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Measurement of the Isobaric Vapor−Liquid Equilibria of Dimethyl Carbonate with Acetone, 2-Butanone, and 2-Pentanone at 101.3 kPa and Density and Speed of Sound at 298.15 K

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Densities and speeds of sound have been measured at $T = 298.15$ K and atmospheric pressure for acetone, 2-butanone, and 2-pentanone + dimethyl carbonate over the whole composition range. Excess molar volumes and deviations in isentropic compressibility were fit to the Redlich−Kister polynomial for the binary systems. Isobaric vapor−liquid equilibrium data for binary systems acetone + dimethyl carbonate, 2-butanone + dimethyl carbonate, and dimethyl carbonate + 2-pentanone have been experimentally determined at 101.3 kPa. The experimental data were correlated with the Wilson, NRTL, and UNIQUAC equations.

Introduction

Dimethyl carbonate is a nonirritating and nontoxic chemical that can be used as a fuel additive. Recent research shows that the performance of the engine is more consistent with dimethyl carbonate addition. At the same time, carbon dioxide and smoke decrease with increasing carbonate addition, and NO_x does not increase with an increase in dimethyl carbonate.[1] As the use of dimethyl carbonate increases, the thermophysical property data will become more important.

This work is a continuation of our systematic research program concerning the study of the VLE of binary mixtures containing dimethyl carbonate.[2−4] This paper reports experimental densities and speeds of sound of binary mixtures of some ketones and dimethyl carbonate at 298.15 K and atmospheric pressure. Of the studied systems, earlier excess molar volumes[5] were found in the literature for comparison.

VLE data are always required for engineering, such as designing a distillation tower, which is the most common operation performed in the chemical industry for the separation of liquid mixtures. The VLE data for the binary systems acetone + dimethyl carbonate, 2-butanone + dimethyl carbonate, and dimethyl carbonate + 2-pentanone have been experimentally determined at 101.3 kPa and have been tested for thermodynamic consistency. The experimental data were correlated with the Wilson,[6] NRTL,[7] and UNIQUAC[8] equations. The interaction parameters and root-mean-square deviations of temperature and vapor-phase composition obtained from the correlation equations were presented. The VLE data for these binary mixtures are not available in the literature.

Experimental Section

Chemicals. The liquids used in this work were obtained from Merck. The materials were Lichrosolv quality. The pure components were degassed ultrasonically, dried over freshly activated molecular sieves (types 3 and 4 Å, supplied by Aldrich) for several weeks before use to reduce the water content, and protected in an inert argon atmosphere. When this treatment was finished, the content of water was determined using a Metrohm 737 KF coulometer because the water quantities were inappreciable. Chromatographic (GLC) tests of the solvents showed purities that fulfilled purchaser specifications. The mass fraction purities were >99.0% for dimethyl carbonate, >99.8% for acetone, and >99.5% for 2-butanone and 2-pentanone. We have compared the measured densities and boiling points with the literature values, and the data are listed in Table 1.

Table 1. Comparison of the Density at 298.15 K and Normal Boiling-Point Temperature of Pure Components with Literature Data

	ρ/g·cm^{-3}		T_{bp}/K	
component	exptl	lit	exptl	lit
dimethyl carbonate	1.06333	1.0632[a]	363.46	363.50[b]
acetone	0.78437	0.7844[c]	329.27	329.25[d]
2-butanone	0.79970	0.79974[e]	352.78	352.72[f]
2-pentanone	0.80139	0.80139[g]	375.36	375.41[h]

[a] Pal et al.[9] [b] García de la Fuente et al.[10] [c] Marino et al.[11] [d] Jiang et al.[12] [e] Comelli and Francesconi.[13] [f] Hiaki et al.[14] [g] Brocos et al.[15] [h] Riddick et al.[16]

Apparatus. The mixtures were prepared by transferring known masses of the pure liquids via syringe into stoppered bottles to prevent preferential evaporation, using a Mettler AX-205 Delta Range balance with a precision of $\pm 10^{-5}$ g. The estimated uncertainty in the mole fraction was ±0.0001.

The density and speed of sound of the pure liquids and mixtures were measured with an Anton Paar DSA-5000 digital vibrating tube densimeter and sound velocity meter. The repeatability and uncertainty in our measured densities and speed of sound were found to be lower than $\pm 2.0 \times 10^{-6}$ and $\pm 10^{-5}$ g·cm^{-3} for the density and ±0.01 and ±0.1 m·s^{-1} for the speed of sound.

A glass Fischer LABODEST VLE apparatus (model 602/D, manufactured by Fischer Labor und Verfahrenstechnik, Germany) was used in the equilibrium determinations. The equilibrium apparatus was a dynamic recirculating still equipped with a Cottrell circulation pump. This pump ensures that both the liquid and vapor phases are in intimate contact during boiling and also in contact with

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Table 2. Density ρ, Excess Molar Volume V^E, Speed of Sound u, Isentropic Compressibility k_S, and Deviation in Isentropic Compressibility $\Delta\kappa_S$ at 298.15 K

x_1	ρ g·cm^{-3}	V^E cm^3·mol^{-1}	u m·s^{-1}	κ_S TPa^{-1}	$\Delta\kappa_S$ TPa^{-1}
Acetone (1) + Dimethyl Carbonate (2)					
0	1.06333	0	1198	655	0
0.0447	1.05264	−0.022	1196	664	−3.9
0.0906	1.04154	−0.044	1195	673	−8.2
0.1886	1.01722	−0.082	1192	692	−17.6
0.2886	0.99168	−0.114	1188	714	−24.1
0.3941	0.96386	−0.137	1184	740	−29.0
0.4933	0.93683	−0.148	1180	766	−31.5
0.5988	0.90717	−0.152	1176	797	−31.5
0.7021	0.87706	−0.134	1172	830	−28.8
0.7974	0.84841	−0.110	1168	863	−22.6
0.9053	0.81488	−0.065	1165	905	−12.7
0.9534	0.79951	−0.035	1163	924	−7.1
1	0.78437	0	1162	945	0
2-Butanone (1) + Dimethyl Carbonate (2)					
0	1.06333	0	1198	655	0
0.0499	1.04931	0.005	1199	663	−3.0
0.0999	1.03529	0.015	1198	673	−4.5
0.1994	1.00779	0.025	1196	694	−6.2
0.2996	0.98050	0.031	1194	715	−7.1
0.3986	0.95388	0.036	1192	737	−7.2
0.5027	0.92630	0.037	1191	761	−7.0
0.6014	0.90051	0.034	1190	784	−6.5
0.7102	0.87249	0.027	1190	809	−5.7
0.8038	0.84869	0.020	1191	831	−4.5
0.9043	0.82348	0.007	1191	856	−2.8
0.9514	0.81175	0.002	1191	868	−1.1
1	0.79970	0	1192	880	0
2-Pentanone (1) + Dimethyl Carbonate (2)					
0	1.06333	0	1198	655	0
0.0498	1.04671	0.023	1199	665	0.4
0.1004	1.03033	0.043	1198	676	1.9
0.1996	0.99949	0.079	1197	698	4.1
0.3009	0.96977	0.098	1198	719	5.6
0.3980	0.94267	0.116	1198	739	6.5
0.5036	0.91475	0.122	1200	760	6.9
0.6017	0.89010	0.121	1201	779	6.9
0.7046	0.86552	0.108	1203	798	6.0
0.8012	0.84359	0.079	1206	815	4.6
0.9010	0.82194	0.042	1209	832	2.5
0.9504	0.81155	0.025	1211	841	1.1
1	0.80139	0	1212	849	0

Table 3. Fitting Parameters and Root-Mean-Square Deviations σ for Binary Mixtures to Correlate the Excess Molar Volumes V^E and the Deviations in Isentropic Compressibility $\Delta\kappa_S$

	B_{11}	B_{12}	B_{21}	σ
Acetone (1) + Dimethyl Carbonate (2)				
V^E/cm^3·mol^{-1}	−0.5957	−0.1224	−0.0541	0.001
$\Delta\kappa_S$/TPa^{-1}	−126.95	−24.72	−0.0885	0.33
2-Butanone (1) + Dimethyl Carbonate (2)				
V^E/cm^3·mol^{-1}	0.1492	−0.0290	−0.0431	0.001
$\Delta\kappa_S$/TPa^{-1}	−27.74	9.821	−18.85	0.25
2-Pentanone (1) + Dimethyl Carbonate (2)				
V^E/cm^3·mol^{-1}	0.4929	0.0246	−0.0090	0.002
$\Delta\kappa_S$/TPa^{-1}	28.35	3.668	−6.153	0.19

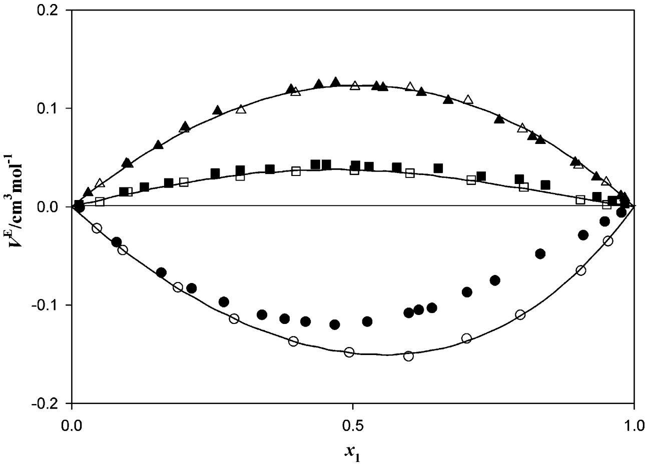

Figure 1. Excess molar volumes, V^E, obtained from eq 3 and comparison with literature data versus mole fraction for the binary mixtures: ○, acetone + dimethyl carbonate; ●, Comelli and Francesconi;[5] □, 2-butanone + dimethyl carbonate; ■, Comelli and Francesconi;[5] △, 2-pentanone + dimethyl carbonate; ▲, Comelli and Francesconi[5] at T = 298.15 K. The solid line corresponds to the Redlich−Kister polynomial.

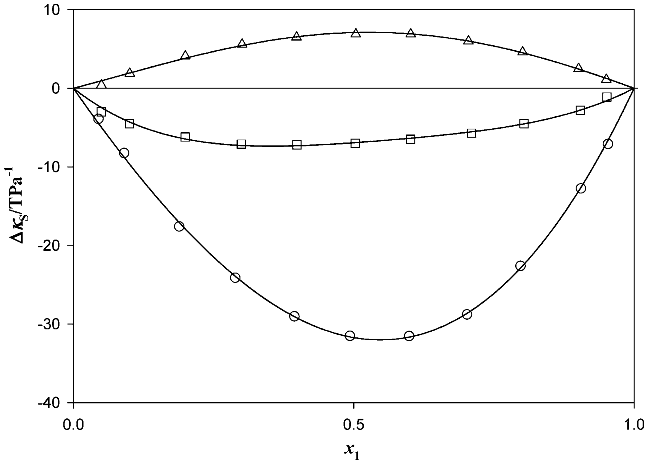

Figure 2. Deviations in isentropic compressibility, $\Delta\kappa_S$, obtained from eq 3 versus mole fraction for the binary mixtures: ○, acetone + dimethyl carbonate; □, 2-butanone + dimethyl carbonate; △, 2-pentanone + dimethyl carbonate at T = 298.15 K. The solid line corresponds to the Redlich−Kister polynomial.

the temperature-sensing element. The equilibrium temperature was measured with a digital Yokogawa model 7563 thermometer with an uncertainty of ±0.01 K. The apparatus is equipped with a glass temperature probe PT 100 with an uncertainty of ±0.01 K. For the pressure measurement, a digital pressure controller (Ruska model 7218) with an uncertainty of ±0.001 kPa, according to the manufacturer, was used. Equilibrium conditions were assumed when constant temperature and pressure were obtained for 30 min or longer. Then, samples of liquid and condensed gas were taken for analysis. The concentration of the liquid and vapor phases at equilibrium were determined on the basis of density−composition curves obtained previously for each of the binary mixtures. The standard deviation in the mole fraction was usually <0.001.

Results and Discussion

The experimental density, speed of sound, excess molar volume, isentropic compressibility (determined by means of the Laplace equation, $\kappa_S = \rho^{-1}u^{-2}$), and deviation in isentropic compressibility of the binary mixtures acetone + dimethyl carbonate, 2-butanone + dimethyl carbonate, and 2-pentanone + dimethyl carbonate at T = 298.15 K are given in Table 2. Excess molar volumes and deviations in isentropic compressibility were calculated from experimental values as follows:

$$V^E = \sum_{i=1}^{N} x_i M_i (\rho^{-1} - \rho_i^{o-1}) \qquad (1)$$

$$\Delta\kappa_S = \kappa_S - \sum_{i=1}^{N} x_i \kappa_{S,i} \qquad (2)$$

Table 4. Vapor−Liquid Equilibrium Data for the Acetone (1) + Dimethyl Carbonate (2) System at 101.3 kPa

T/K	x	y	γ_1	γ_2
360.52	0.0469	0.1270	1.129	0.995
359.88	0.0668	0.1709	1.084	0.985
357.58	0.0989	0.2532	1.150	0.989
355.77	0.1271	0.3185	1.180	0.988
354.45	0.1565	0.3782	1.178	0.975
353.55	0.1802	0.4102	1.136	0.980
352.25	0.2100	0.4556	1.121	0.981
351.25	0.2265	0.4906	1.149	0.970
350.60	0.2438	0.5112	1.132	0.974
349.80	0.2610	0.5370	1.136	0.970
348.82	0.2893	0.5671	1.111	0.976
347.37	0.3288	0.6091	1.093	0.982
346.64	0.3562	0.6402	1.082	0.967
345.10	0.3945	0.6781	1.081	0.972
343.60	0.4309	0.7095	1.080	0.985
342.95	0.4505	0.7276	1.079	0.979
342.13	0.4728	0.7441	1.077	0.988
341.46	0.4957	0.7612	1.071	0.988
340.89	0.5202	0.7793	1.063	0.980
340.32	0.5399	0.7906	1.056	0.991
339.49	0.5834	0.8176	1.035	0.983
338.54	0.6104	0.8335	1.038	0.995
338.21	0.6334	0.8452	1.024	0.995
337.58	0.6589	0.8578	1.018	1.006
336.86	0.6876	0.8710	1.012	1.025
336.65	0.6982	0.8748	1.007	1.038
335.70	0.7238	0.8902	1.017	1.031
335.24	0.7656	0.9035	0.990	1.087
334.51	0.7861	0.9176	1.001	1.047
333.67	0.8225	0.9323	0.997	1.071
332.88	0.8443	0.9422	1.006	1.075
332.06	0.8828	0.9584	1.003	1.062
331.25	0.9176	0.9701	1.002	1.122
330.29	0.9655	0.9879	0.999	1.127

Table 5. Vapor−Liquid Equilibrium Data for the 2-Butanone (1) + Dimethyl Carbonate (2) System at 101.3 kPa

T/K	x	y	γ_1	γ_2
362.62	0.0406	0.0675	1.260	0.996
362.04	0.0712	0.1166	1.260	0.992
361.54	0.1010	0.1576	1.217	0.993
361.06	0.1271	0.1983	1.232	0.988
360.73	0.1518	0.2268	1.190	0.991
360.38	0.1712	0.2585	1.214	0.984
360.02	0.1958	0.2890	1.199	0.984
359.57	0.2199	0.3195	1.195	0.985
359.14	0.2484	0.3486	1.168	0.992
358.62	0.2794	0.3815	1.153	0.999
358.18	0.3094	0.4140	1.144	1.002
357.48	0.3616	0.4647	1.120	1.014
357.12	0.3915	0.4936	1.110	1.019
356.59	0.4366	0.5342	1.094	1.030
356.26	0.4665	0.5577	1.079	1.044
356.14	0.4784	0.5688	1.077	1.046
356.01	0.4910	0.5786	1.071	1.052
355.86	0.5048	0.5917	1.070	1.053
355.72	0.5191	0.6048	1.068	1.054
355.56	0.5357	0.6192	1.064	1.058
355.41	0.5521	0.6357	1.065	1.055
355.04	0.5928	0.6682	1.053	1.070
354.84	0.6169	0.6864	1.046	1.083
354.67	0.6377	0.7053	1.045	1.082
354.44	0.6683	0.7248	1.032	1.113
354.26	0.6935	0.7453	1.028	1.122
353.99	0.7183	0.7694	1.032	1.116
353.79	0.7496	0.7933	1.026	1.133
353.62	0.7791	0.8193	1.024	1.130
353.45	0.8128	0.8448	1.017	1.153
353.30	0.8473	0.8720	1.012	1.172
353.17	0.8821	0.9016	1.009	1.173
352.95	0.9229	0.9322	1.004	1.246
352.84	0.9699	0.9713	0.998	1.358

Table 6. Vapor−Liquid Equilibrium Data for the Dimethyl Carbonate (1) + 2-Pentanone (2) System at 101.3 kPa

T/K	x	y	γ_1	γ_2
375.12	0.0078	0.0194	1.755	0.997
374.04	0.0469	0.0940	1.458	0.989
373.13	0.0874	0.1549	1.322	0.989
372.33	0.1211	0.2014	1.269	0.994
371.56	0.1600	0.2523	1.230	0.996
370.95	0.1954	0.2975	1.208	0.995
370.43	0.2289	0.3363	1.184	0.996
369.98	0.2570	0.3663	1.163	1.000
369.61	0.2861	0.3955	1.140	1.004
369.19	0.3120	0.4243	1.136	1.005
368.69	0.3516	0.4621	1.114	1.012
368.05	0.3925	0.5052	1.111	1.013
367.85	0.4175	0.5233	1.088	1.024
367.52	0.4417	0.5482	1.088	1.023
367.29	0.4671	0.5673	1.072	1.033
367.03	0.4917	0.5873	1.063	1.042
366.71	0.5210	0.6141	1.059	1.044
366.39	0.5539	0.6413	1.050	1.052
366.02	0.5824	0.6727	1.059	1.038
365.86	0.6006	0.6869	1.054	1.043
365.60	0.6280	0.7083	1.047	1.052
365.48	0.6526	0.7245	1.034	1.068
365.33	0.6697	0.7398	1.034	1.066
365.24	0.6850	0.7527	1.031	1.066
365.25	0.6857	0.7523	1.029	1.069
365.02	0.7120	0.7716	1.024	1.084
364.86	0.7343	0.7878	1.018	1.097
364.78	0.7443	0.7953	1.017	1.103
364.65	0.7630	0.8094	1.013	1.112
364.50	0.7858	0.8277	1.011	1.118
364.31	0.8109	0.8485	1.010	1.120
364.08	0.8460	0.8722	1.002	1.169
363.99	0.8613	0.8824	0.999	1.198
363.84	0.8853	0.9033	0.999	1.197
363.67	0.9116	0.9245	0.998	1.219
363.59	0.9308	0.9405	0.997	1.231
363.54	0.9616	0.9667	0.993	1.244

Table 7. Parameters and Root-Mean-Square Deviations between Experimental and Correlated Values for the Binary Systems at 101.3 kPa[a]

equation	parameters						ΔT/K	Δy
Acetone (1) + Dimethyl Carbonate (2)								
Wilson	$\Delta\lambda_{12}$	−1026.9	$\Delta\lambda_{21}$	1929.7			0.34	0.0125
NRTL	Δg_{12}	0.9410	Δg_{21}	297.38	α	−4.37	0.32	0.0132
UNIQUAC	Δu_{12}	1249.4	Δu_{21}	−868.68			0.36	0.0127
2-Butanone (1) + Dimethyl Carbonate (2)								
Wilson	$\Delta\lambda_{12}$	−704.55	$\Delta\lambda_{21}$	1555.75			0.15	0.005
NRTL	Δg_{12}	705.67	Δg_{21}	477.88	α	3.9	0.16	0.005
UNIQUAC	Δu_{12}	595.92	Δu_{21}	−313.14			0.15	0.005
Dimethyl Carbonate (1) + 2-Pentanone (2)								
Wilson	$\Delta\lambda_{12}$	365.98	$\Delta\lambda_{21}$	393.95			0.16	0.0076
NRTL	Δg_{12}	350.00	Δg_{21}	350.00	α	0.90	0.10	0.0084
UNIQUAC	Δu_{12}	634.08	Δu_{21}	−374.80			0.22	0.0071

[a] Fitting parameters of the equations are in units of J·mol^{-1}.

where ρ and ρ_i° are the density of the mixture and of the pure components, respectively, x_i is the mole fraction, k_S is the isentropic compressibility of the mixture, and $k_{S,i}$ is the isentropic compressibility of the pure components.

The binary values were fit to a Redlich−Kister-type equation

$$\Delta Q = x_i x_j \sum_{p=0}^{M} B_p (x_i - x_j)^p \tag{3}$$

where ΔQ_{ij} is the excess property, x is the mole fraction, B_P is the fitting parameter, and M is the degree of the

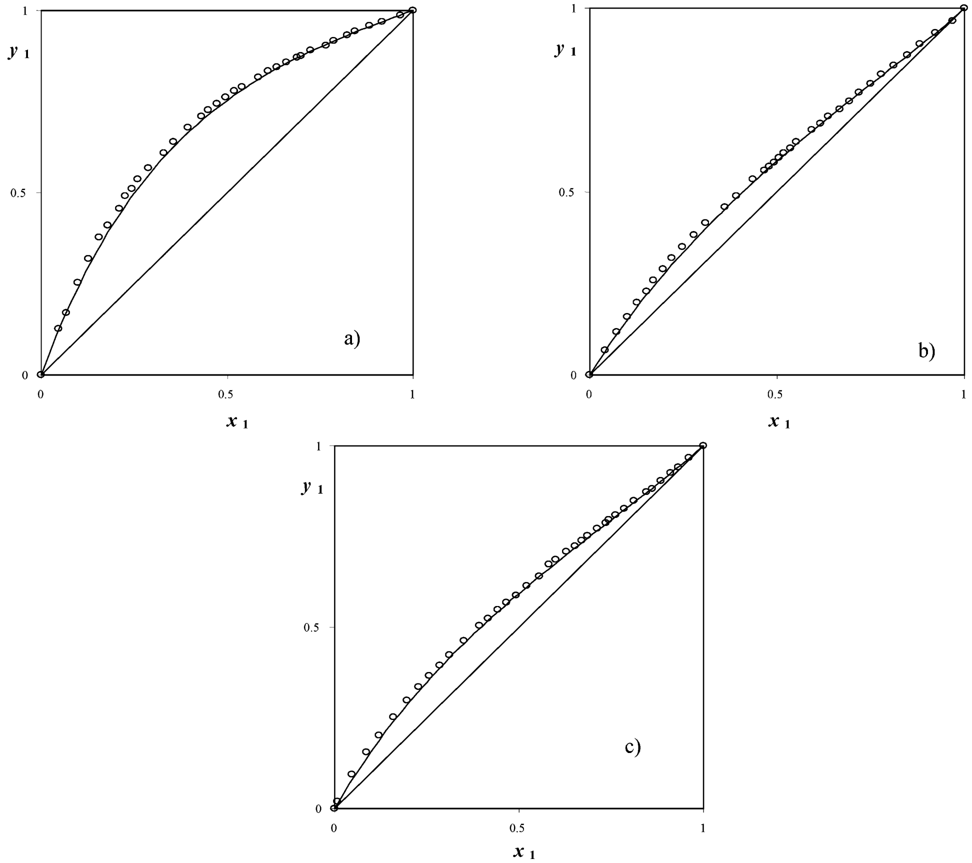

Figure 3. Experimental $y-x$ data and solid lines correspond to the best correlative equation for each binary system at 101.3 kPa. (a) Acetone (1) + dimethyl carbonate: ○, this work; −, Wilson. (b) 2-Butanone (1) + dimethyl carbonate: ○, this work; −, UNIQUAC. (c) Dimethyl carbonate (1) + 2-pentanone (2): ○, this work; −, Wilson.

polynomial expansion. By applying the F-test,[17] we optimized the degree of the polynomial expression. The correlation parameters calculated using eq 3 are listed in Table 3, together with the root-mean-square deviations (σ). This deviation is calculated by applying the expression

$$\sigma = \left(\frac{\sum^{\text{DAT}} (z_{\text{exptl}} - z_{\text{pred}})^2}{\text{DAT}} \right)^{1/2} \qquad (4)$$

where property values and the number of experimental data are represented by z and n_{DAT}, respectively.

Figure 1 shows excess molar volumes for the binary mixtures acetone + dimethyl carbonate, 2-butanone + dimethyl carbonate, and 2-pentanone + dimethyl carbonate at $T = 298.15$ K versus the mole fraction over the whole composition range. A comparison with literature data[5] was made in this Figure. It can be observed that the excess molar volumes are positive over the entire composition range for the binary mixtures 2-butanone + dimethyl carbonate and 2-pentanone + dimethyl carbonate, with the exception of the binary mixture acetone + dimethyl carbonate, which displays an inversion of sign.

Figure 2 shows a deviation in isentropic compressibility for the binary mixtures acetone + dimethyl carbonate, 2-butanone + dimethyl carbonate, and 2-pentanone + dimethyl carbonate at $T = 298.15$ K plotted against mole fraction together with the fitted curve obtained from eq 3. The deviation in isentropic compressibility for the binary mixtures acetone and 2-butanone with dimethyl carbonate is negative over the entire composition range, whereas for the binary mixture 2-pentanone + dimethyl carbonate positive values of this quantity are observed.

Experimental isobaric VLE data, corresponding to the temperature, T, and the liquid-phase and vapor-phase mole fractions, x and y, for the binary systems acetone + dimethyl carbonate, 2-butanone + dimethyl carbonate, and dimethyl carbonate + 2-pentanone at 101.3 kPa are presented in Tables 4 to 6. The activity coefficients, γ_i, were calculated from the equation

$$\ln \gamma_i = \ln \frac{y_i P}{x_i P_i^\circ} + \frac{(B_{ii} - V_i^{\text{L}})(P - P_i^\circ)}{RT} + \frac{P}{2RT} \sum_{j=1}^{n} \sum_{k=1}^{n} y_j y_k (2\delta_{ji} - \delta_{jk}) \qquad (5)$$

where δ_{ji} and δ_{jk} are defined by

$$\delta_{ji} = 2B_{ji} - B_{jj} - B_{ii} \qquad (6)$$

$$\delta_{jk} = 2B_{jk} - B_{jj} - B_{kk} \qquad (7)$$

T and P are the temperature and the total pressure, respectively, V_i^{L} is the molar liquid volume of component i, B_{ii} and B_{jj} are the second virial coefficients of the pure gases, P_i° is the saturation pressure, and δ_{ij} is related to the cross second virial coefficient. The virial coefficients, B_{ii} and B_{ij}, were estimated by the method of Hayden and O'Connell[18] using the molecular parameters given by Prausnitz et al.[19] Critical properties of all components were taken from the DIPPR database.[20] The activity coefficients are listed in the last columns of Tables 4 to 6. Experimental

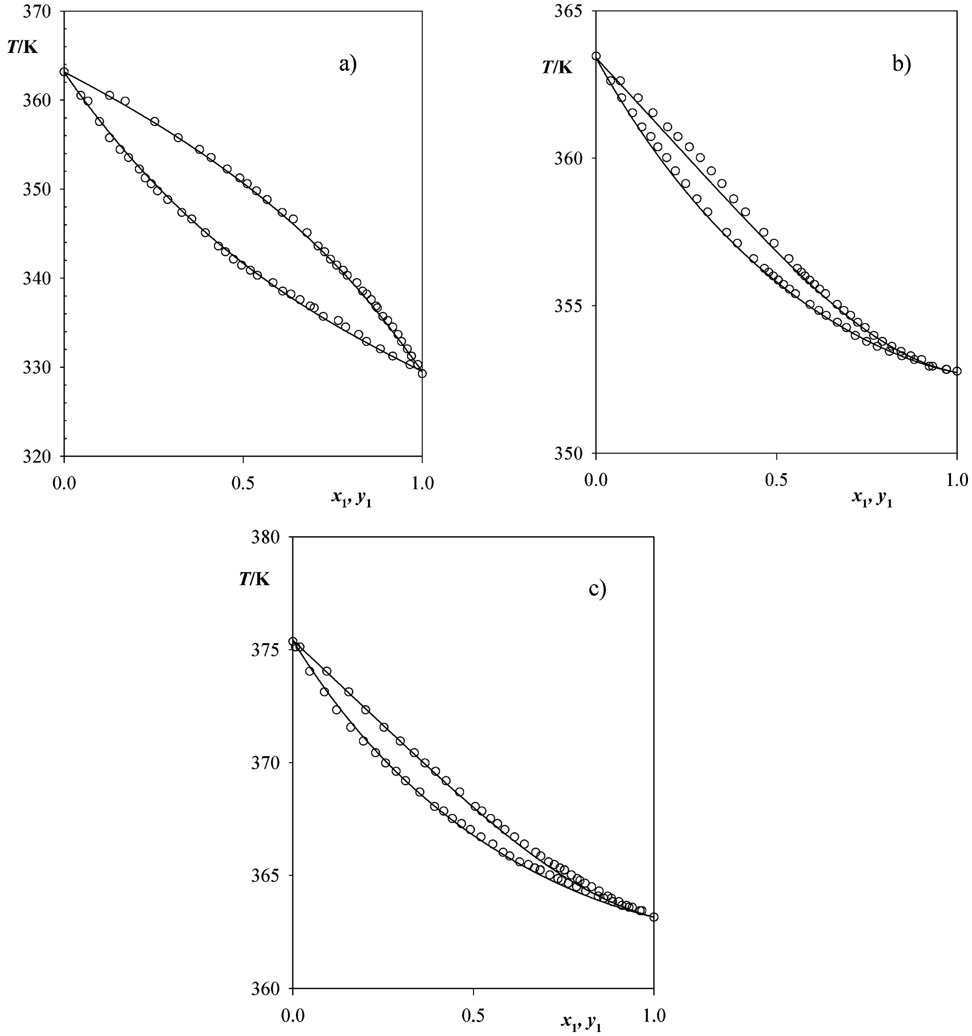

Figure 4. Experimental $T-x,y$ data and solid lines correspond to the best correlative equation for each binary system at 101.3 kPa. (a) Acetone (1) + dimethyl carbonate: ○, this work; −,Wilson. (b) 2-Butanone (1) + dimethyl carbonate: ○, this work; −, UNIQUAC. (c) Dimethyl carbonate (1) + 2-pentanone (2): ○, this work; −, Wilson.

vapor pressures of diethyl carbonate were determined experimentally and published in a previous paper[2], and the Antoine coefficients of the ketones were taken from the DIPPR database.[20]

The VLE data were found to be thermodynamically consistent by the point-to-point method of Van Ness et al.[21] and modified by Fredenslund et al.[22]

The correlation equations of Wilson, NRTL, and UNIQUAC were used. The parameters were optimized by minimizing the objective function

$$\mathrm{OF} = \sum_{j=1}^{np}\sum_{i=1}^{nc}\left[\frac{\gamma_{ij}^{\mathrm{exptl}} - \gamma_{ij}^{\mathrm{calcd}}}{\gamma_{ij}^{\mathrm{exptl}}}\right]^2 \tag{8}$$

The calculated parameters and the root-mean-square deviations in temperature and vapor-phase composition are reported in Table 7. An inspection of the results shows that all models are suitable for correlating the binary data. Figures 3 and 4 show the correlated line corresponding to the best model for each binary system.

Conclusions

In this paper, the experimental density and speed of sound of binary mixtures dimethyl carbonate with acetone, 2-butanone, and 2-pentanone at T = 298.15 K were determined. Excess molar volumes are positive over the whole composition range except for the binary mixture acetone + dimethyl carbonate. Negative values of excess molar volumes suggest that the molecular packing of dimethyl carbonate with ketones is more efficient when the length of the hydrocarbon chain of ketones is increased. The deviation in isentropic compressibility values for binary mixtures of ketones with dimethyl carbonate increases as the molecular mass of the ketone is increased.

Isobaric VLE data for three binary systems containing dimethyl carbonate and ketones (acetone, 2-butanone, and 2-pentanone) were measured at 101.3 kPa in a Labodest dynamic recirculating still. Experimental VLE data are thermodynamically consistent, and the activity coefficients were evaluated with Wilson, NRTL, and UNIQUAC. The correlation of the temperature and liquid- and vapor-phase compositions for the cited equations is satisfactory. In this case, we could suggest that all of the correlation equations produce similar results.

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