE; ○, MTBE.

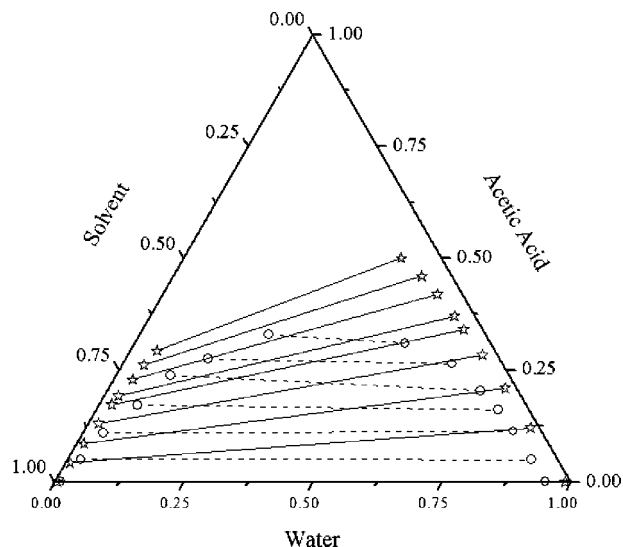


Figure 5. Comparison of the LLE phase diagram for the water (1) + acetic acid (2) + solvent (3) systems at 293.15 K: ☆, solid lines, DIPE; ○, dashed lines, MTBE.

where w is the mass fraction; the superscript I represents the solvent-rich phase and II the water-rich phase.

Figure 4 compares the separation factor of DIPE with that of MTBE at 293.15 K. The LLE phase diagrams of water (1) + acetic acid (2) + solvent (3) at 293.15 K are shown in Figure 5. From Table 4, the value of a separation factor of DIPE is found to be greater than 1 (varying between 2.9747 to 32.0087) for the system investigated here, which means that the extraction of acetic acid from aqueous solution by DIPE is possible. It can be seen that the separation factor of DIPE is greater than that of MTBE at 293.15 K from Figure 4. Figure 5 shows that the area of two-phase region of the water (1) + acetic acid (2) + DIPE (3) system is larger than that of the system of water (1) + acetic acid (2) + MTBE (3) at 293.15 K.

Conclusions

LLE data for the water + acetic acid + DIPE ternary system at (293.15, 303.15, and 313.15) K under atmospheric pressure were determined. The reliability of experimental data was inspected by the use of the Othmer–Tobias and Bachman equations. The experimental results are shown to be reliable. NRTL and UNIQUAC models were used to correlate the experimental data. The rmsd is less than 0.0065. The results show that the LLE of the investigated system could be correlated well with both models. Compared with MTBE, DIPE has a better extraction efficiency.

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