Korean J. Chem. Eng., 37(7), 1212-1217 (2020)
DOI: 10.1007/s11814-020-0534-1

pISSN: 0256-1115
eISSN: 1975-7220

Separation of ethanol from a 2-butanone/ethanol mixture using choline chloride based deep eutectic solvents

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(*Received 10 January 2020 • Revised 3 March 2020 • Accepted 5 March 2020*)

Abstract−At 323.2 K the liquid-liquid equilibria (LLE) of a ternary system of ethanol, 2-butanone, and choline chloride based deep eutectic solvents (DESs) were experimentally determined under atmospheric pressure. The LLE of the same ternary system was also obtained at 303.2 K to investigate the effect of temperature on ethanol separation. In almost all cases no DESs were detected in the raffinate phase. In addition, the values of the distribution coefficient of ethanol in the presence of the applied DESs were higher than those with glycerol at 303.2 K. This could afford a significant advantage because a higher distribution coefficient of ethanol requires a smaller amount of solvent in ethanol separation. The experimental LLE data were correlated using a non-random two-liquid model.

Keywords: Deep Eutectic Solvent, Distribution Coefficient, Liquid-liquid Equilibrium, Selectivity, Correlation

INTRODUCTION

Both ethanol and 2-butanone produced from a gas to liquid process, such as the Fischer-Tropsch reaction [1], cannot be separated by distillation because of the closeness of their boiling points. Owing to their pristine physical properties, extractive distillation [2], azeotropic distillation [3], and extraction [4] in the presence of an extracting agent have been proposed. While organic solvents, such as, 2,2-dimethyl butane, have been used as an extracting agent, they are volatile, flammable, and harmful. Accordingly, there is strong need to replace them.

Ionic liquids have been applied as extracting agent in azeotropic distillation [2,5,6] and extraction [7-10] because they are less volatile and have low flammability and high thermal stability. However, there is a huge barrier to overcome in applying ionic liquids to the separation process because the synthesis process is complicated and strong concerns regarding the environment and human health have been raised [11]. In efforts to replace the ionic liquids, deep eutectic solvents (DESs) have been utilized in many areas, including extraction [4,12,13]. DESs are known to be far more easily synthesized than ionic liquids and are also inexpensive and environmentally benign [14]. DESs and ionic liquids have many common features, including tunability by varying their constituents. In the case of DESs, their synthesis may be adjusted by simply changing the hydrogen bond donor (HBD) or hydrogen bond acceptor (HBA) or the mole ratio of HBD to HBA.

While 2-butanone has HBA only, ethanol has both HBD and HBA, which allows ethanol to associate. In this study, choline chloride based DESs were applied because they have both HBD and HBA, which may allow them to selectively dissolve ethanol. The choice of DESs was made by using the COSMO-RS package. The DESs synthesized in this study included glutaric acid/choline chloride with a molar ratio of 1 : 1 (Gl1C1), ethylene glycol/glutaric acid/choline chloride with a molar ratio of 1 : 1 : 1 (E1Gl1C1), and ethylene glycol/xylitol/choline chloride with a molar ratio of 1 : 2 : 1 (E1X2C1). The DES xylitol/choline chloride with a molar ratio of 2 : 1 (X2C1) was not chosen due to its high viscosity. Based on a naked eye inspection, the viscosity of X2C1 was as high as that of honey at room temperature and atmospheric pressure. The viscosity of E1Gl1C1 was rendered much lower than that of Gl1C1 by adding ethylene glycol as a thinner. The presence of ethylene glycol led to a decrease of viscosity, consistent with an earlier report [15].

In this study, the liquid-liquid equilibria (LLE) of a ternary system of ethanol, 2-butanone, and choline chloride based DESs were performed at 323.2 K and 0.1 MPa. The LLE of the ternary system were also evaluated at 303.2 K to investigate the influence of temperature on ethanol separation. The experimental LLE data were correlated using a non-random two-liquid (NRTL) model.

Table 1. Chemicals* used in this study

Compound	Purity (wt%)	Analysis method	Viscosity (mPa·s)
Ethanol	≥99.50%	GC	-
2-Butanone	≥99.0%	GC	-
Xylitol	≥99%	GC	1.449[a]
Glutaric acid	≥98.5%	GC	18.530[b]
Choline chloride	≥98%	GC	-
Ethylene glycol	≥99.75%	GC	2.58[c]
DMSO-d6	99.9 atom %D		-
D_2O	99.9 atom %D		-

*All chemicals were purchased from Sigma-Aldrich Inc.
[a]Ref. [22] at 293.15 K and m=1.002 (mol/kg of water).
[b]Ref. [23] at 373 K.
[c]Ref. [24] at 298 K and 42.28 wt% in aqueous solution.

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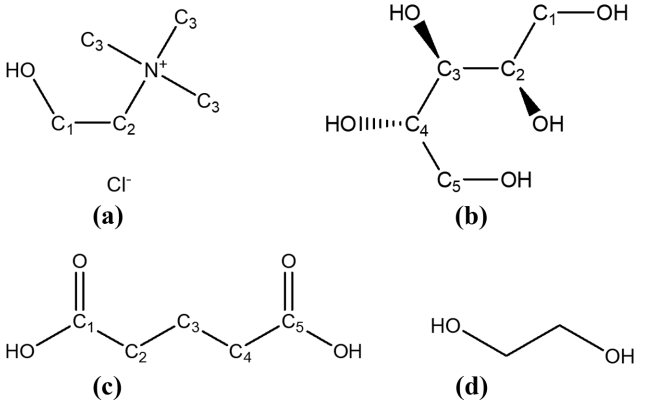


(a) (b) (c) (d)

Fig. 1. Chemical structures of (a) choline chloride, (b) xylitol, (c) glutaric acid, (d) ethylene glycol.

EXPERIMENTAL SECTION

1. Chemicals and DESs Preparation

As shown in Table 1 and Fig. 1, ethanol, 2-butanone, xylitol, glutaric acid, choline chloride, ethylene glycol, dimethyl sulfoxide-d6 (DMSO-d6), and deuterium oxide (D_2O) were purchased from Sigma-Aldrich and used as received. A glove box (Model J-924A) from JISICO Ind. (Seoul, S. Korea) was used to ensure the absence of moisture in handling DESs because the DESs used in this study are hygroscopic. DESs were synthesized by using HBD and HBA in a 500 mL round flask at 353 K. All DES synthesized were analyzed using a ^1H NMR (AVANCE III, 400 MHz, Bruker) spectrometer. A Karl-Fischer titrator (Model V20, Mettler Toledo Inc.) was used to determine water content in DESs, which was analyzed to be less than 0.15 wt%.

2. Selection of Choline Chloride Based DES

As done by several researchers [16,17], we treated DES as an electroneutral mixture [18] and generated the sigma profile using the ADF modeling suite 2017 package [19] to determine which DESs would perform better for ethanol extraction. Fig. 2 shows the sigma profiles of ethanol, 2-butanone and the three DESs chosen for this study. There are three regions divided by two vertical lines at $\sigma = \pm 0.0084$ e/Å^2. The HBD region and HBA region are located $\sigma < -0.0084$ e/Å^2 and $\sigma > +0.0084$ e/Å^2, respectively. While the sigma profile of ethanol appears in both the HBD and HBA regions, that of 2-butanone appears in the HBA region only. All three DESs selected in this study have a broad sigma profile range in the HBD, which may allow for these DESs to serve as an ethanol extractant.

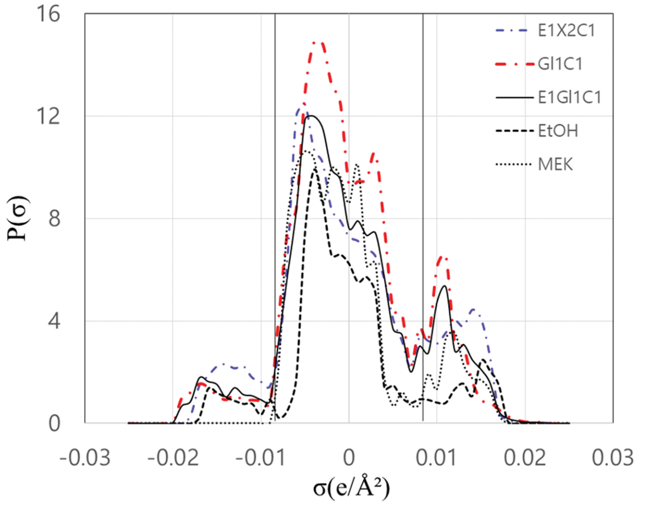


Fig. 2. The sigma profile of DESs selected for this study ethanol and 2-butanone.

3. Experimental Method

A known amount (~15 g) of DES was measured using an analytical balance (Shimadzu ATX 224, Japan) with an accuracy of $\pm 1\times 10^{-4}$ g in a 50 cm^3 round flask containing ethanol and 2-butatnone to prepare several mixtures. They were added into a temperature controlled glass vessel under vigorous mixing for several hours and held for a few hours to obtain equilibrium. A ^1H NMR (JNM-LAMDA, 300 MHz, Jeol, Inc.) spectrometer was used to quantitative analyze each compound in both phases at least three times, as we did earlier [8,13].

The LLE data were experimentally measured at 303.2 and 323.2 K using the tie-line method [9]. The methyl peak in ethanol appearing at 1.0-1.2 was used to determine the amount of ethanol in each phase. Similarly, the methyl peak on beta carbon in 2-butanone in both the raffinate and extract phases appearing at 0.8-0.95 ppm was used to perform a quantitative analysis. When E1X2C1 was used in the LLE experiment, four protons at C1 and C5 in Fig. 1(b) and two protons at C1 in Fig. 1(a) appearing at 4.4 and 3.5 ppm, respectively, were used to perform a quantitative analysis. When both Gl1C1 and E1Gl1C1 were used as an extracting agent, two protons on C3 in Fig. 1(c) and nine protons on C3 in Fig. 1(a) appearing at 1.6 and 3.2 ppm, respectively, were used to measure the amount of DESs in each phase.

RESULTS AND DISCUSSION

1. Experimental LLE Data

Before carrying out ternary LLE experiments, we performed binary LLE experiments to investigate the mutual solubility between 2-butanone and DESs and that of ethanol and DESs. Table 2 shows that the LLE experimental data of the two binary systems were obtained at two temperatures, 303.2 and 323.2 K. Ethanol is completely miscible with the DESs used in this study but 2-butanone is not. This result shows that ethanol has stronger affinity for the DESs than 2-butanone. Interestingly, no DES was detected in the 2-butanone-rich phase from the NMR analytical results. In the case of E1X2C1, a solid phase was observed with both ethanol and 2-butanone, which resulted in failing to obtain binary LLE data.

The LLE experimental data of the three ternary systems were measured at 0.1 MPa and two temperatures, 303.2, and 323.2 K. The distribution coefficient (D_i) for each component i and the selectivity (S) for ethanol were calculated using Eqs. (1) and (2), respectively, to determine the capability of DESs for ethanol separation from a mixture containing 2-butanone.

$$D_i = \frac{w_i^{II}}{w_i^{I}} \tag{1}$$

Table 2. LLE data for the systems 2-butanone(1)-Gl1C1 (2) and 2-butanone(1)-E1Gl1C1(2)

T (K)	2-butanone (1) - Gl1C1 (2)	
	DES-rich phase	
	x_1^{II}	x_2^{II}
303.2 K	0.234	0.766
	0.250	0.750
	0.255	0.745
	0.253	0.747
	0.256	0.744
	0.239	0.761
323.2 K	0.272	0.728
	0.255	0.745
	0.248	0.752
	0.259	0.741
	0.256	0.744
	0.244	0.756
T (K)	2-Butanone (1) - E1Gl1C1 (2)	
	DES-rich phase	
	x_1^{II}	x_2^{II}
303.2 K	0.384	0.616
	0.353	0.647
	0.360	0.640
	0.354	0.646
	0.323	0.677
	0.318	0.682
323.2 K	0.382	0.618
	0.379	0.621
	0.373	0.627
	0.369	0.631
	0.288	0.712
	0.334	0.666

The standard uncertainty is $u(x_i^{II})=0.02$.

Table 3. LLE data, distribution coefficient of ethanol (D_1), and selectivity (S) for the systems ethanol (1) - 2-butanone (2) - DES (3) at 303.2 and 323.2 K at atmospheric pressure

Ethanol (1) - 2-butanone (2) - E1X2C1 (3) at 323.2 K					
Raffinate phase		Extract phase			
w_1^I	w_2^I	w_1^{II}	w_2^{II}	D_1	S
0.4712	0.5137	0.2772	0.0615	0.59	4.91
0.6351	0.3511	0.4719	0.0586	0.74	4.45
0.5794	0.3968	0.3953	0.0654	0.68	4.14
0.5532	0.4028	0.3777	0.068	0.68	4.04
0.6469	0.2868	0.4949	0.0763	0.77	2.88
0.6678	0.2853	0.5244	0.0788	0.79	2.84

Table 3. Continued

Ethanol (1) - 2-butanone (2) - E1Gl1C1 (3) at 323.2 K					
Raffinate phase		Extract phase			
w_1^I	w_2^I	w_1^{II}	w_2^{II}	D_1	S
0.0325	0.9644	0.0352	0.174	1.08	6.00
0.0310	0.9665	0.0301	0.1645	0.97	5.70
0.0702	0.9195	0.0803	0.1934	1.14	5.44
0.0330	0.9647	0.0276	0.1789	0.84	4.51
0.0811	0.9012	0.0902	0.2356	1.11	4.25
0.1316	0.8331	0.1418	0.2560	1.08	3.51
0.1454	0.8012	0.1510	0.2746	1.04	3.03
0.0147	0.9830	0.0048	0.1515	0.33	2.12
Ethanol (1) - 2-butanone (2) - E1Gl1C1 (3) at 303.2 K					
Raffinate phase		Extract phase			
w_1^I	w_2^I	w_1^{II}	w_2^{II}	D_1	S
0.0306	0.9636	0.0412	0.2091	1.35	6.20
0.0323	0.9641	0.037	0.1789	1.15	6.17
0.0281	0.9691	0.0334	0.1912	1.19	6.02
0.0608	0.9284	0.0766	0.2347	1.26	4.98
0.1413	0.8131	0.1586	0.3063	1.12	2.98
0.1830	0.7206	0.1894	0.3784	1.03	1.97
Ethanol (1) - 2-butanone (2) - Gl1C1 (3) at 323.2 K					
Raffinate phase		Extract phase			
w_1^I	w_2^I	w_1^{II}	w_2^{II}	D_1	S
0.0311	0.9689	0.0393	0.1794	1.26	6.82
0.0069	0.9931	0.0066	0.1407	0.96	6.75
0.0571	0.9372	0.0684	0.2041	1.20	5.50
0.0584	0.9363	0.0662	0.1945	1.13	5.46
0.0642	0.9245	0.0739	0.1965	1.15	5.42
0.0053	0.9947	0.0036	0.1322	0.68	5.11
0.0986	0.9014	0.0996	0.1906	1.01	4.78
0.1115	0.8885	0.1046	0.1826	0.94	4.56
0.1667	0.7932	0.1535	0.1985	0.92	3.68
Ethanol (1) - 2-butanone (2) - Gl1C1 (3) at 303.2 K					
Raffinate phase		Extract phase			
w_1^I	w_2^I	w_1^{II}	w_2^{II}	D_1	S
0.0052	0.9948	0.0043	0.1276	0.83	6.45
0.0080	0.9920	0.0061	0.1299	0.76	5.82
0.0592	0.9340	0.0615	0.1828	1.04	5.31
0.0712	0.9194	0.0698	0.1989	0.98	4.53
0.1225	0.8472	0.1073	0.1899	0.88	3.91
0.1718	0.7871	0.1685	0.2284	0.98	3.38

The standard uncertainties are $u(w_i^I)=0.009$ and $u(w_i^{II})=0.02$.

$$S=\frac{D_1}{D_2} \tag{2}$$

where w_i^I and w_i^{II} are the weight fraction of each component *i* in the raffinate phase (I) and that in the extract phase (II), respectively, and the subscripts 1 and 2 refer to ethanol and 2-butanone, respectively.

Table 3 shows the experimentally obtained weight fractions of each phase in the ternary system of ethanol (1), 2-butanone (2), and DES (3). In the case of E1X2C1, the LLE data at 303.2 K were not repeatedly and reliably obtained, partly because solid liquid

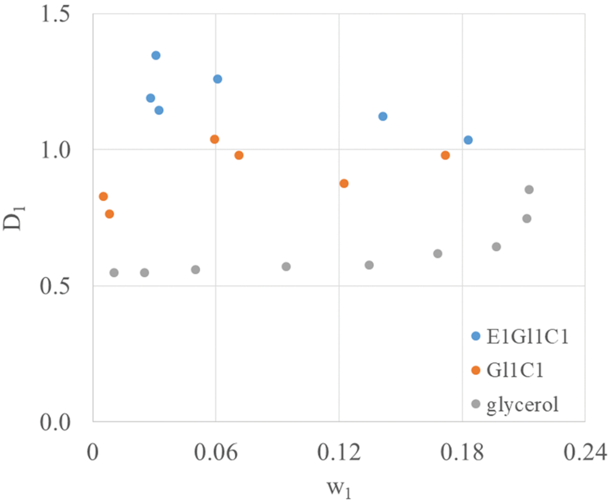


Fig. 3. Distribution coefficient of ethanol (D_1) as a function of ethanol weight fraction (w_1) in the raffinate phase in a ternary system of ethanol (1)+2-butanone (2)+extractant (3) at 303.2 K.

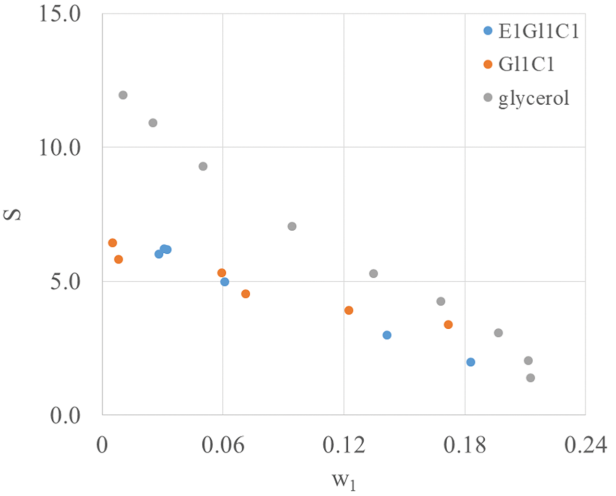


Fig. 4. Selectivity (S) as a function of ethanol weight fraction (w_1) in the raffinate phase in a ternary system of ethanol (1)+2-butanone (2)+extractant (3) at 303.2 K.

equilibria were also observed. As shown in Fig. 3, the values of D_1 remained at about 1.0 in the whole range of the ethanol weight fraction in the raffinate phase at 303.2 K in the presence of DESs used in this study. These values were higher than the value of D_1 in the presence of glycerol [20].

As can be seen in Fig. 4, the effect of the DESs used in this study on the selectivity values was significant. The values of selectivity are inversely proportional to the ethanol weight fraction in the raffinate phase. While the effect of the usage of ethylene glycol on the values of D_1 appears to be significant, as shown in Fig. 3, the effect on the values of selectivity was insignificant, as seen in in Fig. 4. Specifically, the values of D_1 in the presence of E1Gl1C1 and Gl1C1 at a w_1 of 0.06 were 1.20 and 1.04, respectively. The values of S in the presence of E1Gl1C1 and Gl1C1 at a w_1 of 0.06 were 5.50 and 5.31, respectively. However, the effect of temperature on both the distribution coefficient and selectivity is insignificant because the values of D_1 and S were unchanged in a range of ethanol weight fraction from 0 to 0.2 in the raffinate phase at both 303.2 and 323.2 K in the presence of the DESs used in this study.

Table 4. Comparison of ethanol distribution coefficient (D_1) and selectivity (S) for the ethanol (1) in the presence of different solvents at 0.1 MkPa

Solvent	T (K)	D_1	S	Refs.
Glycerol	283.15	0.714-0.865	1.7-15.8	20
	293.15	0.707-0.839	2.0-13.6	
	303.15	0.686-0.906	1.4-12.0	
G4C1[a]	298.15	0.556-.0.811	5.997-22.147	4
G2C1[b]	298.15	0.538-0.765	5.658-21.952	
G4T1[c]	298.15	0.546-0.701	4.827-17.526	
G2T1[d]	298.15	0.587-0.727	5.376-15.802	
E1X2Ch1[e]	323.2	0.59-0.79	2.84-4.91	
E1Gl1C1[f]	303.2	1.03-1.35	1.97-6.20	This study
	323.2	0.33-1.14	2.12-6.00	
G11C1[g]	303.2	0.83-1.04	3.38-6.45	
	323.2	0.68-1.26	3.68-6.82	

*Mole fraction of toluene in the raffinate phase.

[a] Mole ratio between glycerol (G) and choline chloride (C) is 4 : 1.

[b] Mole ratio between glycerol (G) and choline chloride (C) is 2 : 1.

[c] Mole ratio between glycerol (G) and tetramethylammonium chloride (T) is 4 : 1.

[d] Mole ratio between glycerol (G) and tetramethylammonium chloride (T) is 2 : 1.

[e] Mole ratio between ethylene glycol (E), xylitol (X), and choline chloride (C) is 1 : 2 : 1.

[f] Mole ratio between ethylene glycol (E), glutaric acid (Gl) and choline chloride (C) is 1 : 1 : 1.

[g] Mole ratio between glutaric acid (G1), and choline chloride (C) is 1 : 1.

Table 4 summarizes the values of D_1 and S in the presence of glycerol and various DESs. By adding either choline chloride or tetramethylammonium chloride as an HBA to form various DESs, the values of selectivity were enhanced significantly. For example, the values of S with G2C1 (two moles of glycerol and one mole of choline chloride) and with pure glycerol were about 22 and 12, respectively. This result may be explained by the reduction of the viscosity by the formation of a DES [4]. While no significant increase of the values of S was observed in the presence of the DESs used in this study, the values of D_1 with the DES used in this study were higher than those with either the pure glycerol or glycerol based DES. This may also be explained by the decrease of viscosity due to the formation of DES. In addition, this suggests that the usage of choline chloride based DES in ethanol separation from a mixture containing 2-butanone would be more economically favorable than other extracting agents, such as, glycerol.

2. Data Correlation

The liquid-liquid equilibria for a ternary system is defined by Eq. (3):

$$x_i^I \gamma_i^I = x_i^{II} \gamma_i^{II} \qquad (3)$$

where γ_i is the activity coefficient of each component in the ternary system. The NRTL equation [21] was used to correlate the experimentally measured LLE data. The activity coefficient for each component in the ternary system for the NRTL model is given by Eq. (4).

$$\ln\gamma_i = \frac{\sum_{j=1}^{n} x_j\tau_{ji}G_{ji}}{\sum_{k=1}^{n} G_{ki}x_k} + \sum_{j=1}^{n}\frac{x_jG_{ij}}{\sum_{k=1}^{n} G_{kj}x_k}\left(\tau_{ij} - \frac{\sum_{m=1}^{n} x_m\tau_{mj}G_{mj}}{\sum_{k=1}^{n} G_{kj}x_k}\right) \tag{4}$$

where,

$$G_{ij} = \exp(-\alpha_{ij}\tau_{ij}) \tag{5}$$

$$\tau_{ij} = \frac{g_{ij} - g_{jj}}{RT} \tag{6}$$

In this study α was set to 0.2. The binary interaction parameters for the NRTL correlation were carried out by minimizing the objective function (O.F.) defined in Eq. (7) using the SOLVER tool in Microsoft Excel 2013.

$$\mathrm{O.F.} = \min\sum_{i=1}^{c}\sum_{j=1}^{t}\sum_{k=1}^{p}[(x_{ij}^{exp} - x_{ij}^{cal})^2]^k \tag{7}$$

where i, j, k, c, t, p, exp, and cal are the each component, tie-line, phase, number of chemical components, number of tie-lines, number of phases, and experimental and calculated equilibrium data, respectively. The root mean square deviation (RMSD) was defined to test the accuracy of the correlation and is defined in Eq. (8).

$$\mathrm{RMSD} = \sqrt{\frac{\sum_{i=1}^{c}\sum_{j=1}^{t}[(x_{ij}^{I,\,exp} - x_{ij}^{I,\,cal})^2 + (x_{ij}^{II,\,exp} - x_{ij}^{II,\,cal})^2]}{6t}} \tag{8}$$

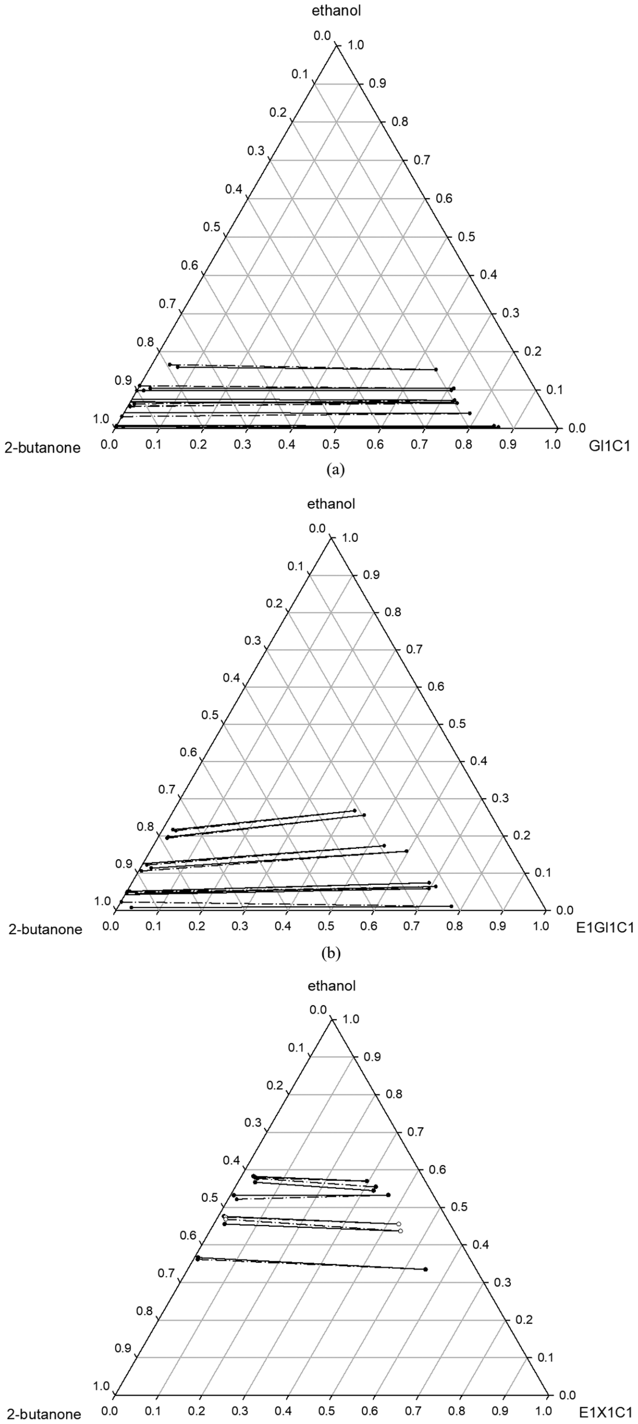
Table 5 shows that the RMSD values are reasonably small, confirming that a good experimental correlation with NRTL was obtained. Fig. 5 shows both the experimentally obtained and correlated LLE data.

CONCLUSIONS

Ternary liquid-liquid equilibrium data for ethanol (1), 2-butanone (2) and DESs (3) were experimentally determined at 303.2 and 0.1 MPa. The values of the distribution coefficient of ethanol with the DESs used in this study were higher than those with pure glycerol or glycerol based DESs as a solvent. Additional ternary data

Table 5. NRTL binary interaction parameters and RMSD for ethanol (1), 2-butanone (2), and DES (3) system at 323.2 K

i-j	Δg_{ij} (J/mol)	Δg_{ji} (J/mol)	α	RMSD
		Ethanol (1)+2-butanone (2)+E1Gl1C1 (3)		
1-2	147.1	5,737.0	0.2	0.00392
1-3	5,683.0	1,296.0		
2-3	11,442.3	207.3		
		Ethanol (1)+2-butanone (2)+E1X2C1 (3)		
1-2	3,938.1	2,367.4	0.2	0.00117
1-3	6,817.9	232,214.7		
2-3	29,011.1	495,165.0		
		Ethanol (1)+2-butanone (2)+Gl1C1 (3)		
1-2	41,399.7	71.9	0.2	0.00219
1-3	1,593.1	1,089.0		
2-3	8,656.8	48,778.8		



(a)

(b)

(c)

Fig. 5. (a) Tie-lines of the ethanol (1)+2-butanone (2)+Gl1C1 (3) at 323.2 K. (b) Tie-lines of the ethanol (1)+2-butanone (2)+E1Gl1C1 (3) at 323.2 K. (c) Tie-lines of the ethanol (1)+2-butanone (2)+E1X2C1 (3) at 323.2 K. Solid line: experimental tie lines; dash-dot line: correlated tie lines.

for ethanol, 2-butanone, and DESs were determined at 323.2 K and 0.1 MPa to investigate the effect of temperature. While the values of D_1 in the presence of the DESs applied in this study were higher than those in the presence of pure glycerol or glycerol based DESs, the values of selectivity with the DESs were lower than those with glycerol. Although there is still not a clear explanation for why the usage of DESs results in higher values of D_1 and lower values of S, it is suggested that the DESs employed in this study may allow an economically feasible process due to higher values of D_1 in ethanol separation from a mixture containing 2-butanone at moderate temperature because viscosity appeared to be an additional process variable in the extraction process. Moreover, ethylene glycol could be added to serve as a thinner to reduce the viscosity in the DES application process. The experimentally obtained LLE data were well correlated with the NRTL model.

ACKNOWLEDGEMENTS

This work was supported by 2019 Hongik University Research Fund.

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