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Excess Molar Volumes at 298.15 K and Isothermal Vapor−Liquid Equilibria at 333.15 K for the Binary Mixtures of Dimethyl Carbonate with Benzene, Toluene, *n*-Heptane, and Isooctane

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Excess molar volumes (V^E) of dimethyl carbonate (DMC) + benzene, DMC + toluene, DMC + *n*-heptane, and DMC + isooctane are obtained from the measured densities at 298.15 K by using a digital vibrating-tube densimeter. All the measured excess molar volumes are correlated with the five-parameter Redlich−Kister polynomial. Isothermal vapor−liquid equilibrium (VLE) data are measured for the binary systems of benzene + DMC, DMC + toluene, DMC + *n*-heptane, and DMC + isooctane at 333.15 K by a using headspace gas chromatography (HSGC) method. The experimental binary VLE data were correlated with common g^E model equations.

Introduction

In the chemical engineering, separation processes are the essential to obtain the final and higher value-added product. These separation processes often rely on knowledge of the vapor−liquid equilibria (VLE) of the mixtures. Dimethyl carbonate (DMC) is an environmentally benign and biodegradable chemical. DMC is mainly produced by the oxidative carbonylation of methanol over a CuCl catalyst. The current worldwide production capacity of DMC is much less than the demand because it is a versatile reagent and solvent and is nontoxic to humans and the environment, as indicated by its toxicological and ecotoxicological properties.[1] DMC is a strong contender to assist the refining industry meeting the Clean Air Act specifications for oxygen in gasoline. DMC has about 3 times the oxygen content as methyl *tert*-butyl ether (MTBE). It does not phase separate in a water stream as some alcohols do, and it has both low toxicity and relatively quick biodegradablity.[2,3]

In this work, excess molar volumes (V^E) are measured for the binary systems of DMC (1) + benzene (2), DMC (1) + toluene (2), DMC (1) + *n*-heptane (2), and DMC (1) + isooctane (2) at 298.15 K. Isothermal VLE are reported of the benzene (1) + DMC (2) system and the other systems at 333.15 K. The measured excess molar volumes were correlated by the Redlich−Kister polynomial, and the experimental VLE data were correlated with the g^E model equations; Margules, van Laar, Wilson, NRTL, and UNIQUAC.

Experimental Section

Materials. DMC and benzene were obtained from Aldrich Chemical Co., and the others were supplied by Merck Co. All the chemicals had a purity of better than $w = 99.8$ %, and these values were verified with gas chromatography. The reagents were used without further purification. The measured densities of all chemicals, literature values, and Antoine constants are listed in Table 1.

Apparatus and Procedure. Densities of the pure components and each binary mixture were determined with an Anton Paar digital vibrating-tube densimeter (DMA 5000) at 298.15 K with an uncertainty of $\pm 1 \times 10^{-5}$ g·cm^{-3}. Bidistilled water and dry air were used for the calibration of the densimeter.

Table 1. Measured Densities at 298.15 K and Antoine Constants of Pure Components

	density/g·cm^{-3}		Antoine constants[a,b]		
chemicals	present study	lit. value[a]	*A*	*B*	*C*
DMC	1.06319	1.06328	6.15885	1253.59	211.600
benzene	0.87356	0.8737	6.00477	1196.76	219.161
toluene	0.86250	0.8623	6.07577	1342.31	219.187
n-heptane	0.68052	0.6795	6.01876	1264.37	216.640
isooctane	0.68804	0.6878	6.12151	1339.49	229.033

[a] Data from Dortmund Data Bank.[8] [b] $\log_{10} P_i^{\mathrm{sat}}/\mathrm{kPa} = A - [B/(t(°\mathrm{C}) + C)]$.

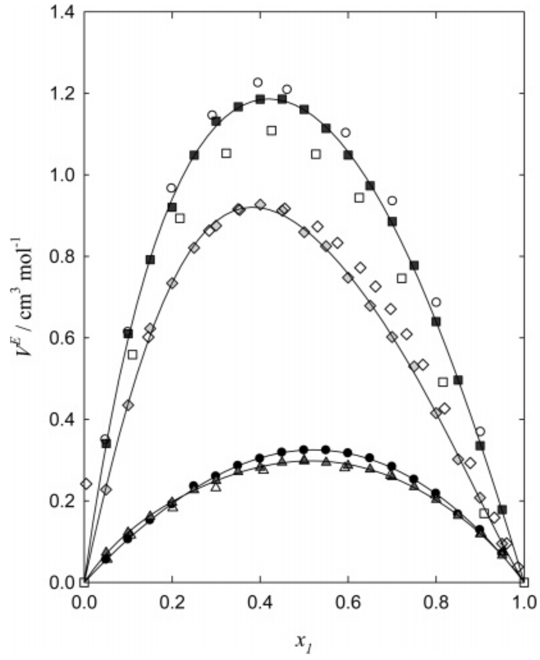

Figure 1. Excess molar volumes for the ●, DMC + benzene; ▲, DMC + toluene; ■, DMC + *n*-heptane; and ◆, DMC + isooctane at 298.15 K. △, DMC + toluene taken from ref 11; □ and ○, DMC + *n*-heptane taken from refs 12 and 13; ◇, DMC + isooctane taken from ref 14. Solid lines, calculated values from Redlich−Kister polynomial.

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Table 2. Measured Densities and Excess Molar Volumes of DMC (1) + Benzene (2), DMC (1) + Toluene (2), DMC (1) + *n*-Heptane (2), and DMC (1) + Isooctane (2) at 298.15 K

x_1	ρ_m/g·cm^{-3}	V^E/cm^3·mol^{-1}	x_1	ρ_m/g·cm^{-3}	V^E/cm^3·mol^{-1}	x_1	ρ_m/g·cm^{-3}	V^E/cm^3·mol^{-1}
				DMC (1) + Benzene (2)				
0.0000	0.87356	0.0000	0.3498	0.93453	0.2859	0.7001	1.00084	0.2836
0.0499	0.88200	0.0553	0.4000	0.94370	0.3033	0.7501	1.01088	0.2520
0.1000	0.89057	0.1055	0.4500	0.95289	0.3182	0.8001	1.02101	0.2177
0.1500	0.89918	0.1521	0.5001	0.96225	0.3240	0.8498	1.03136	0.1670
0.2001	0.90793	0.1917	0.5500	0.97169	0.3241	0.8999	1.04169	0.1284
0.2499	0.91661	0.2357	0.6000	0.98128	0.3167	0.9501	1.05235	0.0706
0.3000	0.92559	0.2596	0.6499	0.99096	0.3044	1.0000	1.06319	0.0000
				DMC (1) + Toluene (2)				
0.0000	0.86250	0.0000	0.3498	0.91998	0.2716	0.7000	0.98994	0.2589
0.0498	0.86990	0.0735	0.4000	0.92922	0.2823	0.7499	1.00114	0.2346
0.0998	0.87768	0.1229	0.4498	0.93857	0.2947	0.8001	1.01277	0.2035
0.1500	0.88575	0.1621	0.4999	0.94826	0.3001	0.8501	1.02473	0.1639
0.1999	0.89396	0.1962	0.5499	0.95827	0.2945	0.8998	1.03703	0.1188
0.2498	0.90239	0.2268	0.5999	0.96851	0.2867	0.9502	1.04989	0.0665
0.2999	0.91110	0.2497	0.6500	0.97906	0.2775	1.0000	1.06319	0.0000
				DMC (1) + *n*-Heptane (2)				
0.0000	0.68052	0.0000	0.3501	0.76395	1.1669	0.7001	0.89223	0.8854
0.0501	0.69016	0.3410	0.4000	0.77905	1.1854	0.7500	0.91572	0.7779
0.0999	0.70047	0.6102	0.4499	0.79507	1.1858	0.8000	0.94109	0.6401
0.1500	0.71170	0.7919	0.5001	0.81218	1.1605	0.8501	0.96830	0.4963
0.1998	0.72365	0.9204	0.5498	0.83025	1.1140	0.9001	0.99761	0.3356
0.2501	0.73628	1.0481	0.6000	0.84967	1.0485	0.9501	1.02909	0.1788
0.2999	0.74959	1.1318	0.6499	0.87023	0.9730	1.0000	1.06319	0.0000
				DMC (1) + Isooctane (2)				
0.0000	0.68804	0.0000	0.3498	0.76375	0.9159	0.7000	0.88702	0.6021
0.0497	0.69681	0.2280	0.4004	0.77796	0.9268	0.7500	0.91031	0.5300
0.1000	0.70622	0.4351	0.4498	0.79289	0.9125	0.8000	0.93594	0.4154
0.1500	0.71612	0.6231	0.5002	0.80929	0.8592	0.8499	0.96369	0.3020
0.2001	0.72695	0.7341	0.5499	0.82646	0.8247	0.8999	0.99377	0.2079
0.2499	0.73838	0.8209	0.5998	0.84520	0.7478	0.9498	1.02679	0.0955
0.2998	0.75067	0.8753	0.6502	0.86543	0.6788	1.0000	1.06319	0.0000

Table 3. Fitted Redlich−Kister Parameters and Standard Deviations for Excess Molar Volomes of DMC (1) + Benzene (2), DMC (1) + Toluene (2), DMC (1) + *n*-Heptane (2), and DMC (1) + Isooctane (2) at 298.15 K

	A_1	A_2	A_3	A_4	A_5	σ_{st}/cm^3·mol^{-1}
DMC (1) + benzene (2)	1.2988	0.1166	−0.0368	0.0192	0.0644	0.0033
DMC (1) + toluene (2)	1.1924	0.0721	0.0521	−0.1426	0.3069	0.0021
DMC (1) + *n*-heptane (2)	4.6380	−1.3053	0.7477	−0.7334	0.2619	0.0085
DMC (1) + isooctane (2)	3.4681	−1.6932	0.6212	0.0841	−0.7258	0.0096

Binary isothermal VLE data have been measured by using headspace gas chromatography (HSGC). The HSGC system consists of a commercial gas chromatography (Agilent 6890N) and a headspace sampler (HP19395A), which has an electro-pneumatic sampling system and a precision thermostat, having an uncertainty of in temperature of ± 0.1 K. The HP-FFAP (Hewlett-Packard, poly(ethylene glycol)−TPA modified (50 m × 0.2 mm × 0.3 μm) capillary column fitted with a thermal conductivity detector was used for the analysis. All the sample mixtures (of volume about 3 cm^3) were prepared directly in a 10 cm^3 glass vial, which was the equilibrium cell, using a digital microbalance (AND Co. HA-202M) with an uncertainty of ± 1 × 10^{-5} g. With the HSGC method, the equilibrated vapor phase is automatically analyzed with a electro-pneumatic sampling system, while the liquid-phase compositions were calculated from the thermodynamic relations, and the mass balance was calculated from the feed compositions. According to the HSGC method used in this work, total pressure is not measured but calculated using the chromatogram peak area along with thermodynamic relations. The detailed procedure of the calculation method is described in our previous work.[4−7]

Results and Discussion

The pure component properties, stored in the DDB,[8] were used to calculate the true liquid compositions with the SRK equation.[9] Vapor pressures of the pure component at $T = 333.15$ K were calculated from the Antoine equation. The used Antoine constants are listed also in Table 1.

The excess molar volumes for the binary mixtures were calculated from the measured densities of the pure substance and mixtures using

$$V^E/\text{cm}^3\cdot\text{mol}^{-1} = \frac{(x_1M_1 + x_2M_2)}{\rho_m} - \left(\frac{x_1M_1}{\rho_1} + \frac{x_2M_2}{\rho_2}\right) \qquad (1)$$

where x_i, M_i, ρ_i, and ρ_m are the mole fraction, molar mass, and pure component density of the i component and mixture density, respectively. The experimental densities and excess molar volumes at 298.15 K for the binary systems of DMC (1) + benzene (2), DMC (1) + toluene (2), DMC (1) + *n*-heptane-(2), and DMC (1) + isooctane (2) are listed in Table 2 and shown in Figure 1. All the measured excess molar volumes showed positive deviations from the ideal behavior. DMC (1) + benzene (2) and DMC (1) + toluene (2) binaries showed nearly symmetric figures while excess molar volumes of DMC (1) + *n*-heptane (2) and DMC (1) + isooctane (2) systems inclined to the DMC-poor region. The maximum deviation of excess molar volume of DMC (1) + benzene (2) was bigger than that of DMC (1) + toluene (2), which was 0.3241 cm^3·mol^{-1} and 0.3001 cm^3·mol^{-1}, respectively. This deviation

Table 4. Isothermal VLE for Binary Systems of Benzene (1) + DMC (2), DMC (1) + Toluene (2), DMC (1) + *n*-Heptane (2), and DMC (1) + Isooctane at 333.15 K

P(cal)/kPa	x_1	y_1	γ_1	γ_2	P(cal)/kPa	x_1	y_1	γ_1	γ_2	P(cal)/kPa	x_1	y_1	γ_1	γ_2
Benzene (1) + DMC (2)														
35.41	0.0169	0.0282	1.1340	1.0018	42.56	0.3498	0.4800	1.1180	0.9737	49.24	0.7499	0.8104	1.0191	1.0684
35.60	0.0338	0.0449	0.9052	1.0072	43.35	0.3997	0.5186	1.0771	0.9952	49.76	0.7999	0.8415	1.0025	1.1280
35.99	0.0498	0.0785	1.0859	0.9990	44.71	0.4497	0.5798	1.1040	0.9774	50.51	0.8500	0.8864	1.0088	1.0947
36.59	0.0999	0.1204	0.8445	1.0235	45.28	0.4996	0.6049	1.0500	1.0233	51.11	0.9000	0.9216	1.0024	1.1478
37.49	0.1499	0.2126	1.0188	0.9940	45.98	0.5499	0.6425	1.0289	1.0455	51.65	0.9501	0.9604	0.9999	1.1757
38.69	0.1999	0.2882	1.0684	0.9853	46.83	0.5996	0.6871	1.0276	1.0477	51.84	0.9659	0.9734	1.0004	1.1601
40.07	0.2497	0.3641	1.1191	0.9719	47.44	0.6499	0.7218	1.0091	1.0790	52.03	0.9831	0.9866	1.0001	1.1768
41.36	0.2998	0.4267	1.1275	0.9694	48.55	0.6999	0.7790	1.0350	1.0234					
DMC (1) + Toluene (2)														
19.24	0.0170	0.0530	1.7150	1.0006	27.76	0.3496	0.5381	1.2227	1.0641	33.52	0.7499	0.8201	1.0492	1.3014
19.87	0.0343	0.0979	1.6246	1.0020	28.86	0.3996	0.5887	1.2169	1.0669	34.00	0.8000	0.8517	1.0361	1.3606
20.38	0.0501	0.1328	1.5470	1.0041	29.74	0.4497	0.6276	1.1880	1.0862	34.33	0.8500	0.8801	1.0175	1.4814
21.91	0.1000	0.2322	1.4563	1.0086	30.55	0.4997	0.6633	1.1606	1.1095	34.62	0.9000	0.9149	1.0073	1.5916
23.32	0.1495	0.3150	1.4062	1.0136	31.13	0.5498	0.6907	1.1195	1.1544	34.80	0.9502	0.9550	1.0011	1.6954
24.66	0.1996	0.3866	1.3671	1.0198	31.85	0.5998	0.7263	1.1040	1.1759	34.87	0.9661	0.9703	1.0023	1.6527
25.71	0.2496	0.4403	1.2981	1.0350	32.50	0.6499	0.7586	1.0860	1.2093	34.92	0.9830	0.9840	1.0006	1.7731
26.94	0.2997	0.4994	1.2846	1.0392	32.93	0.6996	0.7828	1.0546	1.2847					
DMC (1) + *n*-Heptane (2)														
30.34	0.0168	0.0895	4.6383	1.0007	46.28	0.3492	0.5296	2.0092	1.1915	46.74	0.7505	0.6370	1.1355	2.4220
32.25	0.0335	0.1566	4.3168	1.0025	46.63	0.3996	0.5411	1.8074	1.2695	46.21	0.8005	0.6582	1.0875	2.8201
33.91	0.0500	0.2094	4.0667	1.0051	47.03	0.4496	0.5580	1.6705	1.3453	45.26	0.8504	0.6875	1.0474	3.3674
37.93	0.0996	0.3222	3.5131	1.0170	47.22	0.4999	0.5693	1.5395	1.4486	43.46	0.9006	0.7381	1.0194	4.0765
40.62	0.1489	0.3895	3.0410	1.0379	47.33	0.5496	0.5810	1.4321	1.5684	40.16	0.9500	0.8308	1.0053	4.8423
42.79	0.1990	0.4415	2.7170	1.0626	47.41	0.5999	0.6058	1.3703	1.6643	38.71	0.9663	0.8745	1.0028	5.1317
44.45	0.2492	0.4812	2.4569	1.0941	47.42	0.6503	0.6177	1.2892	1.8470	37.01	0.9833	0.9288	1.0007	5.6087
45.46	0.2995	0.5066	2.2006	1.1406	47.75	0.7003	0.5922	1.1559	2.3145					
DMC (1) + Isooctane (2)														
30.76	0.0125	0.0800	5.6229	1.0015	45.25	0.3496	0.5102	1.8902	1.1912	45.96	0.7503	0.6428	1.1272	2.2975
32.45	0.0336	0.1392	3.8522	1.0101	45.83	0.3994	0.5317	1.7462	1.2490	45.34	0.8062	0.6671	1.0740	2.7217
33.91	0.0500	0.1887	3.6616	1.0121	46.19	0.4493	0.5484	1.6136	1.3240	44.29	0.8503	0.7024	1.0472	3.0767
37.40	0.0995	0.2942	3.1649	1.0246	46.42	0.4998	0.5634	1.4977	1.4162	42.69	0.9004	0.7507	1.0188	3.7358
40.39	0.1490	0.3749	2.9084	1.0368	46.57	0.6001	0.5923	1.3156	1.6593	39.65	0.9503	0.8418	1.0053	4.4079
41.94	0.1992	0.4151	2.5009	1.0706	46.49	0.6501	0.6085	1.2455	1.8181	38.39	0.9660	0.8816	1.0028	4.6758
43.44	0.2493	0.4563	2.2761	1.0997	46.31	0.7001	0.6236	1.1807	2.0319	36.86	0.9829	0.9324	1.0008	5.0868
44.54	0.2993	0.4874	2.0762	1.1388										

was caused by CH_3 bond in toluene, which makes weak hydrogen bond in the mixture with DMC. The maximum positive deviations of excess molar volumes of DMC (1) + *n*-heptane (2) and DMC (1) + isooctane (2) were 1.1858 $\text{cm}^3\cdot\text{mol}^{-1}$ and 0.9268 $\text{cm}^3\cdot\text{mol}^{-1}$, respectively. The mean radius of gyration of *n*-heptane is 4.267, and that of isooctane is 4.171.[10] It is thought that the small molecule mixed with DMC caused the small positive deviation. In Figure 1, some reference values[11−14] of DMC + toluene, DMC + *n*-heptane, and DMC + isooctane are also plotted with experimental data.

The measured data were correlated with a five-parameter Redlich−Kister polynomial:[15]

$$V^{\text{E}}/\text{cm}^3\cdot\text{mol}^{-1} = x_1x_2\sum_{i=1}^{5} A_i(x_1 - x_2)^{i-1} \tag{2}$$

where, A_i values are the adjustable parameters. The standard deviation of fit (σ_{st}) is defined by

$$\sigma_{\text{st}}/\text{cm}^3\cdot\text{mol}^{-1} = \left[\frac{\sum_i (V^{\text{E}}_{\text{cal}} - V^{\text{E}}_{\text{exp}})_i^2}{N - n}\right]^{1/2} \tag{3}$$

where N is the number of experimental data and n is the number of the fitted parameters.

The fitted parameters of the Redlich−Kister polynomial and standard deviations are listed in Table 3. With a standard deviation of less than 0.1 %, the correlated values are in good agreement with the experimental data. In Figure 1, the solid lines represent the calculated values with the fitted Redlich−Kister polynomial.

Table 4 gives experimental values of calculated total pressures, equilibrium liquid and vapor compositions, and activity coefficients for the binary systems. The total pressures of this

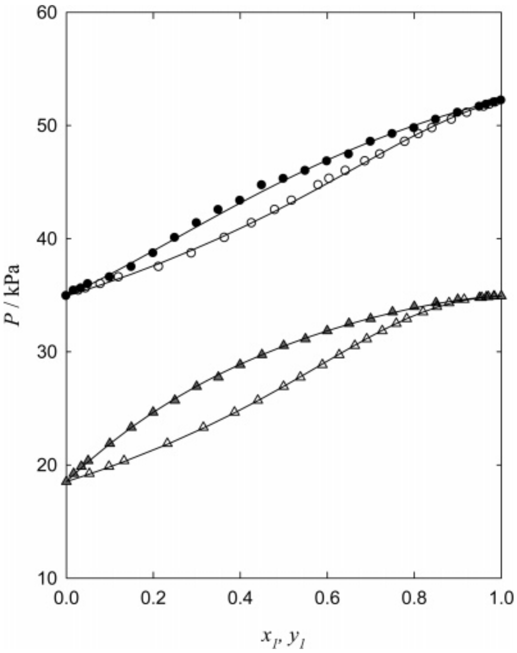

Figure 2. Isothermal VLE for the ●, benzene + DMC; and ▲, DMC + toluene at 333.15 K. Solid lines, correlated values by NRTL equation.

Table 5. g^E Model Parameters and Mean Deviations between the Calculated and Experimental Vapor-Phase Mole Fraction (Δy_1) for the Binary Systems at 333.15 K

model equation	A_{12}	A_{21}	α	$\Delta y_1{}^a$
Benzene (1) + DMC (2)				
Margules	0.0109	0.2249		0.0076
van Laar	0.0727	0.2629		0.0085
Wilson	−1018.6404	3157.1340		0.0085
NRTL	3773.4821	−2390.0506	0.3000	0.0082
UNIQUAC	−920.4507	920.4498		0.0088
DMC (1) + Toluene (2)				
Margules	0.4526	0.5702		0.0031
van Laar	0.4557	0.5797		0.0029
Wilson	743.6415	876.0205		0.0029
NRTL	1882.8962	−272.7719	0.3000	0.0029
UNIQUAC	790.9875	−459.8205		0.0029
DMC (1) + *n*-Heptane (2)				
Margules	1.4862	1.7514		0.0063
van Laar	1.4923	1.7646		0.0059
Wilson	3918.1411	2159.8006		0.0054
NRTL	3478.9245	2204.8273	0.4086	0.0040
UNIQUAC	−19.2680	1568.6058		0.0054
DMC (1) + Isooctane (2)				
Margules	1.4234	1.6220		0.0067
van Laar	1.4268	1.6304		0.0064
Wilson	4131.4235	1408.0842		0.0043
NRTL	3334.0818	2250.6764	0.5593	0.0046
UNIQUAC	−389.1129	1960.6350		0.0060

[a] $\Delta y_1 = |y_{1,\mathrm{exp}} - y_{1,\mathrm{calc}}|/N$; N = number of data.

work are calculated values. Although the total pressure is the calculated value, the calculated total pressure of this HSGC method have been shown good agreement with direct measurement within experimental error.[16] The benzene (1) + dimethyl carbonate (DMC) (2) and DMC (1) + toluene (2) have no azeotropic point while DMC (1) + *n*-heptane (2) and DMC (1) + isooctane (2) binary systems show the minimum boiling azeotrpoes. The azeotropic points were $x_1 = 0.6076$ for the DMC (1) + *n*-heptane (2) system and $x_1 = 0.5891$ for the DMC (1) + isooctane (2) system, which were determined by interpolation from the VLE data. The total pressures at these points are 47.41 kPa and 46.55 kPa, respectively.

The activity coefficients of the experimental binary systems were correlated with the most common g^E models (Margules, van Laar, Wilson, NRTL, and UNIQUAC). These comparisons are listed in Table 5 together with the correlated g^E model parameters. According to the Renon and Prausnitz's result,[17] the non-randomness parameter, α, was fixed at 0.3000 if the adjusted value was not converged between 0.1 and 0.8. So α of the benzene (1) + DMC (2) and DMC (1) + toluene (2) binary systems was fixed at 0.3000. The mean deviation of vapor-phase mole fraction (Δy_1) means

$$\Delta y_1 = |y_{1,\mathrm{exp}} - y_{1,\mathrm{calc}}|/N \tag{4}$$

where N is the number of experimental data. Wilson, NRTL, and UNIQUAC parameters (A_{ij}) for the binary systems are as follows:[18]

$$\text{Wilson:}\quad A_{ij} = (\lambda_{ij} - \lambda_{ii})/\mathrm{J{\cdot}mol^{-1}}$$

$$\text{NRTL:}\quad A_{ij} = (g_{ij} - g_{jj})/\mathrm{J{\cdot}mol^{-1}}$$

$$\text{UNIQUAC:}\quad A_{ij} = (u_{ij} - u_{jj})/\mathrm{J{\cdot}mol^{-1}}$$

The mean deviations between calculated and experimental vapor compositions, Δy_1, are less than 1 mol % for almost all g^E model equations. These small deviations indicate the quality of the measured data indirectly. To check the consistency of the measured VLE, the Redlich−Kister thermodynamic consistency test has been applied, which showed good agreement within ± 1 %. The equilibrium pressure and compositions ($P-x-y$) for each of the binary systems are shown in Figure 2 and Figure 3. The solid lines in Figure 2 and Figure 3 are those calculated by the best correlated equation of NRTL except DMC (1) + isooctane (2) of Wilson equation.

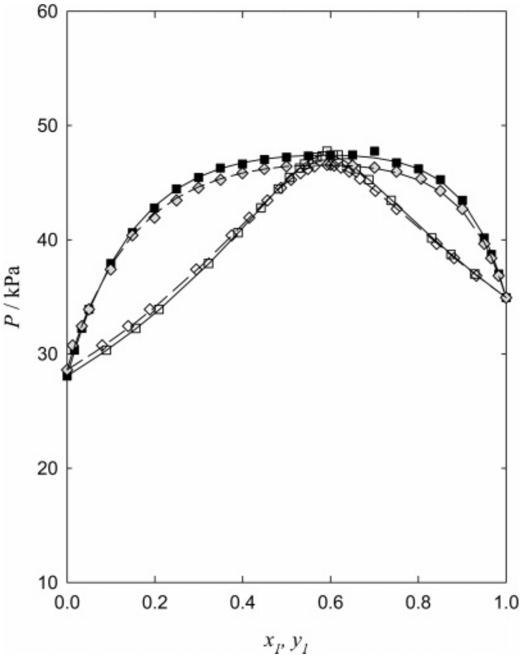

Figure 3. Isothermal VLE for the ■, DMC + *n*-heptane; and ◆, DMC + isooctane at 333.15 K. Solid line, correlated values by NRTL equation. Dashed line, correlated values by Wilson equation.

Conclusions

Excess molar volumes (V^E) were obtained from the measured densities at 298.15 K for DMC + benzene, DMC + toluene, DMC + *n*-heptane, and DMC + isooctane. All the measured V^E values had positive deviations from ideal mixing. Measured V^E values were correlated by the five-parameter Redlich−Kister polynomial, and their deviations between measured and calculated values were less than 1 %. Isothermal VLE data at 333.15 K for benzene + DMC, DMC + toluene, DMC + *n*-heptane, and DMC + isooctane were obtained with the HSGC method. VLE data showed positive deviations from Raoult's law. The binary systems of DMC (1) + *n*-heptane (2) and DMC (1) + isooctane (2) had minimum boiling azeotropes. All the binary systems could be correlated well with common g^E model equations with the deviation of vapor mole fraction of 1 %.

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