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Isobaric Vapor−Liquid Equilibrium for Methanol + Methyl Acetate + 1-Octyl-3-methylimidazolium Hexafluorophosphate at 101.3 kPa

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ABSTRACT: Vapor−liquid equilibrium (VLE) data for methanol + methyl acetate + 1-octyl-3-methylimidazolium hexafluorophosphate ([OMIM][PF_6]) at 101.3 kPa were measured. The experimental VLE data were correlated by the nonrandom two-liquid (NRTL) activity coefficient model, and the binary parameters were obtained. The results show that the ionic liquid [OMIM][PF_6] produces a notable salting-out effect, which enhances the relative volatility of methanol to methyl acetate. The effect of [OMIM][PF_6] on methanol + methyl acetate system was compared with that of *o*-xylene.

INTRODUCTION

As green slovents, ionic liquids (ILs) have excellent properties, such as nonvolatility, high chemical stability, less causticity, and good performance in improving the separation efficiency.[1−3] In recent years, ILs have been used as promising entrainers in extractive distillation for the separation of azeotropic mixtures. Arlt et al. reported the effects of various ILs on different systems such as ethanol + water, propanone + methanol, water + acetic acid, oxolane + water, methanol + trimethylborate, and hex-1-ene + hexane.[4−11] Lei et al. studied the isobaric vapor−liquid equilibrium (VLE) for isopropyl alcohol + water + 1-butyl-3-methylimidazolium tetrafluoroborate and the isobaric VLE for isopropyl alcohol + water + 1-ethyl-3-methylimidazolium tetrafluoroborate.[12,13] VLE data for IL-containing systems are essential for the design of separation process and the development of thermodynamic models; nevertheless, these data are still rare up to now.

Methanol and methyl acetate are involved in the industrial manufacturing process of poly(vinyl alcohol) (PVA). During the production of PVA, methanol is a feedstock, and methyl acetate is a byproduct.[14−16] Because methanol and methyl acetate can form an azeotrope, they are usually separated by extractive distillation. Orchilles et al.[17] used 1-ethyl-3-methylimidazolium trifluoromethanesulfonate ([EMIM][triflate]) as an entrainer for extractive distillation to eliminate the azeotropic point of methyl acetate + methanol, and methyl acetate is the volatile component in this process. Jimenez et al.[18,19] proposed a reactive extractive distillation process to convert methyl acetate with butan-1-ol to butyl ethanoate and methanol. In such process, *o*-xylene is selected as entrainer, and it makes methanol as a volatile component, but the separation of *o*-xylene from the reaction mixture would take much effort. In this paper, we aim to select an IL as entrainer to separate methanol−methyl acetate, making methanol as a volatile component, and this work is part of our research on converting methyl acetate with butan-1-ol to butyl ethanoate and methanol by reactive extractive distillation with ILs as an entrainer and catalyst.

To select a suitable IL entrainer for the reactive extractive distillation, we calculated the infinite dilution activity coefficients of methanol and methyl acetate in hundreds of ILs using the COSMO-SAC model.[20,21] We found 1-octyl-3-methylimidazolium hexafluorophosphate ([OMIM][PF_6]) was a promising solvent to make methanol as a volatile component, for the separation of azeotropic mixture of methanol + methyl acetate. We measured the VLE for the ternary mixture methanol (1) + methyl acetate (2) + [OMIM][PF_6] (3) at atmospheric pressure (101.3 kPa). The VLE data of the ternary mixture were correlated by the nonrandom two-liquid (NRTL) model, and the entrainers [OMIM][PF_6] and *o*-xylene for the separation of methanol + methyl acetate were compared according to the relative volatility of methanol to methyl acetate.

EXPERIMENTAL SECTION

Materials. Methanol and methyl acetate were purchased from Jiangtian Chemical Reagents Co., Tianjin, China. These chemicals were of analytical grade, and GC analysis gave a purity greater than 0.998 (mass fraction). The water mass fraction in each chemicals determined by Karl Fischer titration was less than 0.001.

Entrainers. The IL [OMIM][PF_6] was used as an entrainer. It was purchased from Chengjie Chemical Reagents Co., Shanghai, China, with a minimum mass fraction of 0.99 (observed by liquid chromatography). The water mass fraction in IL was verified by Karl Fischer titration (less than 0.001). The IL was used without further purification but was carefully degassed.

Apparatus and Procedure. The VLE for the ternary mixture methanol (1) + methyl acetate (2) + 1-octyl-3-methylimidazolium hexafluorophosphate ([OMIM][PF_6]) (3) was measured by a circulation VLE still (a modified Othmer still). A detailed description of the apparatus is available in our previous publication.[22] After the mixture in the equilibrium still was maintained in the constant boiling temperature for about 30 min; then samples were taken every 20 min, from the vapor and liquid phase of the system, respectively. To verify the equilibrium state, samples were taken until the standard deviation of the last five samples was less than 0.0015 for both vapor and liquid phase.

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Table 1. Vapor−Liquid Equilibrium Data for the Ternary System Methanol (1) + Methyl Acetate (2) + [OMIM][PF$_6$] (3) at P = 101.3 kPa

x_3	T/K	x_1'	y_1	α_{12}
0.200	337.62	0.000	0.000	
0.201	335.02	0.102	0.175	1.867
0.199	333.56	0.192	0.285	1.677
0.198	333.25	0.301	0.380	1.423
0.202	333.32	0.412	0.481	1.323
0.200	333.55	0.523	0.565	1.185
0.201	334.36	0.601	0.612	1.047
0.200	335.32	0.698	0.683	0.932
0.203	336.62	0.792	0.771	0.884
0.201	338.52	0.903	0.872	0.732
0.202	341.68	1.000	1.000	
0.400	349.88	0.000	0.000	
0.401	345.52	0.090	0.192	2.403
0.401	343.21	0.199	0.355	2.215
0.400	342.05	0.290	0.439	1.916
0.397	341.52	0.391	0.540	1.828
0.402	341.51	0.502	0.635	1.726
0.400	341.53	0.620	0.730	1.657
0.399	341.88	0.713	0.792	1.533
0.401	342.52	0.788	0.841	1.423
0.400	343.42	0.901	0.920	1.264
0.403	345.21	1.000	1.000	
0.601	368.38	0.000	0.000	
0.598	361.14	0.100	0.241	2.858
0.603	357.26	0.208	0.422	2.780
0.599	354.47	0.311	0.542	2.622
0.600	353.52	0.399	0.634	2.609
0.602	351.95	0.500	0.711	2.460
0.602	351.23	0.601	0.783	2.396
0.601	350.45	0.701	0.849	2.398
0.601	350.87	0.792	0.902	2.417
0.600	351.23	0.900	0.956	2.414
0.599	350.28	1.000	1.000	

The total sampling process lasted for about 2 h, so that the sampling process could ensure the vapor and liquid phases are in equilibrium state. In each VLE experiment, the pressure was kept at 101.3 ± 0.05 kPa. The solutions for VLE measurement were prepared gravimetrically using an electronic balance (Acculab Alc 210.4) with a standard uncertainty of 0.0001 g.

Sample Analysis. Gas chromatography (GC) was used to analyze the compositions of the condensed vapor and the concentrations of methanol and methyl acetate in liquid phase. The GC (SP-1000) was equipped with a flame ionization device (FID) detector, and the column was SE-30 (50 m × 0.32 mm × 0.5 μm). The calibration correction factor was obtained using calibration samples prepared gravimetrically. The quality of the calibration was evaluated by measuring samples of known compositions. The results showed that the standard deviation between the known compositions and the GC measurements was below 0.001 (mole fraction). The expanded uncertainty of the gas chromatographic composition analysis was below 0.006 in mole fraction (with 95 % confidence).

High-performance liquid chromatography (HPLC) with an ultraviolet detector (water 490E) was utilized to analyze the compositions of methyl acetate and IL in the liquid phase. The UV detector wavelength was 240 nm, and the mobile phase was methanol + water (v/v = 1:1). The calibration curve was obtained using a series of standard solutions prepared gravimetrically, and the correlation coefficient (R^2) of the calibration curve was 0.99964. To evaluate the quality of the calibration curve, we measured five samples of known compositions. The deviations between the compositions of the gravimetrically composed samples and the HPLC measurements indicated a standard deviation of less than 0.002 (mole fraction). The expanded uncertainty of the HPLC composition analysis was assumed to below 0.007 (mole fraction, with 95 % confidence). In this way, the ratio of the IL to methyl acetate was obtained by HPLC, and the ratio of methanol to methyl acetate was obtained by GC, so the mole fraction of the methanol, methyl acetate, and [OMIM][PF$_6$] in the liquid phase can be calculated.

RESULTS AND DISCUSSION

Experimental Data. The reliability of our experimental method has been verified by the VLE data of methanol (1) + methyl acetate (2) in our previous work.[22] The measurement for the ternary system of methanol (1) + methyl acetate (2) + [OMIM][PF$_6$] (3) was conducted at 101.3 kPa, and the concentrations of IL added to the system were kept at x_3 = 0.2, 0.4, and 0.6 (mole fraction), respectively. The isobaric VLE data for the methanol (1) + methyl acetate (2) + IL (3) are listed in Table 1. In the table, x_3 represents the mole fraction of IL in the liquid phase, and x_1' represents the mole fraction of methanol in the liquid phase excluding IL; y_1 is the mole fraction of methanol in the vapor phase, T is the equilibrium temperature, and α_{12} is the relative volatility of methanol to methyl acetate. Since the vapor pressure of IL can be neglected, there are only methanol and methyl acetate in the vapor phase.

Correlation of the Phase Equilibrium. The NRTL model is commonly used to correlate the VLE data.[23] Gmehling and co-workers,[24−26] Orchilles and co-workers,[17,27] and Li and co-workers[12,13] have used the NRTL model to correlate various VLE systems containing ILs, and it gives good agreement with the experimental results. In this work, we also used the NRTL model to correlate the VLE data. The NRTL model we used is as follows:

$$\ln \gamma_i = \frac{\sum_j \tau_{ji} G_{ji} x_j}{\sum_k G_{ki} x_k} + \sum_j \left[\frac{x_j G_{ij}}{\sum_k G_{kj} x_k} \left(\tau_{ij} - \frac{\sum_k \tau_{kj} G_{kj} x_k}{\sum_k G_{kj} x_k} \right) \right] \quad (1)$$

$$\tau_{ji} = B_{ji}/T \quad (2)$$

$$G_{ji} = \exp(-a_{ji}\tau_{ji}) \quad (3)$$

where B_{ij} is the binary interaction parameter, K; a_{ji} is the nonrandomness parameter; T is the temperature, K.

The binary interaction parameters (B_{12} and B_{21}) and the nonrandomness parameter (a_{12}) for the methanol (1) + methyl acetate (2) system were obtained from the database in commercial

Table 2. Values of Binary Parameters in the NRTL Model

i component	*j* component	a_{ij}	B_{ij}/T	B_{ji}/T
methanol (1)	methyl acetate (2)	0.296	223.376	146.111
methanol (1)	[OMIM][PF_6] (3)	0.381	508.857	29.956
methyl acetate (2)	[OMIM][PF_6] (3)	0.156	1333.943	−991.742

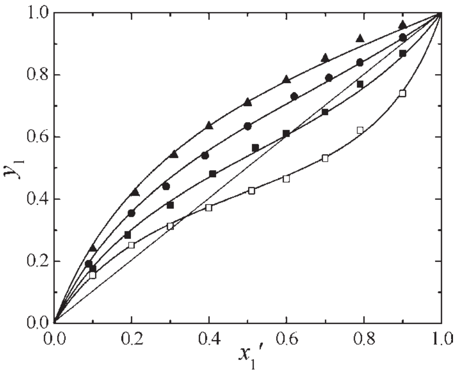

Figure 1. Isobaric VLE diagram for methanol (1) + methyl acetate (2) + [OMIM][PF_6] (3) system at 101.3 kPa: □, $x_3 = 0$; ■, $x_3 = 0.2$; ●, $x_3 = 0.4$; ▲, $x_3 = 0.6$; solid lines, calculated by the NRTL model.

software ChemCAD, and the other binary interaction parameters (B_{13}, B_{23}, B_{31}, and B_{32}) and the nonrandomness parameters (a_{13}, a_{23}) were correlated from ternary experimental VLE data by minimization of the objective function *F*:[28]

$$F = \sum_{j=1}^{N}\left(\sum_{i=1}^{C}\left(\frac{y_{j,i}^{\text{cal}} - y_{j,i}^{\text{exp}}}{\sigma_y}\right)^2 + \left(\frac{T_j^{\text{cal}} - T_j^{\text{exp}}}{\sigma_T}\right)^2 + \left(\frac{P_j^{\text{cal}} - P_j^{\text{exp}}}{\sigma_P}\right)^2 + \sum_{i=1}^{C}\left(\frac{x_{j,i}^{\text{cal}} - x_{j,i}^{\text{exp}}}{\sigma_x}\right)^2\right) \quad (4)$$

where N is the number of data points; C is the number of components; y is the mole fraction in vapor phase; x is the mole fraction in vapor phase; T is the equilibrium temperature, K; P is the equilibrium pressure, kPa; σ_y, σ_T, σ_P, and σ_x are estimated standard deviations for y, T, P, and x, respectively ($\sigma_y = 0.002$, $\sigma_T = 0.07$ K, $\sigma_P = 0.05$ kPa, $\sigma_x = 0.002$); the indices exp and cal denote the experimental and calculated values, respectively.

The six binary interaction parameters as well as the nonrandomness parameters ($a_{12} = a_{21}$, $a_{13} = a_{31}$, and $a_{23} = a_{32}$) are all given in Table 2.

Figures 1 to 3 show the experimental results and the calculated results by NTRL model. As shown in these figures, the calculated results agree well with the experimental results. The maximum absolute deviation Δy represents the absolute deviation σy and root-mean-square deviation δy between the experimental and calculated values of vapor-phase mole fractions ($\Delta y = \max|y^{\text{exp}} - y^{\text{cal}}|$; $\sigma y = (1/N)\Sigma|y^{\text{exp}} - y^{\text{cal}}|$; $\delta y = [(1/N)\Sigma(y^{\text{exp}} - y^{\text{cal}})^2]^{1/2}$) are 0.014, 0.007, and 0.008, respectively. The maximum absolute deviation ΔT, mean absolute deviation σT, and root-mean-square deviation δT between the experimental and calculated values of equilibrium temperatures ($\Delta T = \max|T^{\text{exp}} - T^{\text{cal}}|$; $\sigma T = (1/N)\Sigma|T^{\text{exp}} - T^{\text{cal}}|$; $\delta T = [(1/N)\Sigma(T^{\text{exp}} - T^{\text{cal}})^2]^{1/2}$) are 0.65 K, 0.157 K, and 0.226 K, respectively.

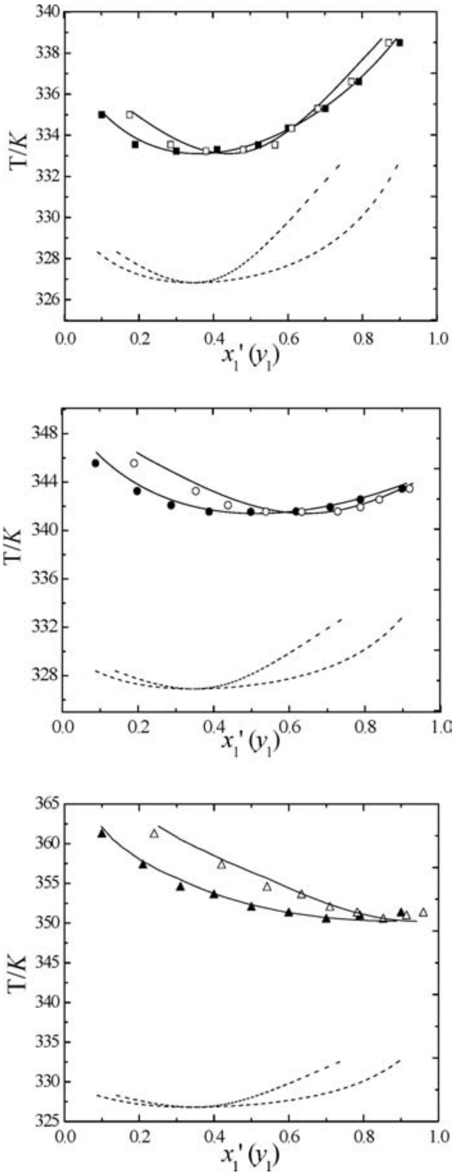

Figure 2. $T-x-y$ diagram for the ternary system of methanol (1) + methyl acetate (2) containing [OMIM][PF_6] (3) at different contents of IL: ■, x_1' ($x_3 = 0.2$); □, y_1 ($x_3 = 0.2$); ●, x_1' ($x_3 = 0.4$); ○, y_1 ($x_3 = 0.4$); ▲, x_1' ($x_3 = 0.6$); △, y_1 ($x_3 = 0.6$); solid lines, calculated by the NRTL model; dashed lines, calculated by the NRTL model for an IL-free system.

For the methanol + methyl acetate system, the boiling points of methanol and methyl acetate are 337.8 K and 330.9 K, respectively. In common terms, methyl acetate is the volatile component. We investigated the VLE of methanol + methyl acetate + 1-ethyl-3-methylimidazolium acetate in our previous work[22] and found that 1-ethyl-3-methylimidazolium acetate ([EMIM][Ac]) can eliminate the azeotropic point of methanol + methyl acetate with methyl acetate as the volatile component. In this work, we choose [OMIM][PF_6] as an entrainer, and [OMIM][PF_6] also can eliminate the azeotropic point of methanol + methyl acetate, but methanol becomes the volatile component (see Figures 1 and 3).

Figures 1 and 3 show that the IL [OMIM][PF_6] produces a notable salting-out effect on methanol for methanol + methyl

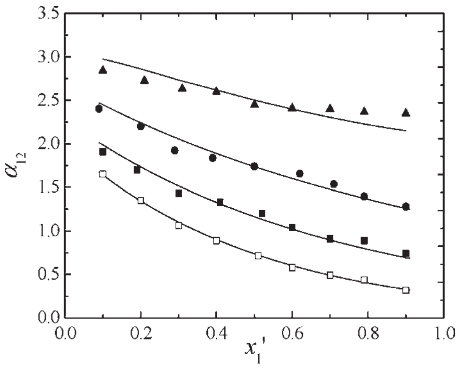

Figure 3. Relative volatility of methanol (1) to methyl acetate (2) at 101.3 kPa: □, x_3 = 0; ■, x_3 = 0.2; ●, x_3 = 0.4; ▲, x_3 = 0.6; solid lines, calculated by the NRTL model.

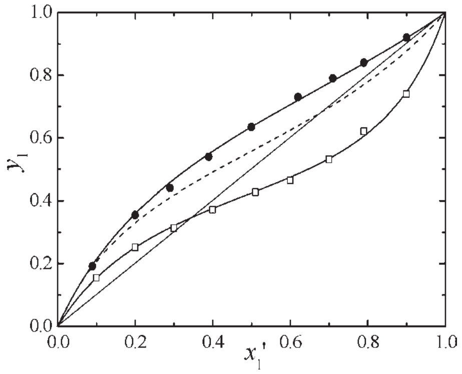

Figure 4. Effects of [OMIM][PF_6] and *o*-xylene on the VLE of the methanol (1) + methyl acetate (2) system at 101.3 kPa with entrainer mole fraction x_3 = 0.4: ●, [OMIM][PF_6], obtained by experiments; dashed line, *o*-xylene, calculated by the modified UNIFAC model; □, IL-free system (ref 22); solid lines, calculated by NRTL model.

acetate system and the salting-out effect of IL increases with its mole fraction in liquid phase. This phenomena may be attributed to the interaction between methanol and [OMIM][PF_6] is less than that between methyl acetate and [OMIM][PF_6], so the relative volatility of methanol to methyl acetate can be increased by [OMIM][PF_6].

Jimenez et al. used *o*-xylene as entrainer to separate methanol + methyl acetate with methanol as volatile component, and the minimum mole fraction of *o*-xylene to eliminate the azeotropic point is 0.48 at 101.3 kPa.[18,19] We used [OMIM][PF_6] as an entrainer to separate methanol + methyl acetate. The minimum mole fraction of [OMIM][PF_6] to eliminate the azeotropic point can be calculated using the binary parameters of NRTL model correlated above, and the value is 0.28 at 101.3 kPa, which is less than that of *o*-xylene. The effects of *o*-xylene and [OMIM][PF_6] are compared in Figure 4.

■ CONCLUSIONS

The isobaric VLE of the ternary mixture methanol + methyl acetate + [OMIM][PF_6] were measured. The results show that the IL [OMIM][PF_6] produces a notable salting-out effect on methanol. The salting-out effect of [OMIM][PF_6] increases with its concentration in the liquid phase.

The NRTL activity coefficient model was used to correlate the VLE data for methanol + methyl acetate + [OMIM][PF_6], and the calculated results agree well with the experimental results. The IL [OMIM][PF_6] is a promising entrainer to enhance the relative volatility of methanol to methyl acetate. It can eliminate the azeotropic point of methanol + methyl acetate if the mole fraction of [OMIM][PF_6] in liquid phase is larger than 0.28.

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