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New high-pressures vapor-liquid equilibrium data for the carbon dioxide + 2-methyl-1-propanol (isobutanol) binary system[*+]

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Abstract: New vapor-liquid equilibria (VLE) data at 333.15, 343.15, and 353.15 K and pressures up to 130.0 bar are reported for the carbon dioxide + 2-methyl-1-propanol (isobutanol) system. The experimental method used in this work was a static analytical method with liquid and vapor phases sampling using a rapid online sampler injector (ROLSI^{TM}) coupled to a gas chromatograph (GC) for analysis. Measured VLE data and literature data for carbon dioxide + 2-methyl-1-propanol system were modeled with the Soave-Redlich-Kwong (SRK) cubic equation of state with classical van der Waals (two-parameter conventional mixing rule, 2PCMR) mixing rules. A single set of interaction parameters that lead to a correct phase behavior was used in this work to model the new VLE data and critical points of the mixtures in a wide range of temperature and pressure. The SRK prediction results were compared to the new data measured in this study and to available literature data.

Keywords: *Carbon dioxide • 2-Methyl-1-Propanol (isobutanol) • SRK; High-pressures • EoS*

1. Introduction

Interest in supercritical fluids is increasing throughout numerous scientific and technological fields. A more efficient use of supercritical fluids as media for separations, reactions, and material productions requires reliable and accurate experimental measurements as well as quantitative prediction of phase equilibria, thermodynamic, and transport properties of supercritical fluid mixtures. High-pressure phase equlibrium data are necessary in a range of processes, such as those related to the oil industry (enhanced oil recovery, the transportation and storage of natural gas, simulation of petroleum reservoirs, study of geological processes), energy (carbon capture and storage, refrigeration and heat-pump cycles), chemical, food, or drugs industries (supercritical fluid chromatography, supercritical fluid extraction, separation of non-volatile mixtures, fractionation, nanoparticles formation, reaction, hydrothermal crystal growing, hydrothermal destruction of hazardous waste, polymer processing, *etc.*) [1-10].

This work is a part of a continuing study [11-28] of carbon dioxide + alkanols of interest in supercritical fluid extraction (SFE) and supercritical fluid chromatography (SFC), in biofuels, in the oil and natural gas industry, in the cosmetic, pharmaceutical, surfactant, and food industries [29,30]. Previously, we have published high-pressure phase equilibrium data for carbon dioxide + 1-alcohols (methanol [19,28,31,32], ethanol [14,20,26], 1-propanol [21], 1-butanol [25], 1-pentanol [13], 1-hexanol [16], 1-heptanol [22], 1-nonanol [15], 1-decanol [33]). Recently, we started to study the influence of the functional group position (hydroxil), *e.g.* carbon dioxide + 2-propanol [27], + 2-butanol [18], or the

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influence of hydrocarbon chain branching in alkanols, *e.g.* carbon dioxide + 2-methyl-2-propanol (*tert*-butanol) [34]. In this study we investigate the phase behavior of carbon dioxide + 2-methyl-1-propanol (isobutanol). The choice for the two branched alcohols firstly examined is motivated by the fact that they are butanol isomers. Our literature survey [2-4,35,36] revealed that the system is not extensively studied. In Table 1 are summarized the experimental conditions of the available information for the carbon dioxide + 2-methyl-1-propanol binary system. Although vapor-liquid equilibrium data or isothermal pressure-liquid phase compositions are reported by several papers [37-45], yet significant scatter can be observed among the sets from different groups.

Therefore, our objectives are to report new experimental data for the carbon dioxide + isobutanol binary system (1-butanol chain isomer) and to represent the phase behavior of this system with a cubic equation of state with classical van der Waals mixing rules, using a single set of binary interaction parameters.

The carbon dioxide + 2-methyl-1-propanol binary system can be atributted to type II fluid phase behavior, according to the classification of van Konynenburg and Scott [46,47], as Buechner [48] reported liquid-liquid equilibrium data at 251.15 K. Type II fluid phase behavior is characterized by a continuous critical liquid - vapor (L = V) loci connecting the critical points of the pure components [49] and a liquid - liquid (L = L) critical line intersecting in an upper critical endpoint (UCEP) with a liquid – liquid – vapor (LLV) three phase equilibrium line.

In this work we report new measurements using a static-analytical method, in a high-pressure visual cell, for carbon dioxide + 2-methyl-1-propanol at several temperatures (333.15, 343.15, and 353.15 K) and pressures up to 130 bar.

Measured and all available literature data for the carbon dioxide + 2-methyl-1-propanol system were modeled with the Soave-Redlich-Kwong (SRK) [50] cubic equation of state coupled with classical van der Waals mixing rules. A semi-predictive modeling approach, using a unique set of binary interaction parameters to predict the phase behavior of the system in a wide range of pressures and temperatures, was used as in our latest papers [11-16].

2. Experimental procedure

2.1. Materials

Carbon dioxide (mass fraction purity >0.997) was provided by Linde Gaz Romania and 2-methyl-1-propanol (mass fraction purity >0.998) was a Sigma product. The chemicals were used without further purification, except for the careful degassing of 2-methyl-1-propanol. Gas chromatographic analysis of 2-methyl-1-propanol give a mole fraction purity of >0.999.

2.2. Apparatus and procedure

The experimental setup was described in detail in earlier papers [11,14,26,27]. The apparatus used in this work is based on a high-pressure visual cell with variable volume [26,27], coupled with a new sampling and analyzing system [11,14]. The sampling system utilized two high-pressure electromechanical sampling valves, the so called rapid on-line sampler injector (ROLSI™, MINES ParisTech/CEP-TEP, – Centre énergétique et procédés, Fontainbleau, France [51]). The ROLSI valves are connected through capillaries to the equilibrium visual cell and to a gas chromatograph (GC). A heating resistance is used to heat the expansion chamber of the sampler injector so the liquid samples are rapidly vaporized. The transferring lines between ROLSI and the GC are heated by means of a linear resistor coupled to an Armines/CEP/TEP regulator. The GC (Perichrom) uses a thermal conductivity detector, TCD, with a HP-Plot/Q column 30 m long and 0.530 mm diameter. The GC carrier gas is helium at a flow rate of 30 mL min^{-1}. The setup was completed with a syringe pump Teledyne ISCO model 500D.

The working procedure is similar to that in our previous studies [13,16,29,30]. The entire internal loop of the apparatus including the equilibrium cell was rinsed

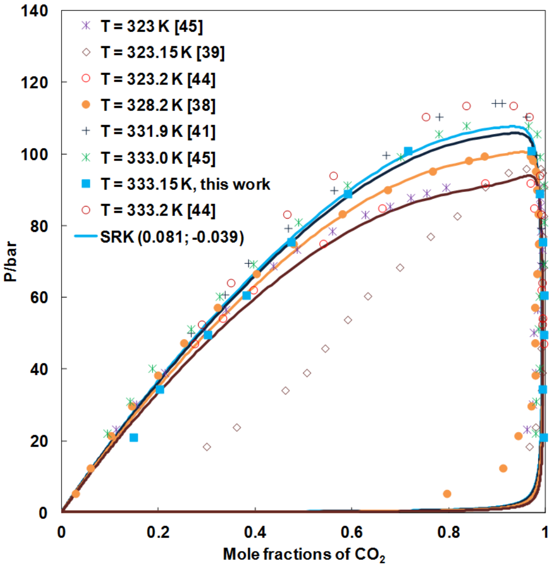

Figure 1. Comparison of new experimental data and literature data for the carbon dioxide + 2-methyl-1-propanol (isobutanol) system and calculations by SRK model: symbols, new data and literature data at different temperatures; solid lines, predictions by SRK (k_{12} = 0.081, l_{12} = -0.039).

Table 1. Literature VLE experimental data for the carbon dioxide + 2-methyl-1-propanol binary system.

T/K	P_{range}/bar	NEXP^{a}	Method	*u*(P)/bar	u(x)	Reference
273.15	6.40-36.00	7	Analytic static	±1	NA	Gainar and Bala [42]
283.15	6.10-35.30	7	Analytic static	±1	NA	Gainar and Bala [42]
288.20	21.00-50.20	10	Analytic static	NA	±0.0015	da Silva et al. [40]
293.15	5.10-43.10	8	Analytic static	±1	NA	Gainar and Bala [42]
298.15	5.70-34.80	7	Analytic static	±1	NA	Gainar and Bala [42]
298.20	6.00-59.00	9	NA	NA	NA	Yun et al. [38]
303.15	5.30-35.40	7	Analytic static	±1	NA	Gainar and Bala [42]
303.20	15.10-69.40	12	Analytic static	NA	±0.0015	da Silva et al. [40]
313.00	21.10-79.20	10	Analytic static	<0.5	<0.12, <0.05	Gutierrez et al. [45]
313.15	41.60-69.50	4	Analytic dynamic	0.5	1%	Inomata et al. [43]
313.15	5.40-32.20	6	Analytic static	±1	NA	Gainar and Bala [42]
313.20	5.00-78.00	12	NA	NA	NA	Yun et al. [38]
313.20	15.40-82.90	13	Analytic static	NA	±0.0015	da Silva et al. [40]
313.20	47.30-78.50	6	Analytic static	0.10	NA	Wang et al. [44]
323.00	23.20-90.70	13	Analytic static	<0.5	<0.12, <0.05	Gutierrez et al. [45]
323.15	18.40-95.90	13	NA	NA	NA	Zhang and Zheng [39]
323.20	47.10-91.90	6	Analytic static	0.10	NA	Wang et al. [44]
328.20	5.30-99.40	14	NA	NA	NA	Yun et al. [38]
331.90	50.10-114.20	8	Analytic static	±0.1	3%	Chen et al. [41]
333.00	22.10-107.90	11	Analytic static	<0.5	<0.12, <0.05	Gutierrez et al. [45]
333.15	21.0-100.9	7	Analytic static	±0.15	<2%	This work
333.20	52.50-113.50	6	Analytic static	0.10	NA	Wang et al. [44]
341.60	50.10-120.10	8	Analytic static	±0.1	3%	Chen et al. [41]
343.15	20.4-119.8	8	Analytic static	±0.15	<2%	This work
343.20	52.10-129.60	7	Analytic static	0.10	NA	Wang et al. [44]
351.30	50.10-120.10	8	Analytic static	±0.1	3%	Chen et al. [41]
353.15	17.3-130.0	8	Analytic static	±0.15	<2%	This work
353.20	43.60-140.40	8	Analytic static	0.10	NA	Wang et al. [44]
373.15	5.00-147.40	16	NA	NA	±1%	Semenova et al. [37]
423.15	10.00-147.00	15	NA	NA	±1%	Semenova et al. [37]
448.15	10.00-143.60	15	NA	NA	±1%	Semenova et al. [37]
493.15	30.00-122.00	11	NA	NA	±1%	Semenova et al. [37]

aNumber of experimental points; NA – not available; u - uncertainty

several times with carbon dioxide. Then, the equilibrium cell was evacuated with a vacuum pump.

The cell was charged with alcohol, which was degassed by using a vacuum pump and vigorously stirring. The lighter component (in this case CO_2) is introduced with the syringe pump into equilibrium cell and the pressure is set to the desired value. Then the cell was heated to the experimental temperature. To facilitate the approach to an equilibrium state, the mixture in the cell was stirred for a few hours. Then the stirrer was switched off, and about 1 h was allowed to pass until the coexisting phases were completely separated. Samples of the liquid and vapor phases are withdrawn by ROLSI and analyzed with the GC. In order to check the repeatability, at least six samples of the liquid phase were normally analyzed at the equilibrium temperature and pressure. The sample sizes being very small, the equilibrium pressure in the cell remains constant.

Table 2. Mole fractions of component 1 in the liquid phase x_1 and mole fractions of component 1 in the vapor phase y_1 at various pressures P and temperatures T for the binary system carbon dioxide (1) + 2-methyl-1-propanol (2).

P/bar	x_1	y_1	P/bar	x_1	y_1
T/K = 333.15 ± 0.1					
21.00	0.1483	0.9954	75.50	0.4740	0.9938
34.40	0.2023	0.9933	88.90	0.5909	0.9874
49.60	0.3018	0.9960	100.90	0.7152	0.9701
60.60	0.3814	0.9967			
T/K = 343.15 ± 0.1					
20.40	0.1152	0.9941	77.40	0.4446	0.9894
42.40	0.2143	0.9969	91.00	0.5305	0.9845
52.50	0.2748	0.9965	111.10	0.7096	0.9665
64.10	0.3407	0.9959	119.80	0.7935	0.9447
T/K = 353.15 ± 0.1					
17.30	0.1009	0.9907	82.20	0.4293	0.9905
40.30	0.2099	0.9940	95.50	0.5187	0.9815
56.00	0.2920	0.9961	111.00	0.5974	0.9652
70.10	0.3806	0.9954	130.00	0.7608	0.9275

The calibration of the TCD for CO_2 and 2-methyl-1-propanol is done by injecting known amounts of each component using gas chromatographic syringes. Calibration data are fitted to quadratic polynomials to obtain the mole number of the component versus chromatographic area. The correlation coefficients of the GC calibration curves were 0.999 for carbon dioxide and 0.997 for 2-methyl-1-propanol.

For the phase equilibrium compositions, the relative uncertainty of the mole fraction in the liquid and vapor phase was calculated using the procedure given by Scheidgen [52], (Eqs. 5-2, 5-3, 5-4, 5-6, p. 194-196). The average relative uncertainty was <2%. As usually in the literature [53], we report the mole fractions with four decimal places.

The uncertainties of the measurements were estimated to be within 0.1 K for temperature The platinum temperature probe connected to a digital indicator was calibrated against the calibration system Digital Precision Thermometer with PT 100 sensor (Romanian Bureau of Legal Metrology). The uncertainty of platinum probe is estimated to be within ± 0.1 K using a similar procedure as described in [53].

The pressure transducer connected to a digital multimeter was calibrated at 323.2 K with a precision hydraulic dead-weight tester (model 580C, DH-Budenberg SA, Aubervilliers, France). The uncertainty of the pressures is estimated to be within ± 0.015 MPa using a similar procedure as described in [53], for a pressure range between 0.5 and 20 MPa.

3. Results and discussion

The vapor–liquid equilibrium compositions for the carbon dioxide + 2-methyl-1-propanol binary system were measured in the temperature range of 323.15 to 353.15 K and pressures between 17.3 and 130.0 bar and the results are given in Table 2. The values are typically averages of six measurements.

Figs. 1 and 2 show a detailed comparison of the new experimental data measured in this study with existing literature data at nearest or same temperatures. Our data at 333.15 K (Fig. 1) are in agreement with those measured by Gutierrez *et al.* [45] and Wang *et al.* [44], except for the higher pressure region of Wang *et al.*' measurements. A good agreement with literature data can be noticed for the new isotherms measured at 343.15 and 353.15 K (Fig. 2). The most significant disagreement among literature data can be observed at 323 K, where the highest difference in pressure at the same composition is about 30 bar.

A high degree of scatter can be also observed in the temperature range of 273.15 to 313.15 K (Figs. 3 and 4). In addition, some data sets have few experimental points measured at relatively low pressure or only the liquid phase composition is reported (Fig. 3). Several literature isotherms measured at higher temperatures are plotted in Fig. 5. It should be noted that the isotherms determined by a research group are represented with the same symbol (different colours) in all figures.

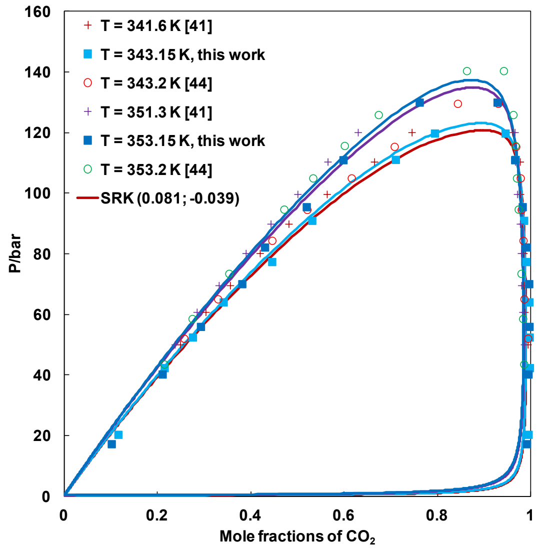

Figure 2. Comparison of new experimental data and literature data for the carbon dioxide + 2-methyl-1-propanol (isobutanol) system and calculations by SRK model: symbols, new data and literature data at different temperatures; solid lines, predictions by SRK (k_{12} = 0.081, l_{12} = -0.039).

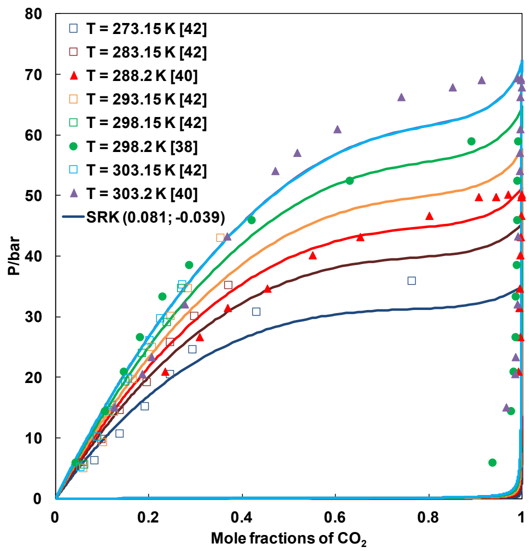

Figure 3. Comparison of literature data for the carbon dioxide + 2-methyl-1-propanol (isobutanol) system and calculations by SRK model: symbols, literature data at different temperatures; solid lines, predictions by SRK (k_{12} = 0.081, l_{12} = -0.039).

Table 3. Critical data and acentric factor [56] for carbon dioxide and 2-methyl-1-propanol (isobutanol).

Component	T_c/K	P_c/bar	ω
CO_2	304.21	73.83	0.224
$isoC_4H_{10}$	547.80	42.95	0.586

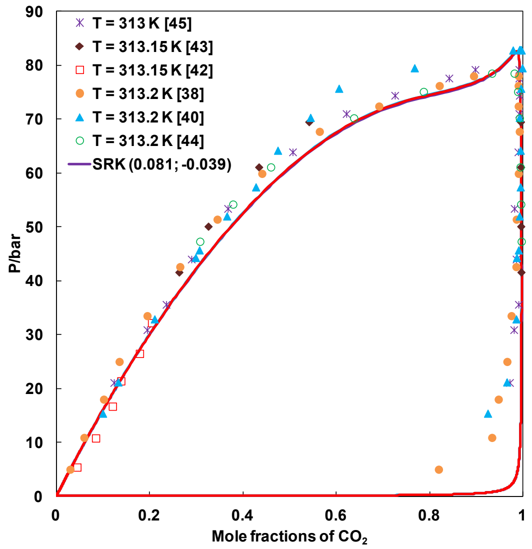

Figure 4. Comparison of literature data for the carbon dioxide + 2-methyl-1-propanol (isobutanol) system and calculations by SRK model: symbols, literature data at different temperatures; solid lines, predictions by SRK (k_{12} = 0.081, l_{12} = -0.039).

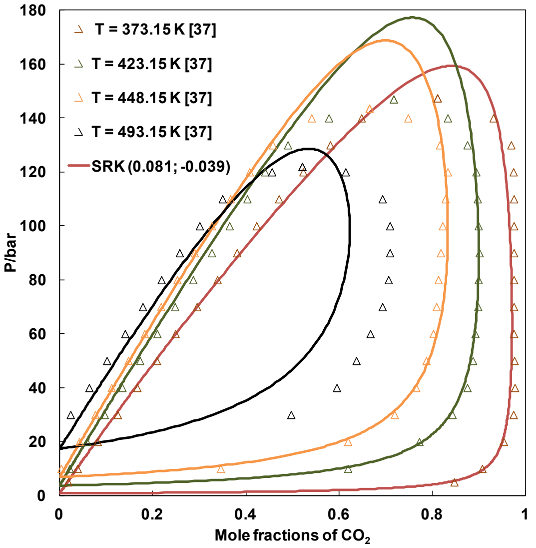

Figure 5. Comparison of literature data for the carbon dioxide + 2-methyl-1-propanol (isobutanol) system and calculations by SRK model: symbols, literature data at different temperatures; solid lines, predictions by SRK (k_{12} = 0.081, l_{12} = -0.039).

Measured and literature data were modeled with Soave–Redlich–Kwong (SRK) equation of state coupled with classical van der Waals mixing rules. The Soave–Redlich–Kwong [50] equation of state is:

$$P = \frac{RT}{V-b} - \frac{a(T)}{V(V+b)} \qquad (1)$$

Table 4. Optimized binary interaction parameters (k_{12}, l_{12}), average absolute deviations in bubble point pressure (*AADP/%*), and average absolute deviations in the vapor phase compositions (*AADY/%*) for carbon dioxide and 2-methyl-1-propanol (isobutanol).

T/K	k_{12}	l_{12}	AADP/%	AADY/%	AADP^a/%	AADY^a/%	Reference
273.15^b	0.1543	0.0214	2.69	-	12.55	-	Gainar and Bala [42]
283.15^b	0.1400	0.0029	2.59	-	7.75	-	Gainar and Bala [42]
288.20	0.0891	-0.0120	2.37	0.38	6.70	0.38	da Silva et al. [40]
293.15^b	0.2161	0.0675	6.82	-	17.26	-	Gainar and Bala [42]
298.15^b	0.2112	0.0604	7.58	-	11.92	-	Gainar and Bala [42]
298.20^b	0.0996	-0.0348	5.39	1.88	7.41	1.88	Yun et al. [38]
303.15^b	0.2055	0.0606	4.39	-	13.46	-	Gainar and Bala [42]
303.20^b	0.1188	0.0075	2.40	0.77	9.16	0.77	da Silva et al. [40]
313.00	0.0918	-0.0386	1.65	0.91	4.79	0.94	Gutierrez et al. [45]
313.15	0.0986	-0.0380	0.45	0.10	9.04	0.13	Inomata et al. [43]
313.15^b	0.2578	0.0919	2.41	-	14.16	-	Gainar and Bala [42]
313.20	0.0909	-0.0433	2.60	3.12	6.84	3.14	Yun et al. [38]
313.20^b	0.1070	-0.0214	1.33	1.31	5.13	1.29	da Silva et al. [40]
313.20	0.0817	-0.0541	0.47	0.36	3.91	0.41	Wang et al. [44]
323.00	0.0857	-0.0515	1.21	0.85	6.20	0.86	Gutierrez et al. [45]
323.15	0.0043	0.0724	2.23	0.67	50.65	0.95	Zhang and Zheng [39]
323.20	0.0834	-0.0466	0.81	0.63	3.34	0.69	Wang et al. [44]
328.20	0.0861	-0.0442	3.06	2.87	5.15	2.92	Yun et al. [38]
331.90	0.0957	-0.0364	1.87	0.31	6.55	0.36	Chen et al. [41]
333.00	0.0795	-0.0594	2.12	0.79	6.83	0.69	Gutierrez et al. [45]
333.15	0.0938	-0.0037	4.50	0.33	8.10	0.41	This work
333.20	0.1008	-0.0293	1.04	0.39	6.85	0.77	Wang et al. [44]
341.60	0.0923	-0.0384	0.81	0.50	6.52	1.77	Chen et al. [41]
343.15	0.0829	-0.0266	3.36	0.53	3.43	0.49	This work
343.20	0.0903	-0.0371	1.29	0.76	3.58	0.43	Wang et al. [44]
351.30	0.0948	-0.0309	0.45	0.42	3.68	0.49	Chen et al. [41]
353.15	0.0858	-0.0060	3.00	1.01	8.94	0.98	This work
353.20	0.0922	-0.0264	1.24	0.56	2.84	0.51	Wang et al. [44]
373.15	0.0927	-0.0266	1.03	0.76	2.22	0.77	Semenova et al. [37]
423.15	0.0529	-0.0540	1.52	0.87	3.87	0.68	Semenova et al. [37]
448.15	0.0380	-0.1550	12.71	3.10	6.67	0.03	Semenova et al. [37]
493.15	0.0430	-0.1683	3.53	14.14	8.61	12.43	Semenova et al. [37]

^{a}*Calculated with* $k_{12} = 0.081$ *and* $l_{12} = -0.039$

^{b}*Data sets excluded from the calculations of the average values binary interaction parameters*

where the two constants, *a* and *b*, are:

$$a = 0.42748\frac{R^2T_c^2}{P_c}\alpha(T) \tag{2}$$

$$b = 0.08664\frac{RT_c}{P_c} \tag{3}$$

$$\alpha(T_R,\omega) = \left[1 + m_{SRK}\left(1 - T_R^{0.5}\right)\right]^2 \tag{4}$$

$$m_{SRK} = 0.480 - 1.574\omega - 0.176\omega^2 \tag{5}$$

The two parameter conventional mixing rules are given by:

$$a = \sum_i\sum_j x_i x_j a_{ij} \tag{6}$$

$$b = \sum_i\sum_j x_i x_j b_{ij} \tag{7}$$

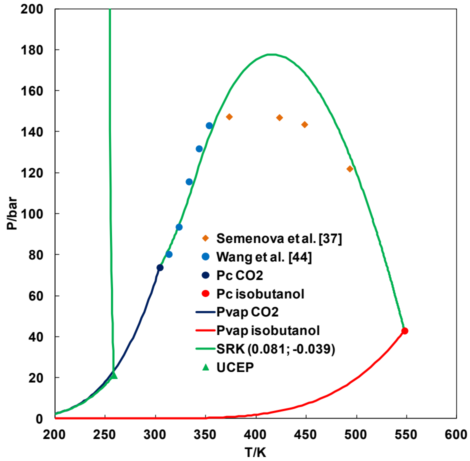

Figure 6. $P-T$ fluid phase diagram of carbon dioxide + 2-methyl-1-propanol binary system: blue full circle (●) [42], orange full diamond (♦) [35], experimental critical curve; dark blue full circle (●) and red full circle (●), experimental critical points of pure components; dark blue and red solid lines (—,—), calculated vapor pressure curves of pure components; green full triangle (▲), UCEP and green solid lines (—), critical curves and LLV line respectively calculated by SRK/ (k_{12} = 0.081, l_{12} = -0.039).

where

$$a_{ij} = \sqrt{a_i a_j}\left(1-k_{ij}\right) \tag{8}$$

$$b_{ij} = \frac{b_i + b_j}{2}\left(1-l_{ij}\right) \tag{9}$$

The calculations were made using the software packages PHEQ (Phase Equilibria Database and Calculations) [54] and GPEC (Global Phase Equilibrium Calculations) [55]. The critical values [53] of the pure carbon dioxide and 2-methyl-1-propanol together with the acentric factors [56] used in the calculations are presented in Table 3.

All available isothermal vapor-liquid equilibrium data were firstly correlated with the SRK EoS coupled with classical van der Waals mixing rules (two-parameter conventional mixing rule, 2PCMR). In Table 4 are presented the optimum values of the binary interaction parameters (k_{12} and l_{12}) together with the values of average absolute deviations in bubble-point pressures (AADP,%) and the average absolute deviations in the vapor-phase compositions (AADY,%). The AADP, respectively AADY are calculated by the equations:

$$AADP = \frac{1}{N_{\exp}}\sum_{i=1}^{N_{\exp}}\left|\frac{P_i^{\exp}-P_i^{calc}}{P_i^{\exp}}\right| \times 100 \tag{10}$$

$$AADY = \frac{1}{N_{\exp}}\sum_{i=1}^{N_{\exp}}\left|Y_i^{\exp}-Y_i^{calc}\right| \times 100 \tag{11}$$

It can be seen that most errors in bubble-point pressures are relatively small with few exceptions, and the overall average absolute deviations in bubble-point pressures for the 32 data sets considered is 2.8%. However, the calculations for several isothermal data lead to liquid-liquid splitting at higher temperatures than expected, as it can be assumed that the experimental UCEP is located ~ 250 K or less, based on the measurement of Buechner [48]. It can be also remarked that the liquid-vapor critical curve is not very well studied, only nine points are available in the literature. Due to the lack of reliable experimental critical curve, our previous modeling strategy [18], by representing well the critical maximum pressure (CPM) of the critical curve, cannot be applied. Therefore, in the present work we obtained a single set of interaction parameters temperature independent by averaging the optimum values of the binary parameters except those which lead to L-L splitting (Table 4). The set of interaction parameters thus obtained is k_{12} = 0.081, l_{12} = -0.039 and it was used to calculate the VLE (Figs. 1-5) and the critical curve(s) (Fig. 6). Compared with the available critical points, the SRK calculations overestimate the CPM. The overestimation of the critical points can be also observed in the pressure-compositions diagram at high temperatures (Fig. 5). The AADP% and AADY% calculated with this unique set of parameters are also reported in Table 4. It can be notted that the highest errors (10%) appear for the unreliable experimental data and the SRK model predictions are reasonably good for most experimental data.

4. Conclusions

New VLE experimental data for the binary system carbon dioxide + 2-methyl-1-propanol (isobutanol) were measured at 333.15, 343.15, and 353.15 K and pressures up to 130.0 bars, with a high-pressure static apparatus using ROLSI valves. Measured and literature data for carbon dioxide + 2-methyl-1-propanol system were modeled with the SRK cubic equation of state using classical van der Waals (two-parameter conventional mixing rule, 2PCMR) mixing rules. The same set of interaction parameters was used to predict the critical and sub-critical phase behavior of the binary mixture studied. The predicted results were compared both with our experimental data and the available literature data for carbon dioxide + 2-methyl-1-propanol binary systems. New experimental vapor-liquid equilibrium data and critical data are required.

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