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Vapor−Liquid Equilibrium in 2-Ethoxyethanol + Methanol at 313.15 to 333.15 K

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The vapor−liquid equilibrium (VLE) isotherms were directly determined by the ebulliometric method for the system 2-ethoxyethanol + methanol. The experimental results were correlated by an equation of state that is capable of reproducing VLE for associating and reacting systems with an accuracy similar to the experiment uncertainty over a reasonable range of pressure and temperature. Such correlations are hard to obtain with equations representing activity coefficients at specific particular isotherms.

1. Introduction

This work is part of an ongoing investigation of the phase equilibrium for systems of industrial interest sponsored by Project 805 of the Design Institute for Physical Property Data, DIPPR, of the American Institute of Chemical Engineers. This paper reports experimental measurements that have been made under Project 805(B)94.

Vapor−liquid equilibrium (VLE) data on binary mixtures of organic compounds are of significant importance for the design of numerous industrial chemical processes or for the purpose of environmental protection. The data for 2-ethoxyethanol + methanol cannot be predicted with sufficient accuracy from pure component properties or by semiempirical methods, such as those based on the group contribution concept like ASOG (Kojima and Tochigi, 1979) or UNIFAC (Fredenslund et al., 1977).

The only data reported in the literature are by Martin et al. (1994). These were obtained by the saturation method. This method enables only determination of the composition of coexisting phases and the equilibrium temperature. There is no possibility of measuring the total pressure.

2. Experimental Section

2.1. Chemicals. *2-Ethoxyethanol* (CASRN. 110-80-5) was purchased from Merck GmbH as 99+% pure. GLC gave 99.5% by mass. The substance was dried by 4A molecular sieves and further purified by distillation through a 25 theoretical plate laboratory column. A final purity of 99.9% was obtained. The content of water determined by GLC analysis with a TCD detector on glass 2.5 m × 3 mm column filled with Chromosorb 101 (60/80 Mesh) was less then 0.02 mass %. *Methanol* (CASRN. 67-56-1) was purchased from Aldrich-Chemie GmbH & Co. KG, as 99.8% pure ACS reagent. GLC gave 99.75% by mass. The substance was dried by 4A molecular sieves and further purified by distillation through a 40 theoretical plate laboratory column. Final purity was 99.94% by mass. The content of water determined by GLC analysis (as above) was less than 0.05 mass %.

2.2. Vapor Pressure Measurements. The measurements of the pure compound vapor pressure were performed in a modified Swietoslawski's ebulliometer described earlier (Rogalski and Malanowski, 1980).

The ebulliometer was connected to the pressure stabilizing system, which consisted of a 0.6 m^3 buffer vessel coupled with a vacuum pump and pressurized argon container. The pressure was manually adjusted using the system of valves and a pressurized rubber balloon until the boiling temperature of the sample in the ebulliometer had achieved the desired constant temperature within ±0.005 K.

The equilibrium temperature was measured with a SYSTEMTEKNIK AB S1228 thermometer with a platinum resistance probe (resolution: 0.001 K). The temperature fluctuation during runs lasting several hours was within ±0.005 K: No systematic deviations of the temperature measurements were observed.

The pressure was determined using a Texas Instruments 144-01 precision pressure gauge with quartz Bourdon tube No. 8 type 2 (resolution: 0.3 Pa), enabling a pressure determination in the range of (1−137) kPa with a resolution of ±0.5 Pa.

The calibration of the thermometer was made with the ice point of water. The pressure meter was calibrated with vacuum to better than 10^{-2} Pa. In addition, the saturation vapor pressure as a function of temperature was measured for pure hexane and compared with literature data (Willingham et al., 1945). The results agree within the claimed accuracy ($\delta P/\mathrm{Pa} = \pm 8$ and $\delta T/\mathrm{mK} = \pm 3$).

The estimated accuracy of the pressure measurement was ±10 Pa. The estimated accuracy of the temperature measurement was ±0.01 K. The ITS-90 was used.

2.3. VLE Measurements. The measurements were performed at isothermal conditions by means of the ebulliometer, enabling the sampling of the liquid phase and vapor condensate, the same as those used for saturation pressure measurements.

First, the pure component sample was introduced to the ebulliometer and heated to boiling with continuous adjustment of pressure until the desired constant temperature was reached with accuracy of ±0.01 K. At this stage readouts of pressure and temperature were taken. Next the desired amount of second component was added, the adjustment of pressure to constant temperature repeated, and the sample of boiling liquid and vapor condensate collected, respectively, for GLC analysis by means of gastight syringes. For changing the sample composition, a known amount of the second component was once more added and the whole procedure repeated until the concentration of second component exceed 50%. Then the same procedure was started from the second pure component.

2.4. Analytical Method. The sample composition was determined by GLC with the use of a 2 m Reoplex packed column, flame ionization detector (FID), and appropriate calibration procedure. A Chrom 5 model gas chromatograph equipped with a FID detector and HP 3380A integrator were used.

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Table 1. Saturation Vapor Pressures Measured for 2-Ethoxyethanol and Methanol

2-ethoxyethanol					
first series		second series		methanol	
T/K	P/kPa	T/K	P/kPa	T/K	P/kPa
313.15	1.766	313.35	1.792	303.34	22.022
318.57	2.406	319.05	2.492	303.35	22.030
323.13	3.109	324.73	3.409	308.20	27.958
328.60	4.173	328.28	4.123	308.19	27.952
333.16	5.278	333.15	5.303	313.11	35.308
338.52	6.899	343.10	8.631	313.13	35.334
343.13	8.608	353.14	13.622	318.14	44.476
348.43	10.999	363.04	20.746	323.15	55.514
352.92	13.446			328.06	68.461
				333.14	84.461
				337.75	101.585

Results

The vapor pressures of pure components are given in Table 1. The measurements for 2-ethoxyethanol were made in two series. The first was at the beginning of the measurements, and the second was at the end. The results of both series agree within 40 Pa. The comparison with the data recommended by DIPPR (Daubert et al., 1995) show discrepancies both for methanol (Figure 1) and 2-ethoxyethanol (Figure 2). The comparison with results of direct measurements given in the literature [for methanol, Ambrose and Sparke (1970) and Boublik and Aim (1972) and for 2-ethoxyethanol, Pick et al., (1955)] exhibit similar deviations as our data (Figures 1 and 2). This indicates that DIPPR recommendations exhibit systematic deviations from experimental data (0.6% for methanol and 4.5% for 2-ethoxyethanol). The errors are within the estimated accuracy of DIPPR (1% for methanol and 10% for 2-ethoxyethanol).

The results of VLE measurements obtained for the equilibrium pressure (P), temperature (T), and the mole fraction of component 1 in the liquid (x_1) and vapor (y_1) phases are listed in Table 2.

Correlation of Vapor Pressure Measurements. First, the measured vapor pressures were correlated by means of the Antoine equation

$$\log(p/\mathrm{kPa}) = A - \frac{B}{C + (T/\mathrm{K})} \tag{1}$$

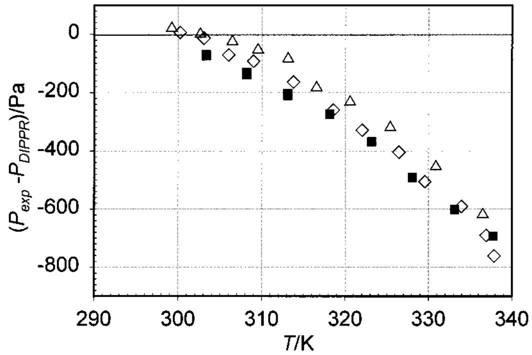

Figure 1. Differences between vapor pressure data recommended for methanol by DIPPR and this work (◆), reported by Ambrose and Sparke (1970) (◇), and by Boublik and Aim (1972) (△).

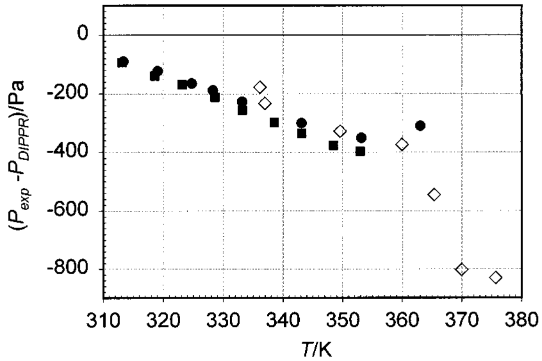

Figure 2. Differences between vapor pressure data recommended for 2-ethoxyethanol by DIPPR and two series of our measurements (■, first series; ●, second series) and reported by Pick et al. (1955) (◇).

where p is the pressure, T is the temperature, and A, B, and C are adjustable parameters.

The results of correlation are summarized in Table 3. The root-mean-square deviations of pressure (RMSD(p)/Pa) are calculated from the equation:

$$\mathrm{RMSD}(p) = \sqrt{\frac{\sum_{i=1}^{n}(p_i^{\mathrm{exp}} - p_i^{\mathrm{calc}})^2}{n - m}} \tag{2}$$

Table 2. VLE in the System Methanol (1) + 2-Ethoxyethanol (2)[a]

T/K = 313.15			T/K = 323.15			T/K = 333.15		
x_1	y_1	P/kPa	x_1	y_1	P/kPa	x_1	y_1	P/kPa
0.0000	0.0000	1.775	0.0000	0.0000	3.113	0.0000	0.0000	5.268
0.0107	0.1696	2.026	0.0121	0.1779	3.648	0.0140	0.1956	6.247
0.0428	0.4995	3.056	0.0436	0.4920	5.281	0.0357	0.4115	7.930
0.1156	0.7482	5.288	0.1116	0.7326	8.513	0.1080	0.7168	13.312
0.2022	0.8500	7.895	0.1774	0.8337	11.644	0.1813	0.8359	18.844
0.2727	0.8992	10.255	0.2600	0.8905	16.183	0.2572	0.8877	24.805
0.3383	0.9182	12.718	0.3435	0.9236	20.482	0.3496	0.9258	31.925
0.4266	0.9480	15.112	0.4221	0.9498	23.815	0.4302	0.9453	37.284
0.5108	0.9640	18.104	0.5109	0.9648	28.851	0.5204	0.9676	44.475
0.5574	0.9706	19.729	0.5528	0.9702	31.152	0.6028	0.9757	52.196
0.6195	0.9786	21.878	0.6219	0.9771	34.637	0.6827	0.9842	58.170
0.6873	0.9845	24.438	0.6978	0.9839	38.394	0.7236	0.9863	61.247
0.7760	0.9915	27.418	0.7700	0.9891	42.818	0.7945	0.9909	67.362
0.8470	0.9930	30.019	0.8344	0.9939	46.435	0.8493	0.9936	72.270
0.9035	0.9969	31.789	0.8900	0.9959	49.149	0.8973	0.9955	75.686
0.9539	0.9984	33.732	0.9546	0.9984	52.882	0.9458	0.9980	79.995
1.0000	1.0000	35.334	1.0000	1.0000	55.514	0.9805	0.9990	82.785
						1.0000	1.0000	84.461

[a] Estimated errors of measurements: $\delta x_1 = \pm 0.001$, $\delta y_1 = \pm 0.002$, $\delta P/\mathrm{Pa} = \pm 30$, $\delta T/\mathrm{mK} = \pm 10$.

Table 3. Correlation of Pure Components Vapor Pressure with the Antoine Equation

	2-ethoxyethanol		
	first series	second series	methanol
temperature range (K)	313−353	313−363	303−338
parameters of Antoine equation (T/K, p/kPa)			
A	6.71644	6.608122	7.226212
B	1628.971	1570.774	1591.237
C	61.388	66.175	32.880
errors: RMSD(p)/Pa	11.49	5.10	19.28
enthalpy of vaporization (H/kJ mol^{-1})			
at T/K = 298.15			
calcd	49.39	49.99	37.92
lit.	none	none	37.43[a] 37.83[b] 38.01[c]
at boiling point T/K =	407.19	407.47	337.69
calcd	41.45	41.09	36.08
lit.	none	none	35.21[a] 34.5[b] 35.26[c]

[a] Majer and Svoboda (1985). [b] TRC m-5000, 1994. [c] Daubert et al. (1995).

where m is the number of adjustable parameters, n the number of experimental points, p_i^{exp} the pressure measured at point i, and p_i^{calc} the pressure calculated from eq 1 at point i. The heats of vaporization calculated from the measured vapor pressure are also given in this table. These values show very small deviations from those reported in the literature and obtained by means of calorimetric method.

The recent development of the equation of state methods (Malanowski and Anderko, 1992; Sandler, 1994) shows that these methods are able to reproduce VLE data within the accuracy of measurement. Another advantage of the equation of state method is the ability to reproduce binary VLE data over a wide range of pressure and temperature with only one set of parameters.

In previous work (Malanowski, 1990) it has been found that the AEOS [association +equation of state (Malanowski and Anderko, 1992)] equation of state is most suitable for representation of phase equilibria in the systems formed by associating or even chemically reacting compounds (Anderko and Malanowski, 1989). In the AEOS model, the thermodynamic properties of an associated mixture are viewed as a result of chemical equilibrium between associated species and physical interactions between all, associated or inert, species existing in a mixture. The chemical equilibria are assumed to follow a simplified, yet plausible association model, which, in general, depends on the nature of the associating compound. An equilibrium mixture of associated species is treated analogously to a mixture of nonreacting polymeric aggregates.

The use of the AEOS equation leads to the split of the compressibility factor (z) into two parts

$$z = z^{\text{ph}} + z^{\text{ch}} - 1 \tag{3}$$

where z^{ph} and z^{ch} are the physical and chemical contributions to the compressibility factor, respectively. The z^{ph} contribution is equivalent to the equation of state for nonreacting monomeric species. The z^{ch} contribution is equal to the reciprocal mean association number and depends on the association model.

The z^{ch} contribution can be combined in a consistent way with a cubic EOS used for the z^{ph} contribution. To reproduce thermodynamic data, it is sufficient to use a one-constant association model. For such a model the equilibrium constants for the consecutive association reactions

$$A_i + A_1 = A_{i+1} \qquad i = 1, ..., \infty \tag{4}$$

can be expressed as

$$K_{i,i+1} = f(i)\,K \qquad i = 1, ..., \infty \tag{5}$$

where $f(i)$ is a function of the number of monomers within a multimer. In this case the chemical contribution to the compressibility factor of a pure associating substance is an algebraic function of the product RTK/V, where V is the molar volume of the system

$$z^{(\text{ch})} = F\left(\frac{RTK}{V}\right) \tag{6}$$

For an infinite-equilibria linear Mecke−Kempter-type association model, $f(i) = 1$ for $i = 1, ..., \infty$ and z^{ch} becomes

$$z^{(\text{ch})} = \frac{2}{1 + \sqrt{1 + 4RTK/V}} \tag{7}$$

This model has been found to give a good fit to a variety of pure compounds such as alcohols, phenols, ketones, amines, pyridine bases, and other compounds. The AEOS equation has been chosen for the systems investigated in this paper.

The auxiliary parameters necessary for AEOS equation are given in Table 4, while the results of the correlation of the vapor pressure data are given in Table 5.

The comparison of correlation of vapor pressure by the Antoine and AEOS equations is given in Figures 3 and 4. There is no discernible difference between the correlation ability of both equations. In both cases the distribution of errors is random. Higher differences in the case of 2-ethoxyethanol agree with the estimation of errors in the course of measurements.

Correlation of VLE Measurements. In the case of mixtures containing any number of associating components, the model equations cannot be rigorously solved and approximate expressions are needed. An accurate approximate expression has been found for mixtures containing n associating components whose self- as well

Table 4. Molecular Parameters and Critical Constants for 2-Ethoxyethanol and Methanol (Daubert et al., 1994)

compound	mol. wt.	T_c/K	p_c/atm	V_c/mL	Z_c	ω	d_{25}/(g/mL)
2-ethoxyethanol	90.123	569.0	41.85	294.0	0.264	0.7582	0.9261
methanol	32.042	512.6	79.91	118.0	0.224	0.5640	0.7896

Table 5. Correlation of Pure Component Vapor Pressure with the AEOS Equation of State

compound	T_c'/K	p_c'/atm	ω_H'	$-\Delta H°$/kJ mol^{-1}	$-\Delta S°$/J mol^{-1} K^{-1}	$-\Delta C_p$/J mol^{-1} K^{-1}	RMSD(P)/Pa
ethoxyethanol	575.57	39.55	0.4822	2.8632	54.29	77.94	10.63
methanol	437.64	89.61	0.1612	19.7287	85.40	23.66	7.18

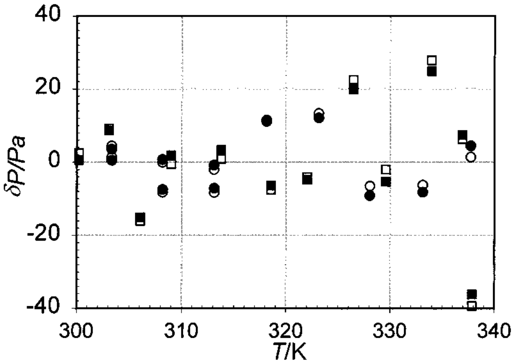

Figure 3. Comparison of the representation of methanol vapor pressure data by Antoine and AEOS equations: ●, this work; ■, Pick et al. (1955) (solid symbols, AEOS equation; hollow symbols, Antoine equation).

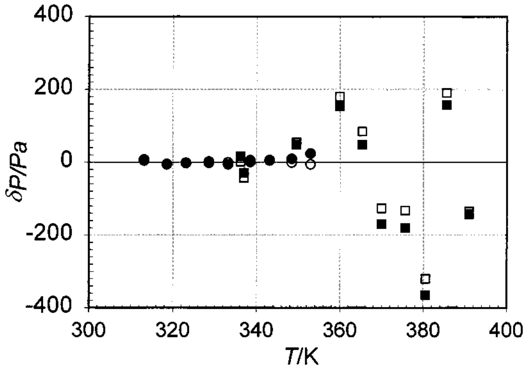

Figure 4. Comparison of the representation of 2-ethoxyethanol vapor pressure data by Antoine and AEOS equations: ●, this work; ■, Ambrose and Sparke (1970) (solid symbols, AEOS equation; hollow symbols, Antoine equation).

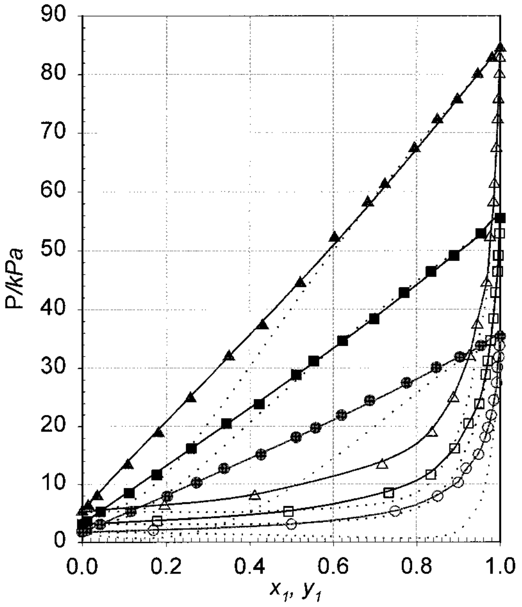

Figure 5. Constant temperature VLE in the system methanol + 2-ethoxyethanol. Dotted line, prediction by AEOS from pure components properties (Table 4); solid line, correlation with mixing rules 11−13, using parameters *A* and *B* from Table 6. Experimental data: ●, *T*/K = 313.15; ■, *T*/K = 323.15; ▲ *T*/K = 333.15. (Solid symbols, bubble point; hollow symbols, dew point.)

as cross-association is represented by the continuous linear association model

$$z^{(\mathrm{ch})} = \sum_{i=1}^{n} \frac{2x_{A_i}}{1 + \sqrt{1 + 4RT(\sum_{j=1}^{n} K_{ij}x_{A_j})/v}} + \sum_{k=1}^{r} x_{B_k} \quad (8)$$

where K_{ij} is either the self-association constant (for $i = j$) or the cross-association constant (for $i \neq j$). Equation 8 has been found to be very useful for multicomponent mixtures containing many possible combinations of alcohols, phenols, ketones, amines, etc., as well as nonpolar components. In all cases the temperature dependence of the association constant can be expressed by assuming that the standard enthalpy ΔH°_{ij} and entropy ΔS°_{ij} of association are linearly dependent on temperature (the appropriate values of C_p are given in Table 5)

$$\ln K_{ij} = \frac{-\Delta H^\circ(T_0) + \Delta C^\circ_p T_0}{RT} + \frac{1}{R}[\Delta S^\circ(T_0) - \Delta C^\circ_p - \Delta C^\circ_p \ln T_0] + \frac{\Delta C^\circ_p}{R} \ln T \quad (9)$$

The z^{ph} contribution (eq 3) was calculated from the cubic equation of state of Yu and Lu (1987)

$$z^{(\mathrm{ph})} = \frac{v}{v - b} - \frac{a(T)v}{RT[v(v + c) + b(3v + c)]} \quad (10)$$

where *a(T)*, *b*, and *c* are generalized as functions of the critical temperature T_c, critical pressure P_c, and acentric factor ω of a pure component. The detailed equations are given in paper by Yu et al. (1987).

The complete equation of state for an associating compound (eq 3) has five characteristic parameters. These are the standard enthalpy ΔH°_{ii} and entropy ΔS°_{ii} of association and T'_c, the critical temperature, P'_c, the critical pressure, and ω', the acentric factor of a hypothetical monomeric compound with nonspecific interactions identical to those in the associating substance but incapable of forming associates. These parameters were determined by

Table 6. Parameters of the AEOS Equation and Root-Mean-Square Deviation of Pressure (*P*) and Vapor-Phase Composition (*y*) for Binary Mixtures

system	*T*/K	K_{12}	θ_{12}	RMSD(*P*)/Pa	RMSD(*y*)
(1) Correlation. K_{12} and θ_{12} Values Obtained by Direct Fit to Each Isotherm					
methanol + 2-ethoxyethanol	313.15	2.1253×10^{-5}	−0.0428	167	0.0173
	323.15	1.7992×10^{-5}	−0.0434	239	0.0241
	333.15	1.5066×10^{-5}	−0.0465	514	0.0269
(2) Prediction. K_{12} and θ_{12} Values Computed for Each Isotherm by Eq 14					
parameters: *A* =		$1.187\,45 \times 10^{-4}$	6.0549×10^{-3}		
B =		$-3.114\,8 \times 10^{-7}$	1.55×10^{-4}		
methanol + 2-ethoxyethanol	313.15	$2.121\,04 \times 10^{-5}$	−0.0425	167	0.0169
	323.15	$1.808\,88 \times 10^{-5}$	−0.0440	240	0.0250
	333.15	$1.497\,39 \times 10^{-5}$	−0.0456	530	0.0265

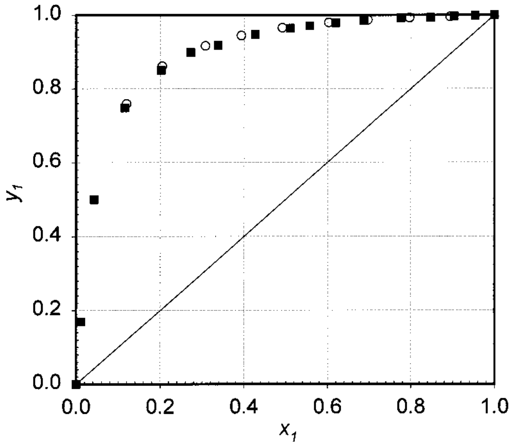

Figure 6. VLE in the system methanol + 2-ethoxyethanol: ■, this work; ○, Martin et al. (1994).

fitting the equation to all available vapor pressure and liquid density data. The values are given in Table 5. Subsequently, the parameters obtained from pure component data were used unchanged for the mixture calculations.

The determination of pure component parameters is the crucial step in the application of the AEOS equation. It is not sufficient to obtain a good fit to pure component data. It is essential ensured that the relative magnitude of the z^{ph} and z^{ch} terms be correct, i.e., the effects of association and nonspecific interactions on the compressibility factor be correctly partitioned. This can be, in principle, accomplished by using physically meaningful values of the association parameters ΔH_{ii}° and ΔS_{ii}°.

For mixtures, the parameters *a*, *b*, and *c* are calculated using the classical quadratic mixing rules

$$a = \sum_i \sum_j x_i x_j \sqrt{a_i a_j}(1 - \theta_{ij}) \qquad (11)$$

$$b = \sum_i x_i b_i \qquad (2)$$

$$c = \sum_i x_i c_i \qquad (13)$$

Similarly as for nonpolar mixtures, these mixing rules contain only one binary parameter θ_{ij}. The correlation results are summarized in Table 5. All results prove to be thermodynamically consistent within the desired experimental accuracy.

The K_{12} and θ_{12} values given in part 1 of Table 5 were fitted to the equation

$$K_{12}^{T} \text{ or } \theta_{12}^{T} = A + B\cdot T \qquad (14)$$

representing the temperature dependence of both parameters. The values computed for each temperature are given in part 2 of Table 6 together with the root-mean-square deviations of pressure and vapor-phase composition.

The comparison of the correlation made for each isotherm with the prediction by means of eqs 9 and 14 shows very satisfactory results.

In the literature there is only one VLE data set for methanol + 2-ethoxyethanol (Martin et al., 1994), and they were made by a transpiration method. By this method only the temperature and the composition of coexisting phases can be determined. The comparison of the Martin et al. data (isotherm at 298 K) with our data (isotherm at 313 K) is given in Figure 6. The agreement is very good.

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