Liquid–liquid equlibria of the system dimethyl carbonate + methanol + water at different temperatures

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Abstract

In this work, experimental liquid–liquid equilibria (LLE) data of the dimethyl carbonate + methanol + water system are presented. The LLE of this system has been measured from 283 to 333 K. On the other hand, LLE and LVE of the binary system dimethyl carbonate + water have been measured. The equilibrium data presented are correlated using NRTL and UNIQUAC equations. The reliability of these models is tested by comparison with experimental results. Finally, the VLE for the system DMC + water at 101.3 kPa was predicted using the UNIQUAC model, with the adjusted parameters obtained from the LLE data. This prediction was successful when is compared with the experimental VLE data.
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1. Introduction

In the past decade, the number of papers and patents related to dimethyl carbonate (DMC) have increased considerably, as it is an environmentally benign and biodegradable chemical with the LD50 value close to ethyl/butyl acetates [1], and it is able to substitute phosgene as a carbonylation intermediate for manufacturing polycarbonate and isocyanate [2,3]. The most intriguing market opportunities of DMC are as gasoline additive [1], and painting solvent [4]. Recently, methyl *tert*-buthyl ether (MTBE), a widely used gasoline additive for octane and oxygen enhancement, was found polluting the groundwater and being not biodegradable [5], as a result, the research activity related to DMC has increased greatly.

DMC can be prepared, for example, by reacting carbon monoxide, methanol and an acid by using copper chloride; by trans-esterifying a cyclic carbonate, such as ethylene/propylene carbonate, with methanol in the presence of a catalyst, and by vapour phase reaction of carbon monoxide and nitrite in the presence of a catalyst [1].

However, in any of these methods, dimethyl carbonate is obtained as a mixture of DMC, methanol and water so the separation of these components is indispensable for purifying dimethyl carbonate [1]. Dimethyl carbonate and methanol form an azeotropic mixture at a composition ratio of 30:70 (weight ratio), and thus it is difficult to separate the mixture by distillation at atmospheric pressure.

It has been reported that DMC and water form another azeotropic mixture [1], but experimental data for this system are not been reported in literature till present. Finally, to the best of our knowledge, also no experimental data for the ternary system (DMC + methanol + water) are available in literature.

Many investigations have been carried out on the method to separate DMC from the mixture of both DMC and methanol, and various proposals have been made, including a method to obtain a crystalline product enriched in dimethyl carbonate by cooling [6], a method of separation of the mixture by distillation by breaking the azeotrope with pressurization [7], a method of separation by distillation by adding a hydrocarbon [8], a method of using extraction and distillation with water [9] or organic solvents [10,11], and a method of pervaporation using crosslinked chitosan membranes [12,13].

Unfortunately, the study of the viability of some of these techniques is limited by the lack of data on the thermodynamic behavior of systems containing DMC, water and methanol.

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Examination of the literature shows that the binary system DMC + methanol has been widely studied. ENIChem has a German patent showing that the percentage methanol in the binary DMC + methanol azeotrope increases with pressure [14]. The thermodynamic properties of the binary methanol + dimethyl carbonate under atmosphere pressure have been reported, as well as the variation of the azeotrope temperature with pressure [7,15]. Yunhai et al. measured the isothermal VLE of DMC + methanol at elevated pressure [16]. Other authors measured VLE of this binary system at atmospheric pressure [17–20].

This work tries to solve the lack of information in the literature on the ternary system DMC + methanol + water. The LLE for this system have been measured from 283 to 333 K. On the other hand, LLE and LVE for the binary system dimethyl carbonate + water have been measured. The equilibrium data presented are correlated using the NRTL and UNIQUAC equations. Finally, the reliability of these models is tested by comparison with experimental results.

2. Experimental section

2.1. Chemicals

Water from NANO-pure (Wasserlab) was used. Methanol (Aldrich) and dimethyl carbonate (Aldrich) had the normal purities of >99.9 and >99 mass%, respectively. Prior to the measurements, chemical purities were checked by gas chromatography. The purities, densities and refractive indices of all chemicals used in this study are presented in Table 1.

2.2. Equilibrium measurements

LLE measurements were made at six temperatures for the ternary system. Equilibrium data were obtained by preparing mixtures of known overall composition by mass, followed by stirring at least an hour and setting for at least 24 h at constant temperature. The accuracy of the temperature measurements was ±0.1 K. Liquid mixtures were prepared in test tubes, which were filled almost completely. At the end of the setting period, samples were taken from both phases and analyzed by gas chromatography (HP 6890 Series chromatograph equipped with a TCD and an HP3395 integrator). Good separation of the three components was obtained on a 2 m × 1 m/8 in. column packed with Porapack
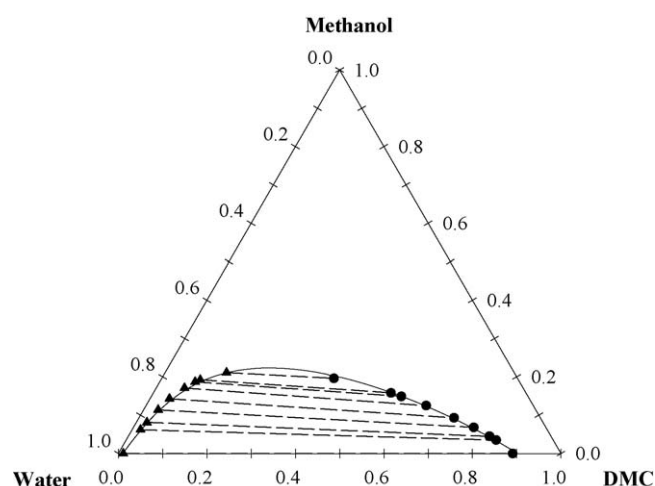

Fig. 1. LLE of DMC (1) + methanol (2) + water (3) at 283.15 K. Experimental data: (▲) organic phase; (●) aqueous phase. Calculated data using the UNIQUAC model (with the parameters of Table 4): (—) binodal curve and (- - -) tie-lines.

Q-S 80/100. The accuracy for the mole fraction measurements was ±0.001.

The results of the concentrations of the three components of both conjugate phases, and the data of the initial composition mixture were used to check the mass balance [26]. For the LLE of the binary system [DMC + water] the same experimental procedure was used.

Also some VLE data of the DMC + water system has been determined in order to compare the experimental VLE behaviour with that simulated by CHEMCAD v5.2, using the selected model parameters obtained from binary LLE data. The experimental VLE method has been reported in a previous work [27].

3. Results and discussion

3.1. Experimental data

The liquid–liquid equilibrium (LLE) data of the ternary system DMC (1) + methanol (2) + water (3) at 283.15, 293.15, 303.15, 313.15, 323.15 and 333.15 K and atmospheric pressure together with the selectivity are presented in Table 2. All concentrations are expressed in mole fractions. As an example, in Figs. 1 and 2 have been plotted the experimental data at 283.15

Table 1
Purity (%), densities ρ, refractive indexes n_D, and UNIQUAC structural parameters of the pure components

Compound	Purity (%)	ρ (298.15 K) (kg m^{-3})		n_D (298.15 K)		UNIQUAC parameters	
		Experimental	Lit.	Experimental	Lit.	r_i[a]	q_i[a]
DMC	>99.9	1063.33	1063.50[b]	1.3672	1.3670[c]	3.0613	2.8160
Methanol	>99	786.49	786.47[d]	1.3262	1.3265[c]	1.4311	1.4320
Water	Nano-pure	997.06	997.05[e]	1.3325	1.3325[e]	0.9200	1.3990

[a] DECHEMA [23].
[b] Garcia et al. [21].
[c] DIPPR [22].
[d] TRC [24].
[e] Riddick et al. [25].

Table 2
Liquid–liquid equilibrium data and selectivity of the system DMC (1) + methanol (2) + water (3)

T (K)	Organic phase		Aqueous phase		Selectivity (S)
	x_1	x_2	x_1	x_2	
	0.891	0.000	0.011	0.000	
	0.836	0.035	0.019	0.062	77.48
	0.816	0.045	0.024	0.081	61.94
	0.769	0.068	0.033	0.114	39.37
283.15	0.712	0.093	0.044	0.143	24.66
	0.633	0.125	0.064	0.171	13.58
	0.565	0.149	0.080	0.187	8.89
	0.537	0.158	0.089	0.192	7.36
	0.874	0.000	0.011	0.000	
	0.775	0.052	0.030	0.078	38.56
	0.734	0.069	0.037	0.099	28.77
	0.677	0.093	0.050	0.125	18.21
293.15	0.634	0.109	0.059	0.137	13.54
	0.566	0.132	0.076	0.155	8.74
	0.472	0.158	0.103	0.172	4.99
	0.422	0.168	0.121	0.179	3.70
	0.849	0.000	0.012	0.000	
	0.759	0.046	0.031	0.061	32.61
	0.723	0.061	0.039	0.080	24.02
	0.684	0.077	0.049	0.097	17.55
303.15	0.627	0.097	0.060	0.116	12.43
	0.543	0.126	0.084	0.140	7.22
	0.503	0.136	0.094	0.147	5.73
	0.433	0.150	0.116	0.157	3.89
	0.825	0.000	0.014	0.000	
	0.769	0.029	0.026	0.032	32.91
	0.737	0.047	0.032	0.055	26.67
313.15	0.700	0.058	0.042	0.067	19.29
	0.649	0.078	0.055	0.090	13.49
	0.579	0.100	0.069	0.107	9.04
	0.508	0.120	0.089	0.124	5.90
	0.800	0.000	0.014	0.000	
	0.763	0.017	0.022	0.013	27.28
	0.723	0.034	0.030	0.034	24.56
	0.705	0.043	0.035	0.044	20.48
323.15	0.653	0.062	0.046	0.065	14.89
	0.618	0.074	0.055	0.078	11.79
	0.572	0.089	0.069	0.091	8.45
	0.532	0.102	0.086	0.100	6.08
	0.483	0.118	0.089	0.114	5.27
	0.770	0.000	0.017	0.000	
	0.746	0.018	0.024	0.013	23.23
	0.713	0.032	0.030	0.028	20.70
333.15	0.652	0.056	0.047	0.054	13.28
	0.602	0.077	0.066	0.073	8.73
	0.546	0.090	0.083	0.084	6.14
	0.482	0.101	0.094	0.095	4.86

and 333.15 K respectively, together with the tie-lines and binodal curve calculated using UNIQUAC model. The plots for the other temperatures are very similar, with a slightly change in the tie-line slopes.

Two-phase regions were observed at all temperatures investigated. As can be observed in Fig. 3, the size of the two-phase region decreases with an increase in temperature but the effect is small. The system exhibits type I liquid–liquid phase behaviour, having one pair of partially miscible components

(DMC + water) and two pairs of completely miscible components (DMC + methanol and methanol + water), in the temperature range investigated.

The reliability of experimental results (tie-lines) can be ascertained by applying the Othmer–Tobias correlation [28]:

$$\left[\frac{1-w_1}{w_1}\right]_{\text{organic phase}} = a\left[\frac{1-w_3}{w_3}\right]^{b}_{\text{aqueous phase}} \tag{1}$$
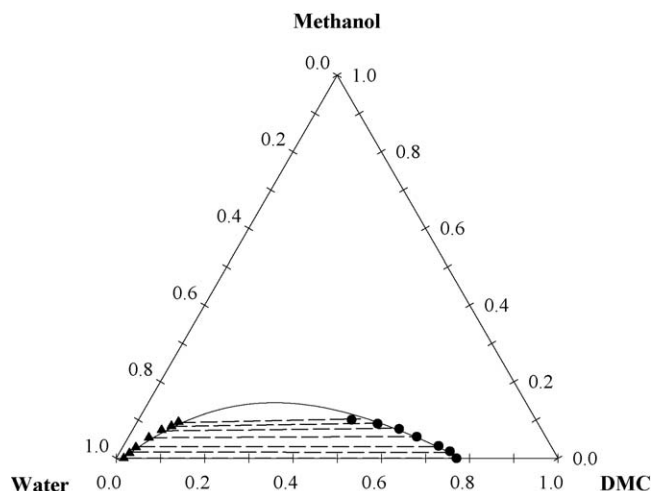
Fig. 2. LLE of DMC (1) + methanol (2) + water (3) at 333.15 K. Experimental data: (▲) organic phase; (●) aqueous phase. Calculated data using the UNIQUAC model (with the parameters of Table 4): (—) binodal curve and (- - -) tie-lines.

where w_1 is the mass fraction of DMC; w_3 the mass fraction of water and a and b are constants in Eq. (1). Fig. 4 shows the plot on logarithmic scale of $[(1 - w_1)/w_1]_{\text{organic phase}}$ against $[(1 - w_3)/w_3]_{\text{aqueous phase}}$ at all temperatures for the system under study. The linearity of these plots indicates the degree of consistency of related data. The parameters of this correlation are given in Table 3.

3.2. Data correlation

The UNIQUAC [29] and NRTL [30] models were used to correlate the experimental data for the ternary system discussed here. In fitting the UNIQUAC interaction parameters, the structural parameters, (r_i and q_i) recommended by DECHEMA [23] were used for the pure components and are listed in Table 1. The non-randomness parameter (α_{ij}) of the NRTL model was set to
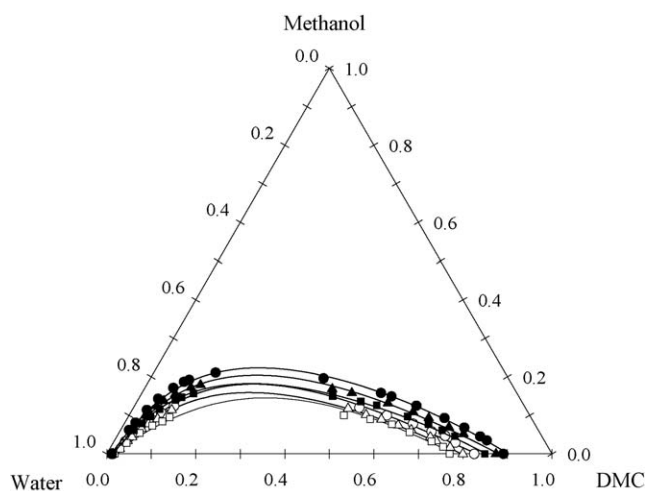

Fig. 3. LLE of DMC (1) + methanol (2) + water (3) at all temperatures. Experimental values: (●) 283.15 K; (▲) 293.15 K; (■) 303.15 K; (○) 313.15 K; (△) 323.15 K; (□) 333.15 K. (—) Binodal curves calculated using the UNIQUAC model (with the parameters of Table 4).
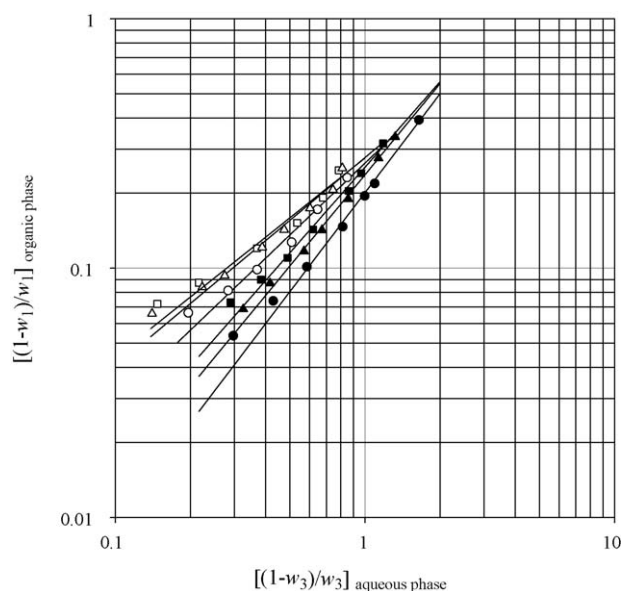

Fig. 4. Othmer–Tobias plot of DMC (1) + methanol (2) + water (3) at all temperatures. Experimental data: (●) 283.15 K; (▲) 293.15 K; (■) 303.15 K; (○) 313.15 K; (△) 323.15 K; (□) 333.15 K. Curve fit: solid lines.

0.1, 0.2, and 0.3 and the results given in Tables 4 and 5 are the best.

There are two effective binary interaction parameters for a pair of substances. Therefore, six effective binary interaction parameters are required for a ternary system. The corresponding sets of binary interaction parameters were determined by minimizing the differences between the experimental and calculated mole fractions for each of the components over all the tie-lines. The objective function (OF) used is

$$\text{OF} = \sum_{k=1}^{M} \sum_{j=1}^{2} \sum_{i=1}^{3} (x_{ijk} - \hat{x}_{ijk})^2 \tag{2}$$

where M is the number of tie-lines, x indicates the experimental mole fraction, $\hat{x}$ the calculated mole fraction, and subscripts i, j and k denote, respectively, component, phase and tie-line.

Two different kinds of correlations were made. First the correlation of experimental data was carried out separately at each temperature. The parameters (A_{ij}) calculated in this way are given in Table 4. Also included in this table is the root-mean-

Table 3
Parameters of Othmer–Tobias correlation for the system DMC (1) + methanol (2) + water (3)

T (K)	a	b	R^2
283.15	0.2008	1.3188	0.9986
293.15	0.2370	1.2156	0.9994
303.15	0.2539	1.1408	0.9985
313.15	0.2637	0.9575	0.9976
323.15	0.2777	0.8368	0.9961
333.15	0.2764	0.7968	0.9937

Table 4
UNIQUAC and NRTL binary interaction parameters for the system DMC (1) + methanol (2) + water (3)

T (K)	ij	UNIQUAC parameters		RMSD (%)	NRTL parameters			RMSD (%)
		A_{12} (J mol^{-1})	A_{21} (J mol^{-1})		α	A_{12} (J mol^{-1})	A_{21} (J mol^{-1})	
283.15	1–2	3360.95	−1633.94		0.2	2114.19	−1563.69	
	1–3	3499.66	959.24	0.45	0.2	1921.54	9828.95	0.73
	2–3	562.87	−4006.06		0.3	9453.14	−6864.12	
293.15	1–2	2122.54	−2074.77		0.2	3719.03	−1629.21	
	1–3	3179.75	1063.15	0.32	0.2	1599.44	9816.65	0.70
	2–3	−1232.05	−3771.39		0.3	8193.84	−5996.10	
303.15	1–2	4872.51	−2041.86		0.2	5491.66	−1427.00	
	1–3	3159.65	951.49	0.39	0.2	1148.47	10206.84	0.71
	2–3	−832.13	−2436.42		0.3	1475.97	−5474.28	
313.05	1–2	6021.87	−1372.43		0.2	4164.60	−1625.96	
	1–3	3459.64	596.70	0.47	0.2	989.41	10333.14	0.54
	2–3	4055.67	−3916.96		0.3	10099.09	−6578.77	
323.15	1–2	3853.53	−1828.58		0.2	7125.19	−1382.35	
	1–3	3181.93	705.48	0.29	0.2	535.61	10889.20	0.71
	2–3	529.25	−3916.92		0.3	7615.74	−4643.01	
333.15	1–2	−2698.06	1914.79		0.2	7387.01	−1508.81	
	1–3	2941.44	895.89	0.50	0.2	509.17	10369.55	0.89
	2–3	−3351.41	1728.94		0.3	9067.85	−4197.19	

square deviation (RMSD) in the phase composition:

$$\mathrm{rmsd} = 100 \times \left(\sum_{k=1}^{M} \sum_{j=1}^{2} \sum_{i=1}^{3} \frac{(x_{ijk} - \hat{x}_{ijk})^2}{6M} \right)^{1/2} \tag{3}$$

The RMSD is a measure of the agreement between the experimental and calculated data. In Table 4, it can be observed that the UNIQUAC model provides a slightly better correlation of the experimental tie-lines than NRTL based on RMSD values and although a good fit is obtained for all temperatures, the parameters determined for each temperature have no relation between them. So, a simultaneous correlation of all the experimental LLE data of this system was carried out in order to obtain a unique set of parameters valid for the range of temperatures studied. Table 5 lists the optimized UNIQUAC and NRTL interaction parameters (A_{ij}) obtained in a simultaneous correlation of all data assuming temperature independent parameters. As was expected, the RMSD values were higher than when the individual correlation at each temperature was made. In any case, the overall magnitude of RMSD values suggests that the NRTL and UNIQUAC models provide an adequate representation of the phase behavior of the ternary system DMC (1) + methanol (2) + water (3) at all temperatures.

3.3. Selectivity

The effectiveness of a solvent can be expressed by the selectivity S. In fact, the effectiveness of methanol extraction by water is given by its selectivity, which is an indication of the ability of water to separate methanol from DMC, and is given by

$$S = \frac{(x_2/x_1)_{\mathrm{aqueous\ phase}}}{(x_2/x_1)_{\mathrm{organic\ phase}}} \tag{4}$$

where the subscript 1 represents DMC and 2 represents methanol. As shown in Table 2, the selectivity values are greater than 1 (these values vary between 3 and 77) for the system reported here, which means that extraction of methanol by water is possible. The selectivity values are not constant over whole two-phase region; they decreased as the concentration of methanol increased; therefore the higher the concentration of methanol in the feed the lower the selectivity of water. The extracting power of the solvent (water) at each temperature is shown in Fig. 5 and it can be observed that the higher the temperature, the lower the selectivity. Similar behaviour was also correctly predicted using the UNIQUAC model as shown in the same figure. In Fig. 6, a good agreement between the experimental and calculated selectivity values is shown. In fact, the mean
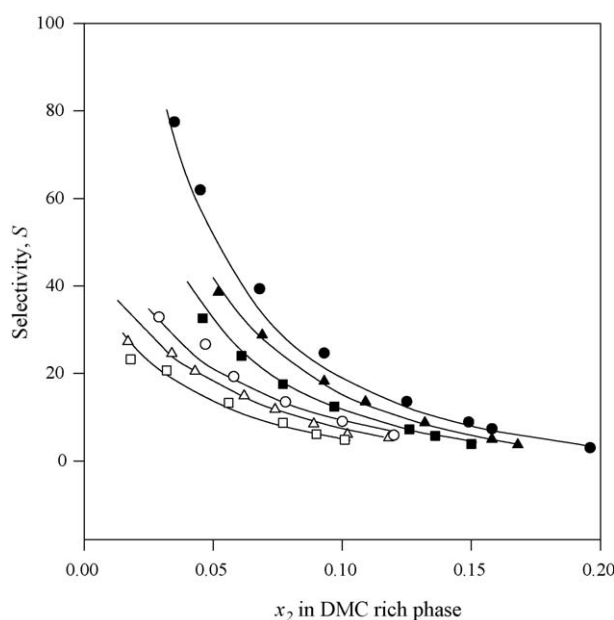
Table 5
Optimized temperature independent binary interaction parameters for the system DMC (1) + methanol (2) + water (3) fitted to all isotherms

ij	UNIQUAC parameters		RMSD (%)	NRTL parameters			RMSD (%)
	A_{ij} (J mol^{-1})	A_{ji} (J mol^{-1})		α	A_{ij} (J mol^{-1})	A_{ji} (J mol^{-1})	
1–2	1937.29	−1008.46		0.2	278.85	−1064.16	
1–3	3420.77	478.75	1.79	0.2	1360.58	8366.16	2.04
2–3	2782.80	−3772.64		0.3	10711.04	−5142.28	

Fig. 5. Effect of temperature on measured and calculated selectivity *S*, for DMC (1) + methanol (2) + water (3). Experimental data: (●) 283.15 K; (▲) 293.15 K; (■) 303.15 K; (○) 313.15 K; (△) 323.15 K; (□) 333.15 K. Predicted by UNIQUAC (with the parameters of Table 4): solid lines.

absolute deviation (MAD) between experimental and calculated selectivity was 1.64.

3.4. Prediction of vapor–liquid equilibria

In this paper, an attempt was made to examine the capability for predicting the isobaric VLE of the partially miscible system [DMC (1) + water (3)] using the parameters determined from the LLE data. Tables 6 and 7 show the experimental LLE and VLE

Table 6
Liquid–liquid equilibria for the system DMC (1) + water (3) at 101.3 kPa

T (K)	Organic phase (x_1)	Aqueous phase (x_1)
278.15	0.898	0.012
283.15	0.891	0.011
288.15	0.882	0.011
293.15	0.874	0.011
303.15	0.849	0.012
313.15	0.825	0.014
323.15	0.800	0.014
333.15	0.770	0.017

Table 7
Vapor–liquid equilibria for the system DMC (1) + water (3) at 101.3 kPa

T (K)	Liquid phase (x_1)	Vapor phase (y_1)
351.53[a]	0.559[a]	0.559[a]
352.39	0.814	0.576
356.31	0.905	0.751
359.13	0.943	0.856
364.85	0.004	0.281

[a] Azeotrope.

data corresponding to this binary system. The predicted VLE data, using the interaction parameters (pair 1–3) obtained by correlation with the UNIQUAC model, are compared with the experimental values in Fig. 7. As can be observed the UNIQUAC model is capable of reproducing the VLE of this system, and the agreement between experimental and predicted VLE and LLE values is very good.
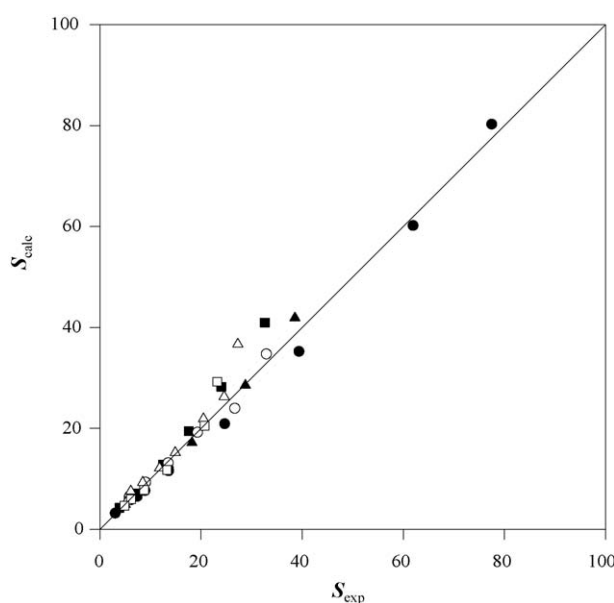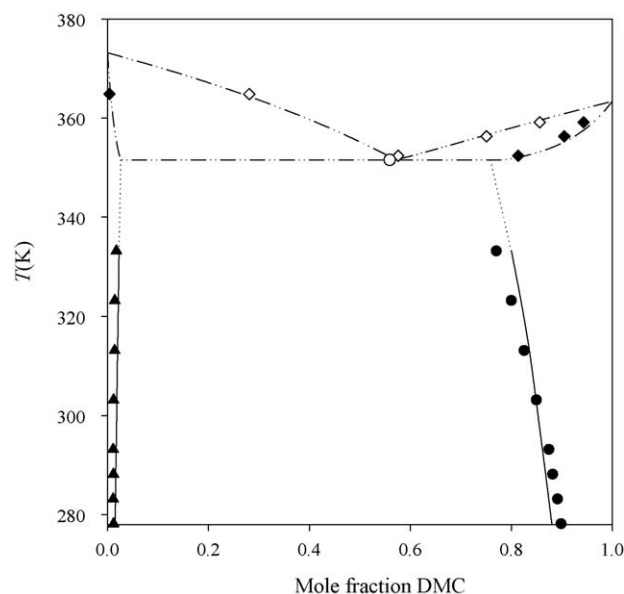

Fig. 7. VLE and LLE experimental and predicted results for DMC (1) + water (3). (a) Experimental LLE data: (▲) organic phase; (●) aqueous phase; (—) calculated by UNIQUAC; (······) extrapolate line. (b) Experimental VLE data: (◆) liquid phase; (◇) vapor phase; (▬··▬··) predicted by UNIQUAC. (○) Experimental azeotrope.

Fig. 6. Measured and calculated selectivity *S*, for DMC (1) + methanol (2) + water (3): (●) 283.15 K; (▲) 293.15 K; (■) 303.15 K; (○) 313.15 K; (△) 323.15 K; (□) 333.15 K.

4. Conclusions

Liquid-liquid equilibrium of the DMC + methanol + water system has been measured at different temperatures. The LLE data were correlated using the NRTL and UNIQUAC activity coefficient models. The correlation with the UNIQUAC equation gives better results than the NRTL equation and fits the experimental data satisfactorily. The simultaneous correlation of the six isothermal data sets gives a unique set of parameters in the range of the temperature considered. Finally, the VLE for the system DMC + water at 101.3 kPa was predicted using the UNIQUAC model, with the adjusted parameters obtained from the LLE data. This prediction was successful when is compared with some experimental VLE data.

List of symbols

a, b	constants of Othmer–Tobias correlation
A	interaction parameters
M	number of tie-lines
q	area parameter in UNIQUAC equation
r	volume parameter in UNIQUAC equation
R	correlation coefficient
RMSD	root mean square deviation
w	composition of liquid phase, mass fraction
x	composition of liquid phase, mole fraction
y	composition of vapor phase, mole fraction

Greek letter

α	non-randomness factor in NRTL equation

Superscript

ˆ	calculated

Subscripts

i	component i
j	component j
k	component k

Acknowledgments

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