

Isothermal vapor–liquid equilibrium data for the decafluorobutane (R3110) + 1,1,1,3,3-pentafluorobutane (R365mfc) system at temperatures from 333 K to 441 K

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ABSTRACT

The organic Rankine cycle (ORC) is one solution to recover energy from high temperature hot sources. It requires working fluid with high critical coordinate values. It is named for its use for an organic high molecular mass fluid with a liquid–vapor phase change. The knowledge of phase diagram of working fluid is a crucial task in refrigeration process. In this context, a new mixture of decafluorobutane (R3110) and 1,1,1,3,3-pentafluorobutane (R365mfc), is studied by means of experimental measurements and modeling procedures. The purpose is to obtain the isothermal vapor–liquid equilibrium data (R3110+R365mfc) of binary system ranging from (333.26 to 441.61)K temperature, and (0.2016 to 3.0927)MPa pressure. The data were obtained with accurate within $u(T, k=2) = 0.02$ K, $u(P, k=2) = 0.0003$ MPa and $u(z) = 0.004$ for molar composition. In the present work, the static analytic method is another time investigated to achieve a high quality data as it was largely demonstrated previously by the team of our laboratories. The experimental data are correlated using the classical equations: Peng–Robinson equation of state, the Mathias–Copeman alpha function, and the Wong–Sandler mixing rules involving the NRTL model. The predicted critical line is well reproduced.

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1. Introduction

Energy access is a fundamental parameter for human development. Institutions such as the World Bank, the United Nations or the European Union consider it as a key-element for promoting and improving social infrastructures such as electricity, water, health, education and communication. Organic Rankine cycle (ORC) gives us opportunity to produce energy from high temperature hot sources (like high pressure steam for example) and to optimize production of energy. ORC is composed of two exchangers (evaporator and condenser), one turbine (to produce energy) and one pump. The ORC technology can play a non negligible role:

- It can have a beneficial effect on the energy intensity of industrial processes, mainly by recovering waste heat;
- It can have a positive effect on consumptions;
- It can be used to convert renewable heat source into electricity. This mainly includes geothermal, biomass and solar sources,

- During the shifting transition toward electric vehicles, it can be used to increase the well-to-wheel efficiency by waste heat recovery on the exhaust gases, on the EGR and the engine coolant [1].

The knowledge of phase diagram is essential for its selection as possible working fluid. The working fluid is the fluid which circulates inside the thermodynamic system. It transports energy and exchange with the environment (evaporator and condenser). Several criteria (high values of T_c , low GWP, good capacity of heat pump, etc.) [2] have to be taken into account. Our laboratories have already published many articles dealing with this subject, for example, experimental vapor–liquid equilibria data of decafluorobutane + ethane [3], carbon dioxide + decafluoroethane [4] and decafluorobutane + DMF [5]. As R3110 and R365mfc possess high critical temperatures, they seem to be very effective for application in organic Rankine cycle processes.

In this work, we present vapor–liquid equilibrium (VLE) data for the system R3110 + R365mfc at seven isotherms; three isotherms below and four above the critical temperature of R3110. This system has not been yet investigated and the measurements (PTxy) represent new data.

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List of symbols

<i>a</i>	parameter of the equation of state (energy parameter ($\text{J m}^3 \text{ mol}^{-2}$))
<i>b</i>	parameter of the equation of state (molar co volume parameter ($\text{m}^3 \text{ mol}^{-1}$))
<i>c</i>	Mathias–Copeman coefficient
<i>F</i>	objective function
<i>g</i>	molar Gibbs energy (J mol^{-1})
<i>k_{ij}</i>	binary interaction parameter
<i>n_x</i>	number of measurements for liquid phase
<i>n_y</i>	number of measurements for vapor phase
<i>P</i>	pressure (MPa)
<i>R</i>	gas constant ($\text{J mol}^{-1} \text{ K}^{-1}$)
<i>T</i>	temperature (K)
<i>u</i>	uncertainty
<i>x</i>	liquid mole fraction
<i>y</i>	vapor mole fraction

Greek letters

β	constant used in the Eq. (4)
λ_i	parameters used in the Eqs. (4) and (5)
ω	acentric factor
ΔU	deviation ($U_{\text{exp}} - U_{\text{cal}}$)

Superscript

<i>E</i>	excess property
<i>0</i>	initial state

Subscripts

<i>C</i>	critical property
<i>cal</i>	calculated property
<i>exp</i>	experimental property
<i>i,j</i>	molecular species
<i>1</i>	R3110 (C_4F_{10})
<i>2</i>	R365fmc

This data were correlated with the Peng–Robinson equation of state [6], the Mathias–Copeman alpha function [7], with the Wong–Sandler mixing rules [8], and utilizing NRTL activity coefficient model [9]. This model will be used to define the phase diagram of the system. The model parameters have been used to calculate the critical temperature and pressure.

2. Experimental

2.1. Materials

The Perfluorobutane [R3110, CAS number: 355-25-9] was supplied by Pelchem (South Africa) with a certified volume purity greater than 98%, while R365mfc [365mfc, CAS number: 406-58-6] was purchased from DEHON (France) and with 99.99 a purity vol.%. The chemicals were used without any further purification.

2.2. Apparatus

The apparatus used in this work is based on a static-analytic method with liquid and vapor phase sampling. The apparatus used in this work is identical to the one used within the previous one (Madani et al. [10–12]). The equipment is fully described in these 3 previous papers. The following concerns the presentation of experimental uncertainties.

The equilibrium cell is immersed inside a temperature regulated liquid bath. Temperatures are measured with two platinum

probes (Pt100). They are inserted inside upper and lower flanges of the equilibrium cell. These Pt100 probes are calibrated against a 25 Ω reference probe (TINSLEY Precision Instrument) certified by the Laboratoire National d'Essais (Paris) following the International Temperature Scale 1990 protocol.

Pressures are measured using a pressure transducer (Druck, type PTX611, range: 0–100 MPa). This sensor is calibrated against a dead weight pressure balance (5202S model from Desgranges & Huot).

Temperature and pressure data were recorded via a computer linked to an HP unit (HP34970A). The resulting uncertainties in this work are $u(T, k=2) = 0.02 \text{ K}$ and $u(P, k=2) = 0.0003 \text{ MPa}$.

The analytical work was carried out using a gas chromatograph equipped with a thermal conductivity detector (TCD) connected to a data acquisition system.

The analytical column used for the separation is a 5% Krytox on CarboBlack B model with 60/80 mesh (2 mm internal diameter, Silcostell tube, 1.5 m length). The TCD was repeatedly calibrated by introducing known amounts of each pure compound. Special GC syringe are used for the introduction of chemicals in the injector of the gas chromatograph. Taking into account the uncertainties due to calibrations and dispersions of analyses, resulting uncertainties on vapor and liquid mole numbers are estimated to be less than $\pm 2.5\%$. Consequently, the maximum uncertainty on mole fraction is $u(z) = 0.004$.

2.3. Experimental procedure

The experimental procedure is similar to the one presented in previous papers [10,11,13]. The thermodynamic equilibrium is reached when no evolution of pressure and temperature is observed whatever the condition of stirring. At least between 8 and 10 samples are taken. Average composition value and its standard deviation are calculated.

2.4. Data correlations

The critical temperatures (T_c), critical pressures (P_c) for each of the two pure components are provided in Table 1.

Our experimental VLE data are correlated by means of homemade software. We have used the PR EoS [5] with the Mathias–Copeman [6] alpha function for accurate representation of the pure component vapor pressures.

The Wong–Sandler (WS) [7] mixing rule is chosen for its capability to represent VLE data close the mixture critical point as we can use 3 interaction parameters (τ_{ji} and τ_{ij} of the excess Gibbs energy model and k_{ij} the binary interaction parameter). The excess Gibbs energy model chosen is the NRTL [8] local composition model. It is recommended [8] to use non randomness parameter value (α_{ji}) equal to 0.3 for systems like this one. τ_{ji} and τ_{ij} are adjusted directly onto VLE data through a modified Simplex algorithm [14] using the following objective function (Flash algorithm):

$$F = \frac{100}{N} \left[\sum_1^N \left(\frac{x_{\text{exp}} - x_{\text{cal}}}{x_{\text{exp}}} \right)^2 + \sum_1^N \left(\frac{y_{\text{exp}} - y_{\text{cal}}}{y_{\text{exp}}} \right)^2 \right] \quad (1)$$

where N is the number of data points, x_{exp} and x_{cal} are respectively the measured and calculated liquid phase mole fractions, y_{exp} and y_{cal} are respectively the measured and calculated vapor phase mole fractions.

3. Results and discussion

3.1. Vapor pressures data

R365mfc vapor pressures were measured for 24 temperatures from 332.79 K to 447.89 K and used to adjust Mathias–Copeman

Table 1
Critical parameters and Mathias–Copeman coefficients.

Compound	CAS number	T_c (K)	P_c (MPa)	c_1	c_2	c_3	Purity vol.%
R3110	355-25-9	385.84	2.2899	0.9352 ^a	-0.41797 ^a	1.5743 ^a	98.00
R365mfc	406-58-6	460.00	3.2660	1.0031	-1.3302	5.1445	99.99

^a From ref [15].

Table 2
Experimental and calculated vapor pressures^a for R365mfc. Δ deviation from PR EoS using Mathias–Copeman alpha function.

T (K)	P_{exp} (MPa)	P_{cal} (MPa)	ΔP (MPa)
332.79	0.1949	0.1941	0.0008
333.18	0.1971	0.1965	0.0006
342.65	0.2615	0.2624	-0.0009
347.94	0.3039	0.3057	-0.0018
352.87	0.3487	0.3507	-0.0020
357.77	0.4011	0.4002	0.0009
363.03	0.4592	0.4589	0.0003
367.94	0.5198	0.5193	0.0005
372.87	0.5861	0.5859	0.0002
378.04	0.6623	0.6623	0.0000
382.95	0.7414	0.7417	-0.0003
387.88	0.8289	0.8284	0.0005
393.02	0.9272	0.9269	0.0003
398.06	1.0364	1.0319	0.0045
402.92	1.1460	1.1417	0.0043
408.07	1.2715	1.2676	0.0039
413.09	1.4038	1.4004	0.0034
418.00	1.5424	1.5407	0.0017
423.13	1.6986	1.6989	-0.0003
428.15	1.8627	1.8660	-0.0033
433.05	2.0345	2.0415	-0.0070
438.03	2.2254	2.2333	-0.0079
442.99	2.4255	2.4388	-0.0133
447.89	2.6371	2.6568	-0.0197

^a Uncertainty on temperature $u(T, k=2) = \pm 0.02$ K; uncertainty on pressure $u(P, k=2) = \pm 0.0003$ MPa.

alpha function parameters (see Table 1). Experimental and calculated vapor pressures values are reported in Table 2. The absolute relative deviation observed is less than 1.00% for R365mfc and plotted in Fig. 1. Concerning the R3110 the Mathias–Copeman parameters are taken from ref [15] (see Table 1).

3.2. Vapor–liquid equilibrium data for the R3110 + R365mfc mixture

The experimental and calculated VLE data are reported in Table 3 and plotted in Fig. 2. The adjusted parameters corresponding to the WS mixing rules involving the NRTL model, associated to PR EoS, are given in Table 4.

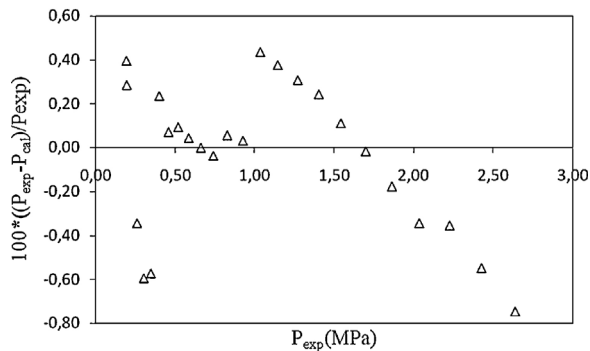


Fig. 1. Relative deviation of R365mfc pure component vapor pressure between experimental data and calculated values using Peng–Robinson equation of state involving Mathias–Copeman alpha function.

Table 3
Vapor–liquid^a equilibrium and phase compositions for the R3110 (1)–R365mfc (2) mixture (standard deviation: $\delta = ((n \sum x^2 - (\sum x)^2) / (n(n-1)))^{1/2}$).

P (MPa)	n_x	x_1	$\delta x_1 * 10^3$	n_y	y_1	$\delta y_1 * 10^3$
333.26 K						
0.3864	7	0.1082	0.4	6	0.4780	1.0
0.4303	8	0.1487	0.4	5	0.5396	0.5
0.4802	8	0.2070	0.7	6	0.6000	1.0
0.5203	7	0.2690	0.8	4	0.6310	7.0
0.5691	6	0.3682	0.8	5	0.6870	1.0
0.6125	6	0.4720	4.0	5	0.7310	1.0
0.6515	6	0.6100	2.0	7	0.7780	1.0
353.34 K						
0.5096	6	0.0566	0.1	5	0.2760	2.0
0.5470	6	0.0736	0.1	6	0.3320	2.0
0.6204	6	0.1130	0.2	6	0.4239	0.8
0.6970	5	0.1630	0.5	4	0.4940	3.0
0.7972	6	0.2450	2.0	6	0.5740	2.0
0.8948	4	0.3590	2.0	4	0.6455	0.7
0.9360	5	0.4240	3.0	4	0.6726	0.1
1.0061	4	0.5430	5.0	4	0.7250	2.0
373.71 K						
0.7822	6	0.0526	0.1	4	0.2000	1.0
1.0045	7	0.1370	0.8	3	0.3653	0.8
1.1261	6	0.2028	0.2	4	0.4705	1.0
1.3102	4	0.3294	0.3	4	0.5737	0.8
1.3958	5	0.4050	0.4	5	0.6120	2.0
1.5033	6	0.5150	1.0	8	0.6690	2.0
1.5901	4	0.6160	1.0	7	0.7260	2.0
1.6823	5	0.7420	2.0	7	0.7990	1.0
393.64 K						
1.0609	5	0.0257	0.0	5	0.0816	0.9
1.2082	3	0.0698	0.9	4	0.2040	1.0
1.6930	5	0.2365	0.3	3	0.4420	1.0
1.8122	7	0.2949	0.9	4	0.4880	2.0
1.8637	6	0.3188	0.5	5	0.5046	0.9
1.9509	7	0.3693	0.7	7	0.5351	0.9
2.0100	7	0.4062	0.7	6	0.5590	2.0
2.0766	5	0.4477	0.3	7	0.5830	1.0
2.1598	6	0.5048	0.5	5	0.6170	2.0
2.2468	5	0.5660	1.0	5	0.6494	0.5
2.3562	6	0.6490	1.0	6	0.7020	1.0
2.4475	4	0.7242	0.9	5	0.7331	0.7
413.65 K						
1.5562	9	0.0257	0.0	4	0.0761	0.6
1.6412	2	0.0420	0.2	5	0.1170	0.7
1.7316	5	0.0615	0.1	1	0.1520	1.0
1.8361	6	0.0853	0.2	5	0.2030	1.0
1.9226	5	0.1062	0.2	3	0.2350	1.0
2.0494	5	0.1409	0.3	5	0.2860	2.0
2.1711	5	0.1748	0.6	3	0.3236	0.3
2.3022	6	0.2182	0.5	5	0.3660	1.0
2.3564	4	0.2367	0.2	5	0.3756	0.5
2.4721	5	0.2755	0.3	6	0.4060	3.0
2.5460	7	0.3057	0.3	5	0.4260	1.0
2.6942	5	0.3671	0.8	3	0.4538	0.2
2.7782	4	0.4049	0.3	5	0.4350	2.0
433.61 K						
2.1163	7	0.0089	0.3	5	0.0211	0.4
2.1893	6	0.0216	0.0	7	0.0479	0.5
2.2579	2	0.0326	0.1	2	0.0675	0.3
2.3487	4	0.0483	0.1	2	0.0976	0.1
2.3946	5	0.0566	0.2	5	0.1137	0.4
2.4427	5	0.0654	0.1	4	0.1260	0.2
2.4934	3	0.0749	0.1	3	0.1394	0.7

Table 3 (Continued)

P (MPa)	n_x	x_1	$\delta x_1 \cdot 10^3$	n_y	y_1	$\delta y_1 \cdot 10^3$
2.5428	4	0.0847	0.1	3	0.1540	2.0
2.5751	4	0.0913	0.0	3	0.1620	1.0
2.6256	4	0.1017	0.1	3	0.1766	0.2
2.6689	4	0.1109	0.1	3	0.1884	0.4
2.7022	3	0.1181	0.1	4	0.1952	0.3
2.7623	10	0.1317	0.0	6	0.2089	0.4
2.8228	9	0.1461	0.1	6	0.2224	0.7
2.8655	5	0.1559	0.1	9	0.2290	0.6
2.9765	6	0.1852	0.1	5	0.2462	0.3
3.0308	13	0.2012	0.1	9	0.2530	3.0
3.0712	8	0.2162	0.2	5	0.2564	0.2
3.0931	5	0.2352	0.6	4	0.2500	4.0
441.83 K						
2.5064	5	0.0203	0.0	5	0.0402	0.1
2.6397	9	0.0419	0.0	9	0.0768	0.2
2.7415	9	0.0595	0.1	7	0.1019	0.3
2.8263	9	0.0748	0.0	9	0.1213	0.4
2.9358	6	0.0962	0.0	5	0.1438	0.4
3.0277	10	0.1157	0.1	6	0.1595	0.4
3.0927	6	0.1313	0.1	5	0.1678	0.1
3.1490	16	0.1484	0.1	6	0.1664	0.4

^a Uncertainty on temperature $u(T, k=2) = \pm 0.02$ K, uncertainty on pressure $u(P, k=2) = \pm 0.0003$ MPa, maximum uncertainty on composition $u(x, y) = \pm 0.004$.

Table 4

Values of the binary parameters at each temperature.

T (K)	τ_{12} (J mol ⁻¹)	τ_{21} (J mol ⁻¹)	k_{12}
333.26	4967	3334	-0.1007
353.34	2675	2652	0.0866
373.71	1596	3001	0.1270
393.64, 413.65, 433.61, 441.83	1477	2840	0.1348

The deviations, average absolute relative deviation (AARDU), and the BIASU (see Table 5), applied on liquid and vapor phase mole fractions, are defined by:

$$\text{AARDU} = \left(\frac{100}{N} \right) \sum \left| \frac{U_{\text{cal}} - U_{\text{exp}}}{U_{\text{exp}}} \right| \quad (2)$$

Table 5

Relative deviations MRDU and BIASU obtained in fitting experimental VLE data with PR EoS, Mathias–Copeman alpha function and WS mixing rules involving NRTL model.

T (K)	Bias $x\%$	MRD $x\%$	Bias $y\%$	MRD $y\%$
333.26	-0.14	0.84	-1.19	1.68
353.34	-0.30	1.11	-2.92	3.25
373.71	0.24	0.90	-3.69	4.08
393.64	0.03	1.90	-3.20	3.66
413.65	0.41	0.93	-1.73	2.62
433.61	0.22	1.09	-1.01	1.25
441.83	2.01	2.24	2.02	2.34

$$\text{BIASU} = \left(\frac{100}{N} \right) \sum \left(\frac{U_{\text{exp}} - U_{\text{cal}}}{U_{\text{exp}}} \right) \quad (3)$$

where N is the number of data points, and $U = x_1$ or y_1 .

3.3. Critical lines computation

The isothermal experimental data have been used to estimate the critical point (composition and pressure). The critical loci for binary mixtures and the near-critical behavior were approximated by the use of extended scaling laws, as proposed previously [16]. In this method the near-critical part of the pressure-composition diagram was represented by complementing the near-critical scaling law with a linear term.

$$y - x = \lambda_1(P_c - P) + \mu(P_c - P)^\beta \quad (4)$$

$$\frac{y+x}{2} - x_c = \lambda_2(P_c - P) \quad (5)$$

Parameters λ_1 , λ_2 , μ , P_c and x_c are adjusted using experimental data close to the mixture critical point. The values are reported in Table 6 and plotted in Fig. 3.

The method used for evaluation of critical using cubic equation of state is identical to the one presented in previous papers. It is based on Heidemann and Khalil [17] algorithm generalized by Stockfleth and Dohrn [18] in 1998. The temperature dependent binary parameters are those obtained by fitting VLE data in the

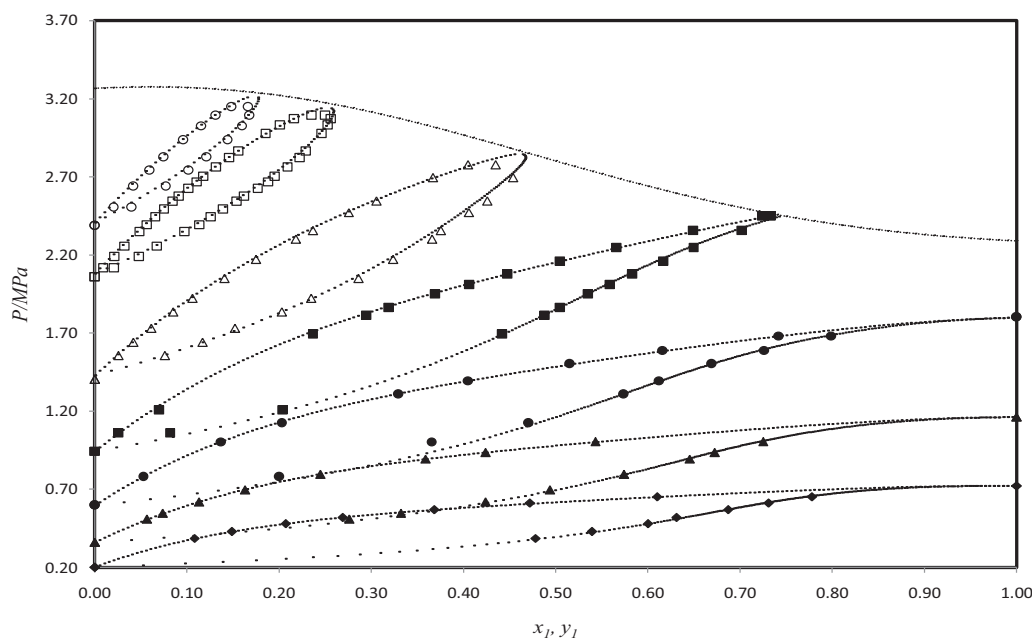


Fig. 2. VLE of the R3110 (1)–R365mfc (2) system at different temperatures \blacklozenge : 333.26 K, \blacktriangle : 353.34 K, \bullet : 373.71 K, \blacksquare : 393.64 K, \blacktriangledown : 413.65 K, \square : 433.61 K, \circ : 441.83 K. —: mixture critical point line. Dotted lines: phase envelopes calculated with PR EoS, Wong–Sandler mixing rules and NRTL activity coefficient model with parameters from Table 4.

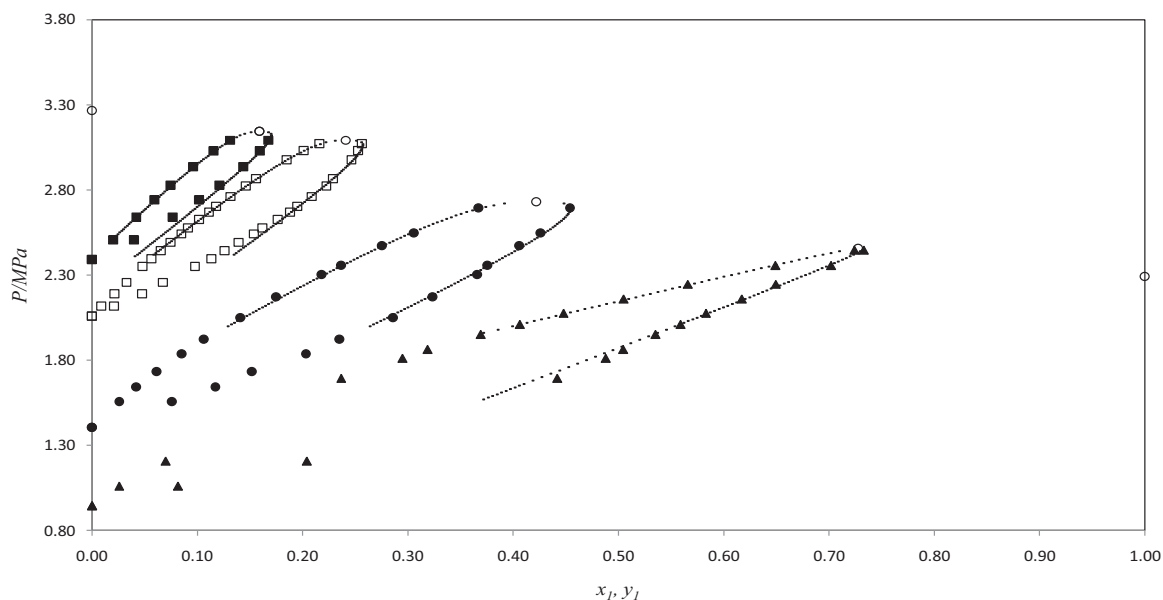


Fig. 3. VLE of the C_4F_{10} (1)–R365mfc (2) system at different temperatures \blacktriangle : 393.64 K, \bullet : 413.65 K, \square : 433.61 K, \blacksquare : 441.83 K, \circ : critique point, $-$: mixture critical point line. Solid lines: phase envelopes calculated with the molecular simulation (above the critical temperature of R3110).

Table 6

Parameters λ_1 , λ_2 , μ adjusted and critical points values determined by applying the scaling laws to the experimental data for the R3110 (1) + R365mfc (2) binary system.

T (K)	$\lambda_1 \cdot 10^4$	$\lambda_2 \cdot 10^4$	$\mu \cdot 10^3$	P_c (MPa)	x_{1c}
393.64	2332	−5529	62	2.455	0.72
413.65	−1441	−3102	266	2.729	0.42
433.61	−758	−2157	145	3.092	0.24
441.83	−976	−1936	113	3.136	0.15

R3110 supercritical domain. Results are plotted in Fig. 2. We have obtained a predicted critical locus line in good agreement with the isothermal phase envelopes.

Regarding the pseudo experimental critical point, we can see from Fig. 3 that the EoS over predict them. It may be interesting to use another experimental equipment to determine directly the critical temperature and pressure for each composition calculated. In order to better calculate their values, it is necessary to couple scaling law and classical EoS theory as presented by Kiselev and Friend [19].

4. Conclusion

In this paper, VLE data at seven temperatures for the R3110 + R365mfc system are presented. They were obtained using a “static-analytic” method. To fit these data the Peng–Robinson EoS, with the Mathias–Copeman alpha function and the Wong–Sandler

mixing rules involving the NRTL model was considered. The complete phase diagram is determined.

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