

Isobaric vapour–liquid equilibrium of binary mixtures of some cyclic ethers with chlorobenzene at 40.0 and 101.3 kPa

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Abstract

A dynamic recirculating still has been used to determine isobaric vapour–liquid equilibrium data for the systems tetrahydrofuran, tetrahydropyran, 2-methyl-tetrahydrofuran, and 2,5-dimethyl-tetrahydrofuran + chlorobenzene at 40.0 and 101.3 kPa. The experimental data for all systems were checked for thermodynamic consistency using the point-to-point method of Van Ness. The systems present negative deviations from ideality and none of them show azeotrope. The VLE data have been satisfactorily correlated with the Wilson, NRTL and UNIQUAC equations. Predictions with the ASOG and UNIFAC methods were also included. © 1999 Elsevier Science B.V. All rights reserved.

Keywords: Experimental VLE; Cyclic ethers; Chlorobenzene; ASOG; UNIFAC

1. Introduction

Our research work has been dedicated to the study of thermodynamic and transport properties of mixtures containing halohydrocarbons and alcohols [1,2] in which the existence of specific interactions is noticeable. Recently, we have extended our interest to another oxygenated compounds, particularly cyclic ethers [3–5] that also exhibit those interactions. The present paper carries on with this working line and reports isobaric vapour–liquid equilibrium data for mixtures of tetrahydrofuran, tetrahydropyran,

2-methyl-tetrahydrofuran, and 2,5-dimethyl-tetrahydrofuran with chlorobenzene at two pressures, 40.0 and 101.3 kPa. The aim of these data is to give more experimental information about the following functional groups: aromatic carbon, cyclic ether and chlorine.

Besides, VLE knowledge is a basic thermodynamic information in the design and optimization of many unit operation processes, such as distillation and liquid–liquid extraction. Accurate VLE data are indispensable in developing and evaluating predictive liquid-phase activity coefficients models, like ASOG or UNIFAC. These group contribution methods need an extensive data base for improving the parameters required in their application.

Experimental (P , T , x_i , y_i) data for these systems are not available in literature.

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2. Experimental

2.1. Materials

The liquids used were tetrahydrofuran (purity better than 99.8 mol%), tetrahydropyran, 2-methyl-tetrahydrofuran, and 2,5-dimethyl-tetrahydrofuran (all better than 99.0 mol%) purchased from Aldrich, and chlorobenzene (99.5 mol%) supplied by Fluka. The purity of chemicals was checked by gas–liquid chromatography, confirming the absence of other significant organic components, so they were employed without further purification.

2.2. Measurements

The still and procedure have been previously described [6]. The apparatus used to study vapour–liquid equilibrium was an all-glass dynamic recirculating still Labodest model equipped with a Cottrell pump. The thermometer used for measuring the equilibrium temperatures was a model F25 from Automatic Systems Laboratories. The pressure was taken with a pressure transducer Druck PDCR 110/W. The experimental error in temperature is ± 0.01 K, and in pressure the accuracy is ± 0.1 kPa.

When equilibrium was reached, (at least after 15 min of constant pressure and temperature), samples of liquid and vapour-condensated phase were taken and their densities analysed at 298.15 K. The apparatus used for this purpose was an Anton Paar DMA-58 vibrating tube densimeter. Prior to this, density-calibration curves for all systems studied were determined [7]. The experimental uncertainty in liquid and vapour mole fractions can be estimated in ± 0.0001 .

The correct running of the different devices and the purity of liquids were tested by measuring the normal

boiling points and the densities for the pure compounds. The results are listed in Table 1, compared with those found in literature [8–12].

3. Results and discussion

Vapour–liquid equilibrium data (T , x_i , y_i), together with calculated activity coefficients at 40.0 and 101.3 kPa are presented in Table 2. All systems show slightly negative deviations from ideality. The activity coefficients of the components, γ_i , have been calculated taking into account the non-ideality of the vapour phase, by using the equations:

$$\gamma_i = \frac{y_i P}{x_i p_i^0} \exp \left[\frac{(B_{ii} - V_i^0)(P - p_i^0) + (1 - y_i)^2 P \delta_{ij}}{RT} \right] \quad (1)$$

$$\delta_{ij} = 2B_{ij} - B_{ii} - B_{jj} \quad (2)$$

where x_i and y_i are the liquid and vapour phase compositions in equilibrium, P is the total pressure, p_i^0 is the pure component vapour pressure, B_{ii} is the second virial coefficient of the pure gas, B_{ij} is the cross second virial coefficient, and V_i^0 is the molar volume of the saturated liquid phase.

The Antoine equation has been used for calculating the p_i^0 , and the constants needed are listed in Table 3. Antoine's constants for tetrahydrofuran and chlorobenzene were obtained from [9], for 2-methyl-tetrahydrofuran and 2,5-dimethyl-tetrahydrofuran were taken from TRC tables [12], and those for tetrahydropyran were obtained from our own vapour pressure measurements. The second virial coefficients B_{ii} have been estimated using the Redlich–Kwong equation [13]. The cross second virial coefficients, B_{ij} , have been calculated by means of the Amdur–Mason equa-

Table 1
Physical properties (densities at 298.15 K and normal boiling points) of the pure compounds

Compound	ρ (kg m ⁻³)		T_b (K)	
	Exptl.	Lit.	Exptl.	Lit.
Tetrahydrofuran	882.09	881.97 [8]	339.12	339.115 [12]
Tetrahydropyran	879.15	879.16 [10]	361.17	361 [9]
2-Methyl-tetrahydrofuran	849.90	848.82 [11]	352.94	353.1 [9]
2,5-Dimethyl-tetrahydrofuran	825.27	–	365.08	365.65 [12]
Chlorobenzene	1100.94	1101.1 [9]	404.86	404.837 [9]

Table 2
Experimental VLE data at the indicated pressure

<i>T</i> (K)	<i>x</i> ₁	<i>y</i> ₁	γ_1	γ_2
Tetrahydrofuran(1) + chlorobenzene(2) at 40.0 kPa				
370.73	0.0258	0.1225	0.782	0.996
369.68	0.0359	0.1577	0.743	1.001
367.53	0.0520	0.2367	0.814	0.991
365.79	0.0612	0.2708	0.828	1.014
364.67	0.0714	0.323	0.873	0.988
358.91	0.1345	0.4833	0.808	0.991
352.82	0.1992	0.6093	0.815	1.010
346.86	0.2551	0.7160	0.891	0.989
340.74	0.3499	0.8034	0.878	0.999
335.69	0.4255	0.8574	0.905	1.008
331.54	0.4974	0.8993	0.931	0.970
327.75	0.5749	0.9288	0.946	0.956
326.81	0.6111	0.9443	0.934	0.852
323.75	0.6626	0.9534	0.968	0.942
320.80	0.7313	0.9715	0.993	0.828
319.01	0.8108	0.9817	0.967	0.821
315.11	0.9397	0.9957	0.978	0.729
Tetrahydrofuran(1) + chlorobenzene(2) at 101.3 kPa				
402.34	0.0178	0.0994	1.124	0.980
400.39	0.0334	0.1466	0.920	0.995
398.33	0.0467	0.2116	0.991	0.987
394.53	0.0751	0.3078	0.971	0.994
390.60	0.1139	0.3988	0.903	1.009
385.89	0.1546	0.4913	0.910	1.028
383.24	0.1837	0.5558	0.921	1.008
381.16	0.2030	0.6035	0.950	0.982
376.64	0.2561	0.6736	0.935	0.997
370.41	0.3478	0.7601	0.906	1.023
365.83	0.4013	0.8231	0.956	0.958
359.47	0.5044	0.8816	0.965	0.965
353.58	0.6169	0.9329	0.983	0.875
350.51	0.6848	0.9528	0.987	0.839
346.26	0.7890	0.9741	0.992	0.808
344.05	0.8685	0.9843	0.973	0.857
340.49	0.9606	0.9960	0.993	0.839
Tetrahydropyran(1) + chlorobenzene(2) at 40.0 kPa				
369.84	0.0692	0.1911	0.868	0.990
368.68	0.0857	0.2353	0.891	0.991
365.47	0.1553	0.3674	0.841	0.989
361.73	0.2195	0.4905	0.885	0.981
358.64	0.2795	0.5755	0.894	0.987
355.67	0.3462	0.6536	0.898	0.988
352.34	0.4313	0.7346	0.898	0.984
349.50	0.4954	0.7916	0.923	0.969
345.87	0.6032	0.8651	0.932	0.917
341.93	0.7065	0.9127	0.959	0.937
339.09	0.7941	0.9518	0.981	0.827
336.56	0.8700	0.9736	1.001	0.795
Tetrahydropyran(1) + chlorobenzene(2) at 101.3 kPa				
400.34	0.0670	0.1695	0.927	1.005
399.18	0.0855	0.2111	0.929	1.006

Table 2 (Continued)

395.67	0.1500	0.3442	0.936	0.992
392.28	0.2061	0.4468	0.957	0.987
386.59	0.3183	0.5973	0.951	0.989
384.27	0.3705	0.6597	0.956	0.970
380.69	0.4415	0.7258	0.966	0.983
377.39	0.5197	0.8035	0.990	0.908
374.45	0.5909	0.8556	1.002	0.861
368.86	0.7453	0.9175	0.993	0.948
366.49	0.8190	0.9468	0.997	0.932
364.31	0.8856	0.9707	1.006	0.875
2-Methyl-tetrahydrofuran(1) + chlorobenzene(2) at 40.0 kPa				
368.70	0.0636	0.1990	0.812	1.012
366.36	0.0996	0.2853	0.792	1.017
361.26	0.1822	0.4662	0.815	0.997
356.59	0.2625	0.5925	0.822	0.997
353.41	0.3131	0.6664	0.851	0.984
347.42	0.4318	0.7952	0.884	0.915
343.78	0.5042	0.8462	0.904	0.908
339.69	0.5935	0.8930	0.925	0.907
334.57	0.7183	0.9420	0.958	0.876
332.04	0.7962	0.9636	0.965	0.846
329.34	0.8624	0.9810	0.998	0.735
326.98	0.9608	0.9965	0.990	0.527
2-Methyl-tetrahydrofuran(1) + chlorobenzene(2) at 101.3 kPa				
400.07	0.0568	0.1767	0.948	0.993
397.53	0.0932	0.2638	0.912	0.991
391.41	0.1771	0.4431	0.925	0.983
385.91	0.2601	0.5706	0.922	0.991
382.22	0.3287	0.6480	0.905	1.002
375.96	0.4475	0.7736	0.928	0.952
372.78	0.5051	0.8153	0.940	0.961
366.90	0.6283	0.8868	0.961	0.952
361.31	0.7459	0.9415	1.003	0.872
359.32	0.8059	0.9563	0.997	0.915
357.37	0.8547	0.9740	1.013	0.780
354.22	0.9583	0.9926	1.010	0.867
2,5-Dimethyl-tetrahydrofuran(1) + chlorobenzene(2) at 40.0 kPa				
370.56	0.0608	0.1561	0.902	1.000
368.62	0.0970	0.2358	0.900	1.004
367.01	0.1279	0.2989	0.904	1.007
364.31	0.1770	0.3967	0.934	1.007
360.60	0.2586	0.5297	0.949	0.992
357.51	0.3360	0.6236	0.941	0.989
352.26	0.4615	0.7437	0.956	1.006
348.75	0.5561	0.8156	0.970	1.003
345.82	0.6475	0.8715	0.977	0.985
342.61	0.7453	0.9175	0.992	0.993
340.22	0.8429	0.9555	0.989	0.955
338.27	0.9259	0.9794	0.986	1.015
2,5-Dimethyl-tetrahydrofuran(1) + chlorobenzene(2) at 101.3 kPa				
401.20	0.0540	0.1459	1.131	0.996
399.07	0.0885	0.2296	1.137	0.988
397.33	0.1220	0.2944	1.099	0.986
393.78	0.1765	0.3910	1.093	1.003

Table 2 (Continued)

<i>T</i> (K)	<i>x</i> ₁	<i>y</i> ₁	γ_1	γ_2
389.02	0.2875	0.5308	1.017	1.026
387.94	0.3025	0.5545	1.036	1.027
382.76	0.4305	0.6904	1.027	1.021
379.09	0.5439	0.7695	0.992	1.063
375.49	0.6405	0.8438	1.013	1.024
371.25	0.7865	0.9151	0.999	1.076
369.49	0.8362	0.9431	1.015	0.996
367.10	0.9265	0.9752	1.011	1.048

Table 3

Constants of Antoine's equation for vapour pressures of the pure compounds (temperature in °C, pressure in kPa)

Compound	<i>A</i>	<i>B</i>	<i>C</i>
Tetrahydrofuran [12]	6.12142	1203.11	226.355
Tetrahydropyran	5.85520	1131.93	205.83
2-Methyl-tetrahydrofuran [12]	5.95009	1175.51	217.80
2,5-Dimethyl-tetrahydrofuran [12]	5.69272	1099.53	205.72
Chlorobenzene [9]	6.30963	1556.6	230

tion [14]. The molar volumes V_i^0 were calculated using the Yen and Woods method [15].

The thermodynamic consistency of the experimental data has been tested using the method of Van Ness, described by Fredeslund et al. [16]. A third-order Legendre polynomial has been used for the excess free energies. This test considers experimental data consistent if the mean absolute deviation between calculated and measured y_1 (Δy_1) is less than 0.01. The results are listed in Table 4, and they indicate that the experimental data are thermodynamically consistent for all systems.

The activity coefficients have been correlated with the Wilson, NRTL and UNIQUAC equations [17]. As recommended by Renon and Prausnitz (1968) the mixture nonrandomness parameter α_{12} in the NRTL equation was set as 0.3. For fitting the parameters of all equations, the following objective function has been used:

$$F = \sum_{i=1}^{i=N} \left[\left(\frac{\gamma_1^{\text{exptl}} - \gamma_1^{\text{cal}}}{\gamma_1^{\text{exptl}}} \right)^2 + \left(\frac{\gamma_2^{\text{exptl}} - \gamma_2^{\text{cal}}}{\gamma_2^{\text{exptl}}} \right)^2 \right] \quad (3)$$

where γ_i are the corresponding activity coefficients

Table 4

Results of the thermodynamic consistency test. Average deviation ΔP and Δy

System	<i>P</i> (kPa)	ΔP (kPa)	Δy
Tetrahydrofuran +	40.0	0.6	0.0045
	101.3	1.7	0.0072
Tetrahydropyran +	40.0	0.2	0.0034
	101.3	0.5	0.0055
2-Methyl-tetrahydrofuran +	40.0	0.5	0.0029
	101.3	0.5	0.0036
2,5-Dimethyl-tetrahydrofuran +	40.0	0.4	0.0051
	101.3	0.7	0.0033
+ Chlorobenzene			

and *N* is the number of experimental data. The method is based on minimization of *F* by means of a non-linear regression procedure [18].

The adjustable parameters A_{12} and A_{21} and the average deviations (ΔT and Δy), along with the activity coefficients at infinite dilution are shown in Table 5. All systems yield similar deviations in *T* and in *y* (less than 0.55 K and 0.007, respectively). Then, it can be concluded that the three equations show a good performance in correlating the activity coefficients.

Although all equations fit experimental data quite satisfactorily, is the Wilson equation the one that has been arbitrarily chosen in VLE calculations to obtain *T*-*x*₁-*y*₁ diagrams. They are graphically represented in Figs. 1–4, together with experimental VLE data. These diagrams are indicative that there does not exist azeotropic behaviour, and the calculations confirm this observation.

The four systems studied at both pressures behave near ideality, with slightly negative deviations. These results are indicative that specific interactions in mixture (Cl-O(ether) and π (aromatic ring)-O(ether)) are a little stronger than those in pure liquids (dipole–dipole interactions, principally). Comparison of these systems with those formed with the same cyclic ethers and chlorocyclohexane [7] suggests that π -O interaction is the responsible for the different behaviour observed.

4. VLE Predictions

ASOG [19] and modified-UNIFAC [20] have been employed to predict VLE. However, in the case of

Table 5

Correlation parameters, average deviations ΔT and Δy , and activity coefficients at infinite dilution

Equation	A_{12}	A_{21}	ΔT (K)	Δy	γ_1^∞	γ_2^∞
Tetrahydrofuran(1) + chlorobenzene(2) at 40.0 kPa						
Wilson	-579.2339 ^a	-80.1915 ^a	0.41	0.0049	0.79	0.69
NRTL	867.3628 ^a	-1517.4872 ^a	0.40	0.0050	0.79	0.70
UNIQUAC	-4.5005 ^a	-552.6615 ^a	0.39	0.0052	0.80	0.70
Tetrahydrofuran(1) + chlorobenzene(2) at 101.3 kPa						
Wilson	-2121.4015	3796.7437	0.35	0.0067	0.89	0.92
NRTL	3832.4520	-3087.4143	0.29	0.0067	0.90	0.85
UNIQUAC	1302.5124	-1460.1952	0.28	0.0070	0.96	0.74
Tetrahydropyran(1) + chlorobenzene(2) at 40.0 kPa						
Wilson	-2088.6920	2299.5661	0.19	0.0039	0.84	0.71
NRTL	2355.2238	-2447.1150	0.22	0.0046	0.83	0.74
UNIQUAC	1335.0194	-1481.8385	0.18	0.0032	0.87	0.69
Tetrahydropyran(1) + chlorobenzene(2) at 101.3 kPa						
Wilson	3242.9761	-2484.6600	0.15	0.0045	0.92	0.87
NRTL	-2665.1990	3043.9615	0.16	0.0046	0.91	0.87
UNIQUAC	-121.0808	-279.3513	0.14	0.0045	0.89	0.89
2-Methyl-tetrahydrofuran(1) + chlorobenzene(2) at 40.0 kPa						
Wilson	-2654.6322	2840.7753	0.34	0.0034	0.77	0.53
NRTL	3005.9574	-3169.5525	0.41	0.0040	0.74	0.58
UNIQUAC	1991.9171	-1938.5921	0.25	0.0035	0.80	0.54
2-Methyl-tetrahydrofuran(1) + chlorobenzene(2) at 101.3 kPa						
Wilson	-2947.8261	4797.3588	0.29	0.0045	0.88	0.89
NRTL	3303.9007	-2905.1517	0.33	0.0045	0.88	0.81
UNIQUAC	885.7692	-1155.8374	0.34	0.0030	0.91	0.78
2,5-Dimethyl-tetrahydrofuran(1) + chlorobenzene(2) at 40.0 kPa						
Wilson	361.6560	-466.0889	0.21	0.0051	0.91	0.92
NRTL	-823.3678	629.4868	0.21	0.0052	0.92	0.92
UNIQUAC	-570.7371	324.7180	0.26	0.0063	0.89	0.94
2,5-Dimethyl-tetrahydrofuran(1) + chlorobenzene(2) at 101.3 kPa						
Wilson	2575.4737	-1307.0600	0.27	0.0038	1.20	1.04
NRTL	-2486.1844	369.3518	0.27	0.0036	1.19	1.02
UNIQUAC	1368.2323	-1237.6115	0.19	0.0049	1.13	1.06

^a J mol⁻¹.

systems containing 2-methyl-tetrahydrofuran and 2,5-dimethyl-tetrahydrofuran, the necessary van der Waals parameters r_i and q_i for the groups c-(CH₂-O-CH) and c-(CH-O-CH) are not available and modified-UNIFAC cannot be applied. Table 6 shows the average deviations in both T and y obtained using these group contribution methods. Both methods yield similar ΔT and Δy , and the results can be considered as moderately satisfactory. The deviations become appreciably smaller when the work pressure is 101.3 kPa. When comparing the two methods, the predictions of ASOG are better than those with mod-

ified-UNIFAC. Anyway, the results disclose that the success and reliability of group contribution methods need a data base as extensive as possible for improving the existing parameters, especially when the systems involved present specific interactions, like happens with the mixtures of this work.

5. Symbols

A_{12} , A_{21} adjustable parameters for VLE correlation equations

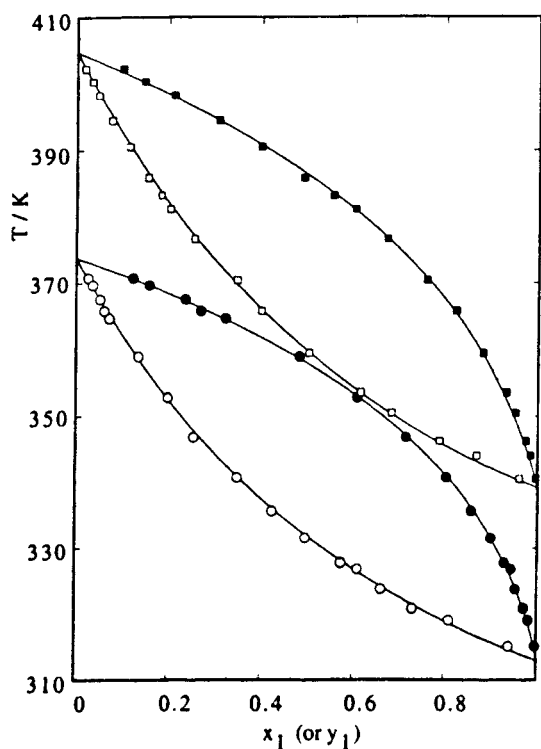


Fig. 1. T - x_1 - y_1 diagram for tetrahydrofuran(1)+chlorobenzene(2): (○, ●) exptl. data at 40.0 kPa; (□, ■) exptl. data at 101.3 kPa; (—) Wilson equation.

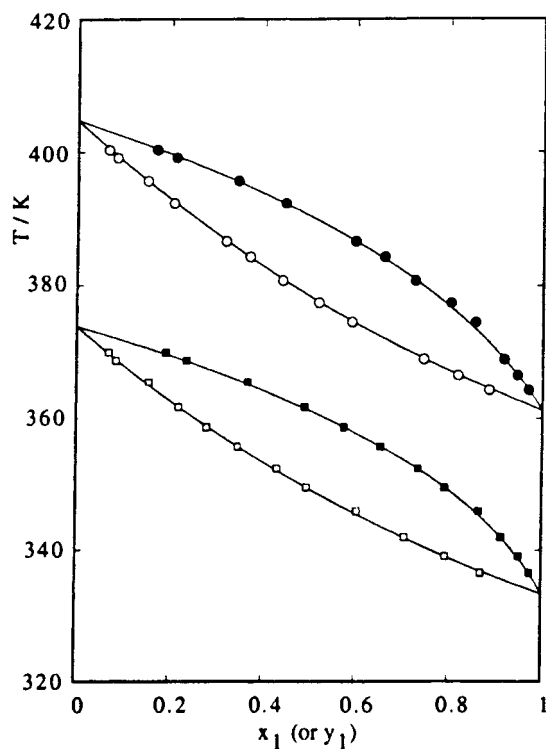


Fig. 2. T - x_1 - y_1 diagram for tetrahydropyran(1)+chlorobenzene(2): (○, ●) exptl. data at 40.0 kPa; (□, ■) exptl. data at 101.3 kPa; (—) Wilson equation.

Table 6

VLE predictions, average deviations ΔT and Δy

System	P (kPa)	Modified-UNIFAC		ASOG	
		ΔT (K)	Δy	ΔT (K)	Δy
Tetrahydrofuran +	40.0	0.97	0.0151	0.63	0.0099
	101.3	0.34	0.0076	0.28	0.0064
Tetrahydropyran +	40.0	0.34	0.0047	0.72	0.0082
	101.3	0.27	0.0036	0.23	0.0013
2-Methyl-tetrahydrofuran +	40.0	—	—	1.88	0.0171
	101.3	—	—	0.54	0.0040
2,5-Dimethyl-tetrahydrofuran +	40.0	—	—	0.54	0.0053
	101.3	—	—	0.78	0.0088

+ Chlorobenzene

B_{ii} second virial coefficient of component i ($\text{m}^3 \text{mol}^{-1}$)
 B_{ij} cross second virial coefficient ($\text{m}^3 \text{mol}^{-1}$)
 F objective function
 N number of experimental data

P total pressure (Pa)
 p_i^0 vapour pressure of component i (Pa)
 R gas constant ($= 8.314 \text{ J K}^{-1} \text{ mol}^{-1}$)
 T temperature (K)
 T_b normal boiling point (K)

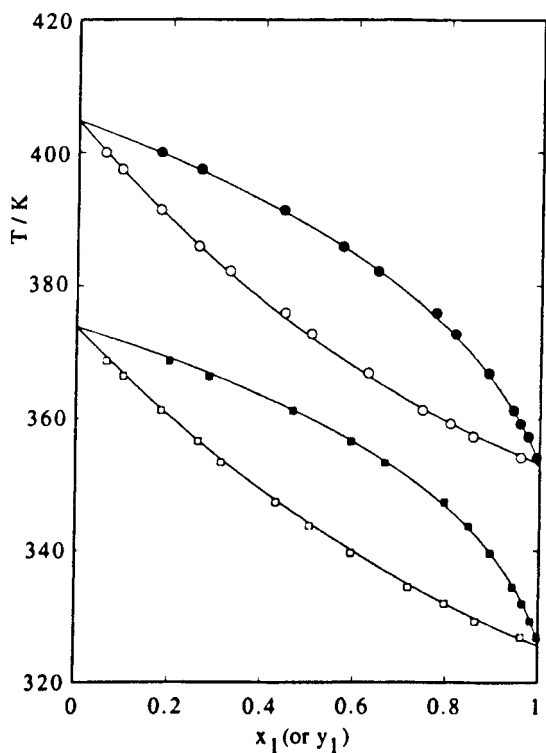


Fig. 3. T - x_1 - y_1 diagram for 2-methyl-tetrahydrofuran(1) + chlorobenzene(2): (○, ●) exptl. data at 40.0 kPa; (□, ■) exptl. data at 101.3 kPa; (—) Wilson equation.

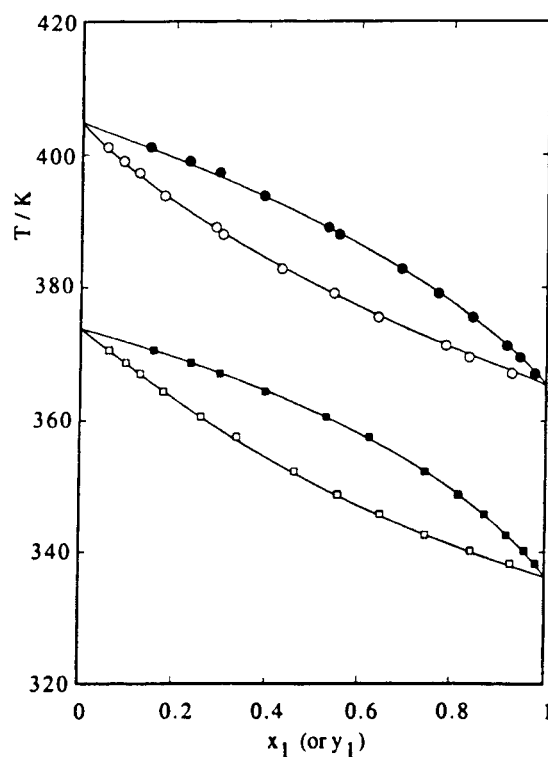


Fig. 4. T - x_1 - y_1 diagram for 2,5-dimethyl-tetrahydrofuran(1) + chlorobenzene(2): (○, ●) exptl. data at 40.0 kPa; (□, ■) exptl. data at 101.3 kPa; (—) Wilson equation.

V_i^0 molar volume of component i ($\text{m}^3 \text{mol}^{-1}$)
 x_i mole fraction of component i in the liquid phase
 y_i mole fraction of component i in the vapour phase
 r_i, q_i van der Waals parameters

5.1. Greek letters

α_{12} nonrandomness parameter in the NRTL equation
 Δ average deviation
 γ_i activity coefficient of component i
 γ_i^∞ activity coefficient of component i at infinite dilution
 ρ density (kg m^{-3})

5.2. Subscripts

i component i

5.3. Superscripts

cal calculated quantity
 exptl experimental quantity

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References

- [1] H. Artigas, C. Lafuente, C.A. Tovar, C. Alvarez-Cerdeirina, J.S. Urieta, *Thermochim. Acta* 306 (1997) 85–92.
- [2] H. Artigas, M. Domínguez, A.M. Mainar, M.C. López, F.M. Royo, *J. Chem. Eng. Data* 43 (1998) 580–584.

- [3] S. Rodríguez, C. Lafuente, J.A. Carrión, F.M. Royo, J.S. Urieta, *Int. J. Thermophys.* 17 (1996) 1281–1288.
- [4] S. Rodríguez, C. Lafuente, P. Cea, F.M. Royo, J.S. Urieta, *J. Chem. Eng. Data* 42 (1997) 1285–1289.
- [5] S. Rodríguez, C. Lafuente, H. Artigas, F.M. Royo, J.S. Urieta, *J. Chem. Thermodyn.* 31 (1999) 139–149.
- [6] H. Artigas, C. Lafuente, M.C. López, F.M. Royo, J.S. Urieta, *Fluid Phase Equilibria* 134 (1997) 163–174.
- [7] S. Rodríguez, Ph.D. Thesis, submitted for publication.
- [8] O. Kiyohara, P.J. D'Arcy, G. Benson, *Can. J. Chem.* 57 (1979) 1006–1010.
- [9] J.A. Riddick, W.B. Bunger, T.K. Sakano, *Organic Solvents. Physical Properties and Methods of Purification, Techniques of Chemistry*, vol. 2, 4th ed., Wiley/Interscience, New York, 1986, pp. 309, 311, 314, 480.
- [10] A. Inglese, J.P.E. Grolier, E. Wilhelm, *J. Chem. Eng. Data* 28 (1983) 124–127.
- [11] L. De Lorenzi, M. Fermeglia, G. Torriano, *J. Chem. Eng. Data* 40 (1995) 1172–1177.
- [12] TRC-Tables, Selected values of properties of chemical compounds, Thermodynamic Research Center Data Project, Texas A&M University, College Station, TX, 1972, p. k-6170.
- [13] O. Redlich, J.N.S. Kwong, *Chem. Rev.* 44 (1949) 233–244.
- [14] I. Amdur, E.A. Mason, *Phys. Fluids* 1 (1958) 370–383.
- [15] L.C. Yen, S.S. Woods, *AIChE J.* 14 (1968) 95–99.
- [16] A. Fredenslund, J. Gmehling, P. Rasmussen, *Vapor–Liquid Equilibria Using UNIFAC*, Elsevier, Amsterdam, 1977, pp. 68–73.
- [17] J. Gmehling, U. Onken, W. Arlt, *Vapor-liquid equilibrium data collection*, vol. 1, part 6a, Dechema Chemistry Data Series, Frankfurt/Main, 1980, pp. xx–xxiv.
- [18] J.A. Nelder, R.A. Mead, *Comput. J.* 7 (1965) 308–313.
- [19] K. Tochigi, D. Tiegs, J. Gmehling, K. Kojima, *J. Chem. Eng. Jpn.* 23 (1990) 453–463.
- [20] J. Gmehling, J. Li, M. Schiller, *Ind. Eng. Chem. Res.* 32 (1993) 178–193.