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Thermochimica Acta 362 (2000) 153–160

thermochimica acta

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

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Received 28 February 2000; accepted 29 June 2000

Abstract

Isobaric vapour–liquid equilibrium data for the binary systems formed by tetrahydrofuran, tetrahydropyran, 2-methyl-tetrahydrofuran, and 2,5-dimethyl-tetrahydrofuran with chlorocyclohexane have been measured at 40.0 and 101.3 kPa using a dynamic recirculating still. All experimental data were checked for thermodynamic consistency by means of the Van Ness method. The systems studied present slightly deviations from ideal behaviour. None of them show azeotrope. The VLE data have been satisfactorily correlated with the equations of Wilson, NRTL and UNIQUAC. Predictions with the ASOG and UNIFAC group contribution methods are included.

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

1. Introduction

Recently, our interest has been directed towards the study of thermodynamic and transport properties of mixtures containing cyclic ethers with chlorine derivatives [1–4]. Continuing this line, in the present paper we report the isobaric vapour–liquid equilibrium data for mixtures of tetrahydrofuran, tetrahydropyran, 2-methyl-tetrahydrofuran, and 2,5-dimethyl-tetrahydrofuran with chlorocyclohexane at two pressures, 40.0 and 101.3 kPa. It is well-known the importance of the availability of accurate VLE data, as well in developing and evaluating predictive liquid-phase activity coefficients models (ASOG, UNIFAC...) as in many industrial processes (distillation, liquid–liquid extraction). In previous papers we have collected experimental information about the following functional groups: aromatic carbon; cyclic ether and chlorine. Then, the objective of this work is both to enlarge the experimental information and to show the different behaviour exhibited by the chlorinated derivative of either cyclohexane or benzene.

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

2. Experimental

2.1. Materials

The liquids used, all supplied by Aldrich, were the following: tetrahydrofuran (purity better than

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PII: S0040-6031(00)00580-3

Nomenclature

Symbols

A_{12}, A_{21}	adjustable parameters for VLE correlation equations
B_{ii}	second virial coefficient of component i ($m^3\ mol^{-1}$)
B_{ij}	cross second virial coefficient ($m^3\ mol^{-1}$)
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 $J\ K^{-1}\ mol^{-1}$)
T	temperature (K)
T_b	normal boiling point (K)
V_i^0	molar volume of component i ($m^3\ mol^{-1}$)
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

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 ($kg\ m^{-3}$)

Subscripts

i	component i

Superscripts

cal	calculated quantity
exptl	experimental quantity

99.8 mol%), and tetrahydropyran, 2-methyl-tetrahydrofuran, 2,5-dimethyl-tetrahydrofuran, and chlorocyclohexane (all better than 99.0 mol%). The purity of chemicals was tested 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 described elsewhere [5]. The apparatus employed 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, samples of liquid and vapour-condensated phase were taken, and their densities analysed at 298.15 K with an Anton Paar DMA-58 vibrating tube densimeter. The density-calibration curves for all systems studied were obtained by Rodríguez et al. [2]. The experimental uncertainty in both liquid- and vapour-phase mole fractions is estimated in ±0.0001.

The correct running of the different devices and the purity of liquids were checked again by measuring the normal boiling points and the densities for the pure compounds. The results are listed in Table 1, and compared with those found in literature [6–10].

3. Results and discussion

Table 2 gathers vapour–liquid equilibrium data (T, x_1, y_1), together with the calculated activity coefficients at 40.0 and 101.3 kPa. The activity coefficients of the components, γ_i, were calculated taking into account the non-ideality of the vapour-phase, using the equations:

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

$$\delta_{ij} = 2B_{ij} - B_{ii} - B_{jj} \tag{2}$$

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

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 [6]	339.12	339.115 [9]
Tetrahydropyran	879.15	879.16 [7]	361.17	361 [10]
2-Methyl-tetrahydrofuran	849.90	848.82 [8]	352.94	353.1 [10]
2,5-Dimethyl-tetrahydrofuran	825.27	–	365.08	365.65 [9]
Chlorocyclohexane	993.23	–	415.76	–

Table 2
Experimental VLE data at the indicated pressure

T (K)	x_1	y_1	γ_1	γ_2
Tetrahydrofuran(1)+chlorocyclohexane(2) at 40.0 kPa				
380.55	0.0138	0.1191	1.102	0.978
370.89	0.0572	0.3905	1.105	0.976
364.04	0.0959	0.5261	1.062	1.007
351.67	0.1879	0.7262	1.056	1.034
342.67	0.2889	0.8293	1.027	1.065
339.22	0.3391	0.8548	1.005	1.131
334.80	0.3956	0.8921	1.037	1.118
329.68	0.5040	0.9341	1.012	1.054
324.15	0.6375	0.9624	0.999	1.074
319.85	0.7599	0.9807	0.997	1.033
317.27	0.8597	0.9888	0.978	1.172
314.99	0.9380	0.9956	0.984	1.176
Tetrahydrofuran(1)+chlorocyclohexane(2) at 101.3 kPa				
411.37	0.0151	0.1384	1.514	0.979
401.45	0.0673	0.3260	0.976	1.055
393.92	0.1045	0.4946	1.118	1.021
385.87	0.1598	0.6103	1.080	1.068
373.81	0.2846	0.7877	1.043	1.007
369.34	0.3412	0.8372	1.036	0.977
362.29	0.4518	0.8955	1.007	0.968
358.03	0.5179	0.9196	1.013	0.991
351.60	0.6467	0.9522	1.008	1.030
347.29	0.7598	0.9719	0.994	1.059
343.68	0.8590	0.9857	0.995	1.066
341.21	0.9380	0.9938	0.992	1.167
Tetrahydropyran(1)+chlorocyclohexane(2) at 40.0 kPa				
379.87	0.0365	0.1384	0.911	1.001
375.20	0.0906	0.2970	0.890	1.008
369.77	0.1584	0.4570	0.908	1.012
364.89	0.2383	0.5900	0.895	1.003
360.63	0.3057	0.6821	0.914	0.996
355.45	0.3901	0.7732	0.949	0.984
349.89	0.5029	0.8519	0.966	0.981
343.90	0.6473	0.9183	0.985	0.975
340.29	0.7598	0.9563	0.988	0.893
337.14	0.8504	0.9761	1.006	0.901
335.01	0.9272	0.9908	1.011	0.784
Tetrahydropyran(1)+chlorocyclohexane(2) at 101.3 kPa				
412.67	0.0376	0.1204	0.900	0.989
408.29	0.0811	0.2342	0.890	1.011
401.98	0.1685	0.4234	0.888	0.998
397.09	0.2383	0.5415	0.897	0.994
392.70	0.3000	0.6314	0.920	0.987
387.19	0.3938	0.7333	0.930	0.973
382.07	0.4790	0.8027	0.951	0.982
374.65	0.6431	0.9003	0.964	0.922
370.50	0.7404	0.9393	0.978	0.888
365.65	0.8587	0.9717	1.000	0.901
363.10	0.9324	0.9901	1.009	0.722
2-Methyl-tetrahydrofuran(1)+chlorocyclohexane(2) at 40.0 kPa				
381.10	0.0184	0.1061	1.088	0.980
373.60	0.0759	0.3311	0.995	0.996
368.70	0.1246	0.4631	0.964	0.999
362.82	0.1858	0.5975	0.980	0.993
356.83	0.2586	0.7002	0.979	1.015
348.97	0.3770	0.8082	0.981	1.052
346.00	0.4445	0.8566	0.967	0.996
341.67	0.5251	0.8973	0.985	1.001
338.17	0.6001	0.9285	1.001	0.963
335.95	0.6716	0.9482	0.984	0.938
331.49	0.7938	0.9759	0.999	0.852
328.17	0.8906	0.9830	1.010	1.324
2-Methyl-tetrahydrofuran(1)+chlorocyclohexane(2) at 101.3 kPa				
412.13	0.0272	0.1188	1.036	0.994
405.23	0.0855	0.3080	0.984	0.996
401.19	0.1218	0.4028	0.984	1.000
393.99	0.1946	0.5436	0.974	1.023
387.97	0.2721	0.6555	0.964	1.022
381.00	0.3693	0.7501	0.961	1.063
376.32	0.4542	0.8199	0.960	1.030
371.91	0.5318	0.8690	0.974	1.012
368.68	0.5997	0.9005	0.975	1.005
365.57	0.6676	0.9272	0.981	0.988
360.08	0.7914	0.9660	1.004	0.897
356.98	0.8811	0.9830	1.003	0.884

Table 2 (*Continued*)

T (K)	x_1	y_1	γ_1	γ_2
2,5-Dimethyl-tetrahydrofuran(1)+chlorocyclohexane(2) at 40.0 kPa				
379.77	0.0380	0.1560	1.136	0.984
374.22	0.0915	0.3274	1.141	0.995
370.39	0.1396	0.4463	1.128	0.983
364.67	0.2174	0.5825	1.106	0.992
359.22	0.2914	0.6876	1.138	0.996
353.91	0.3980	0.7825	1.110	0.993
349.09	0.5019	0.8428	1.100	1.044
344.79	0.6046	0.8957	1.113	1.034
342.58	0.6952	0.9174	1.065	1.161
340.70	0.7485	0.9418	1.081	1.071
339.32	0.8484	0.9619	1.020	1.231
338.17	0.9134	0.9727	0.996	1.620
2,5-Dimethyl-tetrahydrofuran(1)+chlorocyclohexane(2) at 101.3 kPa				
411.40	0.0442	0.1568	1.200	0.986
406.51	0.0915	0.2926	1.196	0.991
401.52	0.1574	0.4315	1.140	0.985
395.46	0.2265	0.5548	1.164	0.997
391.27	0.2944	0.6476	1.150	0.978
384.61	0.4010	0.7432	1.134	1.027
379.11	0.5179	0.8340	1.129	0.980
374.79	0.6240	0.8811	1.105	1.035
372.65	0.6876	0.9100	1.096	1.011
369.07	0.8229	0.9491	1.050	1.138
367.49	0.8786	0.9585	1.037	1.429
367.02	0.9123	0.9721	1.026	1.351

The Antoine equation has been used for calculating the p_i^0. Antoine's constants for tetrahydrofuran were taken from Riddick et al. [10], for 2-methyl-tetrahydrofuran and 2,5-dimethyl-tetrahydrofuran were attained from TRC tables [9], for tetrahydropyran were obtained from our own vapour pressure measurements and those for chlorocyclohexane were taken from Gmehling et al. [11]. All of them are shown in Table 3. The second virial coefficients B_{ii} have been estimated using the Redlich–Kwong equation [12]. The cross second virial coefficients, B_{ij}, have been calculated by means of the Amdur–Mason equation [13]. Finally, the molar volumes V_i^0 were calculated using the Yen and Woods method [14].

Table 3
Constants of Antoine's equation for vapour pressures of the pure compounds (temperature in °C, pressure in kPa)

Compound	A	B	C
Tetrahydrofuran [9]	6.12142	1203.11	226.355
Tetrahydropyran	5.85520	1131.93	205.83
2-Methyl-tetrahydrofuran [9]	5.95009	1175.51	217.80
2,5-Dimethyl-tetrahydrofuran [9]	5.69272	1099.53	205.72
Chlorocyclohexane [11]	5.73540	1235.48	188.647

The thermodynamic consistency of the experimental data has been checked using the point-to-point method of Van Ness, described by Fredenslund et al. [15]. 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 smaller than 0.01. All systems satisfy this condition, thus it can be considered that the experimental data are thermodynamically consistent. The results are reported in Table 4.

The activity coefficients have been correlated with the Wilson, NRTL and UNIQUAC equations [11]. As recommended by Renon and Prausnitz [16], the mixture nonrandomness parameter α_{12} in the NRTL equation was set as 0.3. The estimation of parameters for the three correlation equations is based on minimization of an objective function F which, for a binary system, is given by the expression:

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

where γ_i are the corresponding activity coefficients and N the number of experimental data. The minimization of F has been done with a non-linear regression procedure [17].

Table 4
Results of the thermodynamic consistency test, average deviation ΔP and Δy

System	P (kPa)	ΔP (kPa)	Δy
Tetrahydrofuran+	40.0	0.7	0.0054
	101.3	2.4	0.0088
Tetrahydropyran+	40.0	0.5	0.0016
	101.3	1.1	0.0026
2-Methyl-tetrahydrofuran+	40.0	1.2	0.0047
	101.3	1.2	0.0019
2,5-Dimethyl-tetrahydrofuran+	40.0	0.6	0.0053
+Chlorocyclohexane	101.3	0.9	0.0047

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)+chlorocyclohexane(2) at 40.0 kPa						
Wilson	883.5723a	−503.1581[a]	0.46	0.0066	1.10	1.16
NRT	152.6802a	193.6716[a]	0.47	0.0063	1.11	1.14
UNIQUAC	−68.7249a	104.3476[a]	0.49	0.0068	1.10	1.17
Tetrahydrofuran(1)+chlorocyclohexane(2) at 101.3 kPa						
Wilson	2814.0678	−2166.1981	0.41	0.0094	1.17	1.07
NRTL	−1571.7782	2300.5535	0.43	0.0092	1.16	1.08
UNIQUAC	−1178.3952	1501.5248	0.50	0.0091	1.15	1.10
Tetrahydropyran(1)+chlorocyclohexane(2) at 40.0 kPa						
Wilson	−1318.8832	1466.7000	0.30	0.0021	0.88	0.79
NRTL	2175.3694	−2193.9310	0.28	0.0021	0.88	0.80
UNIQUAC	1041.0813	−1091.5110	0.30	0.0027	0.90	0.77
Tetrahydropyran(1)+chlorocyclohexane(2) at 101.3 kPa						
Wilson	−1691.5890	1948.6381	0.28	0.0020	0.86	0.75
NRTL	2749.0998	−2716.2580	0.27	0.0020	0.85	0.76
UNIQUAC	1682.4389	−1568.0163	0.27	0.0018	0.89	0.72
2-Methyl-tetrahydrofuran(1)+chlorocyclohexane(2) at 40.0 kPa						
Wilson	−2154.6851	5165.0663	0.71	0.0070	0.99	1.58
NRTL	−1901.3131	2317.1870	0.29	0.0045	1.01	0.96
UNIQUAC	−1145.1566	1294.4927	0.33	0.0051	1.02	0.97
2-Methyl-tetrahydrofuran(1)+chlorocyclohexane(2) at 101.3 kPa						
Wilson	−1005.1753	1213.9802	0.30	0.0058	0.95	0.92
NRTL	1919.4107	−1791.9842	0.29	0.0059	0.95	0.92
UNIQUAC	1703.4746	−1470.8674	0.18	0.0049	0.98	0.88
2,5-Dimethyl-tetrahydrofuran(1)+chlorocyclohexane(2) at 40.0 kPa						
Wilson	−2040.2995	5351.0695	0.56	0.0074	1.21	2.35
NRTL	6131.2791	−2978.1951	0.51	0.0072	1.16	2.07
UNIQUAC	3418.1197	−2006.4920	0.60	0.0092	1.24	2.10
2,5-Dimethyl-tetrahydrofuran(1)+chlorocyclohexane(2) at 101.3 kPa						
Wilson	−2378.2621	6202.4909	0.19	0.0036	1.17	2.39
NRTL	6151.5724	−3154.6825	0.31	0.0046	1.14	1.83
UNIQUAC	3846.0756	−2245.8683	0.26	0.0028	1.21	2.09

[a] Joules per mole.

The adjustable parameters A_{12} and A_{21} and the average deviations (ΔT and Δy), along with the activity coefficients at infinite dilution are listed in Table 5. All systems yield similar deviations in both T and y. The greatest value for ΔT is 0.7 K and corresponds to the mixture 2-methyl-tetrahydrofuran+chlorocyclohexane at 40.0 kPa. For Δy, the values are <0.01 and the biggest is obtained for the system tetrahydrofuran+chlorocyclohexane at 101.3 kPa. It can be concluded that all equations show a good performance in correlating the activity coefficients.

The T–x_1–y_1 diagrams were obtained by employing the NRTL equation. They are graphically represented in Figs. 1–4, together with experimental VLE data. These diagrams are indicative that there does not exist azeotropic behaviour. The calculations confirm this observation.

The four studied systems behave near ideality at both pressures, so near in fact that only mixtures containing tetrahydropyran and 2,5-dimethyl-tetrahydrofuran show a definite behaviour. The first ones deviate negatively from ideality while the second

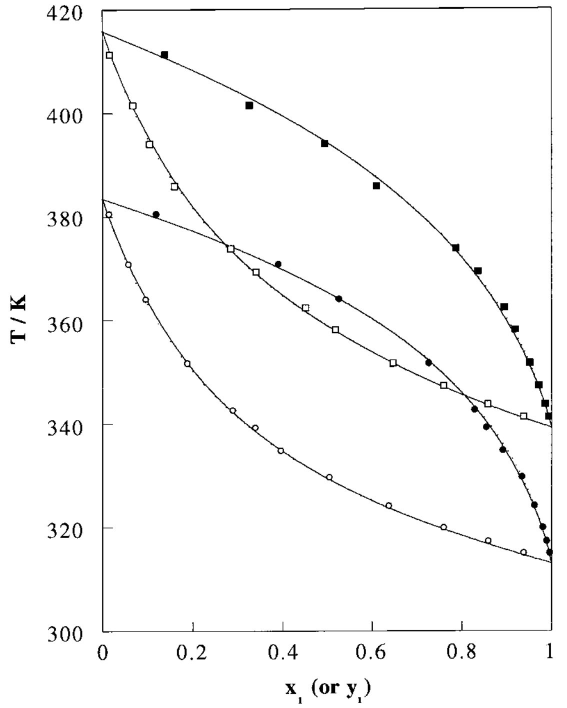

Fig. 1. T–x_1–y_1 diagram for tetrahydrofuran(1)+chlorocyclohexane(2): (○, ●) exptl. data at 40.0 kPa; (□, ■) exptl. data at 101.3 kPa; (—) Wilson equation.

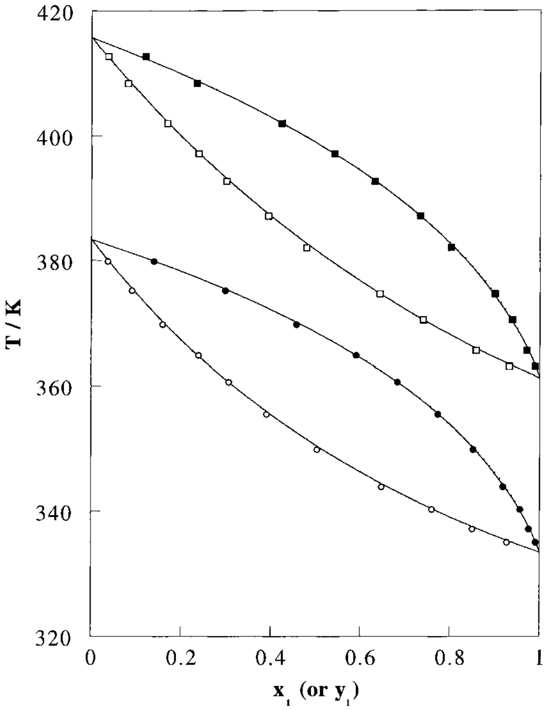

Fig. 2. T–x_1–y_1 diagram for tetrahydropyran(1)+chlorocyclohexane(2): (○, ●) exptl. data at 40.0 kPa; (□, ■) exptl. data at 101.3 kPa; (—) Wilson equation.

mixtures do it positively. These results can be explained considering that the specific interaction Cl–O(ether) existent in the mixture is strong enough to compensate the breaking of the interactions present in the pure liquids (mainly, the dipole–dipole ones). It must be pointed out that other effects, especially those relationed with the branching of the cyclic ether, are important, too.

It is also interesting a comparison between these results and those obtained for systems in which the same cyclic ethers are mixed with chlorobenzene [4]. Excepting tetrahydropyran, the deviations from Raoult's Law are more positive in the case of the mixture with the cyclohexane derivative. This is a result to be expected. On the one hand, the specific π–O(ether) interaction is eliminated. On the other hand, the aliphatic cycle has not the rigid structure of the aromatic ring and therefore hinders in a greater extension the possible interactions. The behaviour of mixtures containing tetrahydropyran is similar with both aliphatic and aromatic derivatives. This could be due to the fact that tetrahydropyran is the worst donor of all the ethers [18], then the π–O(ether) interaction is the weakest. Moreover, the accommodation of tetrahydropyran would be better in chlorocyclohexane than in chlorobenzene because ether and chlorocyclohexane have very similar structures.

4. VLE predictions

ASOG [19] and modified-UNIFAC [20] have been used to predict VLE. The van der Waals parameters r_i and q_i for the groups c-(CH$_2$–O–CH) and c-(CH–O–CH), necessary in the calculations for modified-UNIFAC, are not available. Then this contribution method cannot be applied with systems involving 2-methyl-tetrahydrofuran and 2,5-dimethyl-tetrahydrofuran. In Table 6 are listed the average deviations in both T and y obtained applying these predictive methods. Both of them yield similar ΔT and Δy, with especially satisfactory results for the mixtures containing tetrahydro-

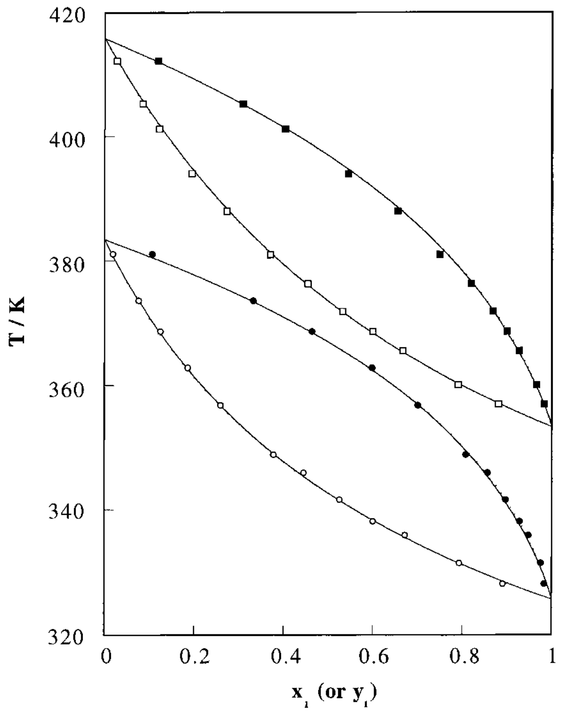

Fig. 3. T–x_1–y_1 diagram for 2-methyl-tetrahydrofuran(1)+chlorocyclohexane(2) : (○, ●) exptl. data at 40.0 kPa; (□, ■) exptl. data at 101.3 kPa; (—) Wilson equation.

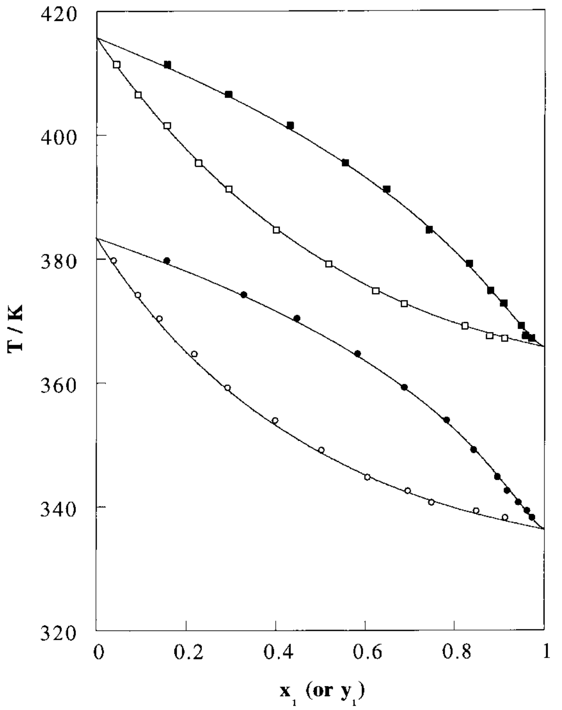

Fig. 4. T–x_1–y_1 diagram for 2,5-dimethyl-tetrahydrofuran(1)+-chlorocyclohexane(2): (○, ●) exptl. data at 40.0 kPa; (□, ■) exptl. data at 101.3 kPa; (—) Wilson equation.

pyran. For the remaining cyclic ethers, the predictions present appreciably greater deviations. The working pressure scarcely affects to the predicted results.

When these values are compared with those obtained for the mixtures chlorobenzene+cyclic ethers [4], it can be seen that the values of ΔT and Δy are bigger in the case of the cyclohexane derivative for both of the group contribution methods. At sight of this, it seems necessary to achieve more experimental information in order to enlarge the available database and, in this way, to revise and improve the existing interaction parameters in mixtures that present either specific interactions (Cl–O this time) or great differences between the boiling points.

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
+Chlorocyclohexane	101.3	–	–	0.78	0.0088

Acknowledgements

The authors are grateful for financial assistance from Universidad de Zaragoza (Proyecto UZ: 96-232-47) and Diputación General de Aragón (Proyecto PCB-0894).

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