Vapour-liquid equilibrium data for the carbon dioxide (CO_2) + carbon monoxide (CO) system

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Abstract

In carbon capture, utilization and storage (CCUS), a thorough understanding of thermophysical behaviour of the candidate fluid is an essential requirement for accurate design and optimised operation of the processes. In this communication, vapour liquid equilibrium data (VLE) of the binary mixtures of $CO+CO_2$ are presented. A static-analytic method was used to obtain VLE data at six isotherms (253.15, 261.45, 273.00, 283.05, 293.05, 298.15) K and pressures up to 12 MPa. The standard uncertainties of the measured temperature and pressure were estimated to be 0.1 K, 0.005 MPa, respectively. Also, the standard uncertainty of the measured molar composition of each phase is found to be less than 1.1%. The measured experimental results are then compared with some predictive thermodynamic equations of state (EoS) (i.e. the Peng Robinson (PR-78) with classical or Wong-Sandler mixing rules, the GERG, and EoS-CG without an with a specific departure function) and available data in the literature. A sound agreement is observed between the results of this work and some of the VLE data published in the open literature. Furthermore, for all isotherms, the best agreement is observed between experimental results and predicted VLE data from the PR-EoS with the Wong-Sandler mixing rules and the EoS-CG with a specific departure function. However, a significant deviation is found between measured results and VLE data calculated using the GERG-EoS.

Keywords: VLE data; Carbon Monoxide; Carbon Dioxide; Thermodynamic Modelling; CCUS.

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1. Introduction

Despite the global roadmaps internationally agreed to control CO_2 emissions and global warming, e.g. Kyoto protocol (1997) [1] and Paris agreement (2015) [2], still much faster solutions are required to overcome the massive daily CO_2 emissions in the world. As a response to this concern, carbon capture utilisation and storage (CCUS) [3] has been proposed as an effective method to control and mitigate this major environmental challenge.

Usually, the captured CO_2 in the first stage of the CCUS is not pure, and various contaminants such as N_2, CO, O_2, H_2 and water can be found in the mixture. These impurities affect thermophysical properties of the fluid (e.g.: phase behaviour, density, viscosity, thermal conductivity, etc.). Therefore, the effect of impurities on the thermophysical properties of CO_2 rich mixtures needs to be addressed carefully as a major technical and safety concern [4,5] [5-8]. Furthermore, because of the broad operational pressure and temperature (P, T) ranges in various stages of the CCUS, investigating the effects of impurities in an extensive (P, T) range is crucial for a safe and efficient design, control and operation of the facilities used to capture, process, transport and storage of the fluids.

Among various thermodynamic models available to predict thermophysical properties of fluids, cubic Equation-Equation-of-State (EoSs) like the Peng-Robinson (PR-78) [6] and the Soave-Redlich-Kwong (SRK) [7] have been widely used in the oil and industry. Despite the simplicity and reliable predictions of these models for most of the hydrocarbon mixtures and industrial fluids, notable deviations from experimental results have been observed for the CCUS candidate fluids in certain (P, T) ranges [8–11].

Another type of predictive model recently been used for accurate determination of thermodynamic properties are multi-parameter equations of state (EOS) which directly calculate thermodynamic properties based on the mathematical differentiation of a thermodynamic potential [12]. In these models, various exponents and fitting coefficients are

computed by fitting the original model on the experimental data available in the literature. For instance, the GERG-EoS [13] is a powerful multi-parameter model for prediction of thermodynamic properties of natural gas and similar mixtures. Despite the accuracy of these models for natural gas mixtures, significant deviations from experimental results can be observed for systems with high concentration ofcarbon dioxide. Over the past few years some models, e.g. EoS-CG for humid gases and CCS mixtures [14], have been developed for more accurate predictions of thermophysical properties of CO_2 rich mixtures. However, for some CO_2 mixtures experimental results are scarce, and generating experimental data is required to improve these models for CCUS applications.

To the best of our knowledge and based on the reported investigations in the open literature, for many CCUS mixtures, significant gaps can be found in the literature data. Therefore, further experimental investigations on CO_2 rich mixtures is necessary to fill the gaps, obtain and optimise mixtures parameters and improve the performance of the predictive tools. In spite of numerous investigations over the past few years in this direction, considerable research work still needs to be performed because of the variety of components and the large domain of pressure, temperature and composition to be covered..

Previously, we performed various experimental and modelling investigations, to obtain thermophysical properties of binary and multicomponent natural gas mixtures with wide ranges of CO_2 content [15–18]. The binary $CO + CO_2$ system was another CCUS fluid with a limited number of experimental data available in the open literature when these new data were measured in 2011. For this mixture, reported VLE measurements were limited to the investigations conducted by Kaminishi et al. [19], Christiansen et al. [20] and Shen [21]. Since then additional measurements have been reported by Blanco et al. [22], Souza et al. [23], and Westman et al. [24]. Details of these investigations including ranges of pressure and temperature are listed in **Table 1**.

The primary objective of this work is to obtain vapour liquid equilibrium data for the binary mixture of CO and CO_2 at pressures up to 12 MPa and in a temperature range between 253.15 K to 298.15 K. The obtained experimental results are then compared to the previously published data in the literature. The results are compared against predictions of the PR-78 [6], E-PR78 [25], PR-WS/NRTL [26,27], GERG [13], EoS-CG [14] and the EoS-CG with a specific departure function for the CO2 – CO binary system [28].

Table 1. Experimental VLE data available in literature for binary mixture of CO+CO₂

Author	Years of Publication	T/K	p/ MPa
Kaminishi at al. [19]	1968	223.15, 253.15, 273.15, 283.15	5.27-13.08
Christiansen et al. [20]	1974	223.15, 243.15, 263.15, 283.15	0.83-14.15
Shen [21]	1991	223.15, 243.15, 261.15	1.57-6.96
Blanco et al. [22]	2014	253.15, 263.15, 273.15, 283.15, 293.15, 323.15, 333.15, 343.15	0.1-20
Souza et al. [23]	2018	218, 233, 243, 258, 273, 288, 303	1.31-13.61
Westman et al. [24]	2018	253, 273, 283, 298	1.97-12.54

2. **Experimental section**

2.1 Materials

Carbon dioxide (CO_2) and carbon monoxide (CO) were purchased from BOC with certified minimum molar purities of 99.995% and 99.90%, respectively, as detailed in Table 2.

Table 2. Composition of the chemical used in this work

Chemical	Symbol	CASRN	Purity (vol)	Supplier
Carbon dioxide	CO_2	124-38-9	0.99995	Air Product
Carbon monoxide	CO	630-08-0	0.9990	Air Product

2.2 Experimental apparatus and uncertainties

In this study, an experimental apparatus is used to investigate phase equilibrium based on a static-analytic method with fluid phase sampling. The apparatus is comprised of a titanium cell with two windows surrounded by an integral water jacket. The cell volume is about 150 ml and it can be operated in temperatures between 243.15 K to 373.15 K and at pressures up to 20 MPa. The temperature of the cell is controlled by circulating coolant from a cryostat within a jacket surrounding the cell. The cryostat can maintain the cell temperature within 0.05 K. A Platinum Resistance Thermometer (PRT) measures the temperature and the pressure is measured by means of a Quartzdyne pressure transducer mounted directly on the cell. To achieve a fast-thermodynamic equilibrium and to provide a good mixing of the fluids, a high-pressure magnetic stirrer (Top Industrie S.A.) was used to agitate the test fluids at around 1,000 RPM with a Rushton type impeller.

The cell is fitted with a moveable capillary sampler. A schematic of the set-up for conducting the Vapour-Liquid Equilibria (VLE) experiments of the CO2+CO mixture - phase behaviour at wide pressure-temeprature range is shown in **Figure 1**. The sampling is carried out using the capillary sampler ROLSI[TM1], which is connected to the top of the cell through a 0.1 mm internal diameter capillary tube. Combining the visual capabilities with the moveable capillary sampler, this system allows for small, microliter samples of any chosen phase to be taken and sent to a Gas Chromatograph (GC) for analysis. As shown in the schematic flow diagram in **Figure 2**, the withdrawn samples are swept into a Varian 3800 GC equipped with a Thermal Conductivity Detector (TCD) for analysis through heated lines (T=453.15 K) to avoid any condensation. The capillary inlet of the sampler can be displaced directly into the vapour or liquid phase and the outlet of the capillary is closed by a movable micro-stem operated by a

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[1] A ROLSI sampler is a proprietary micro-sampling device enabling sampling of very low volumes at high pressure and high temperature

magnet. When the magnet is powered, it opens the outlet of the capillary, and then the sample can flow inside the expansion room which is flushed with the carrier gas. The carrier gas sweeps the sample to the GC column for analysis. The sampler allows direct sampling at the working pressure without disturbing the cell equilibrium due to the relatively small size of the sample. The mass of samples can be adjusted continuously from 0.01 to several mg thanks to an electronic timer. The expansion room of the sampler is heated independently from the equilibrium cell to allow the samples to remain in vapour state and/or to vaporise a liquid sample.
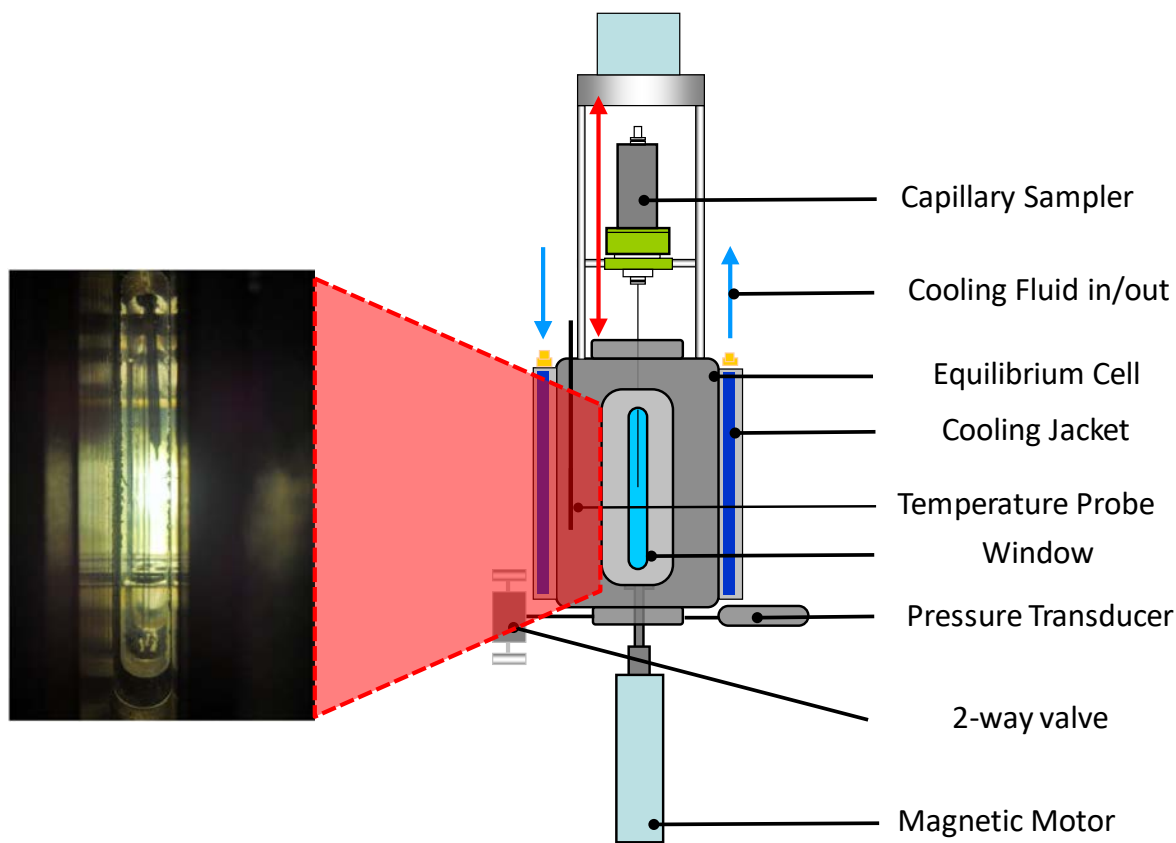

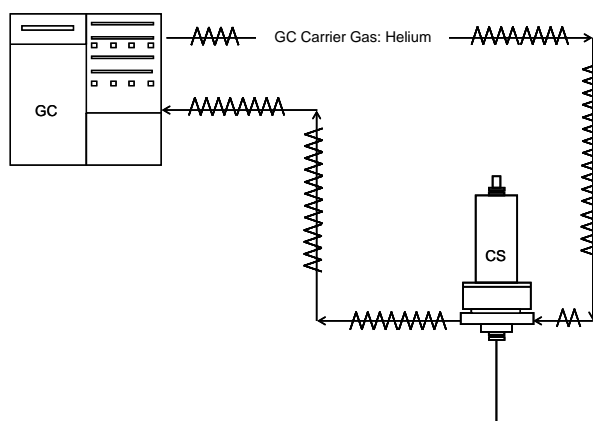**Figure 1. Schematic of the VLE cell**

Figure 2. Flow diagram of apparatus for on-line compositional analysis (GC: Gas Chromatograph, CS: Capillary sampler)

The TCD detector was repeatedly calibrated by introducing known amounts of each pure compound through a syringe in the injector of the gas chromatograph. Taking into account the uncertainties due to calibrations and dispersions of analyses, resulting uncertainties on vapour and liquid mole fractions are reported in **Table 3**.

Table 3. Uncertainty calculation for temperature readings, pressure readings and composition analysis

Uncertainty	absolute value
Maximum uncertainty on T probe[a]	0.05 K
Maximum uncertainty on P probe[a]	0.005 MPa
Maximum uncertainty on TCD for CO_2[b] mole numbers	0.8%
Maximum uncertainty on TCD for CO[b] mole numbers	1.1%

[a] *Uncertainties from temperature probe and pressure probe calibration are considered as the largest deviations that occurred during the calibration.*
[b] *Uncertainty from CO_2 and CO calibration is considered as the largest deviation value occurred during the calibration.*

2.3 Procedures

To start the experiment, the equilibrium cell, connected lines and connections are cleaned and then vacuumed. Using the loading valve, CO_2 is injected into the equilibrium cell. The system

temperature is then set to the desire temperature and enough time is given to the system to reach thermodynamic equilibrium. Thermodynamic equilibrium of the fluid in the system is assumed when the pressure is constant for at least 10 minutes at constant temperature. At each temperature, first vapour pressure is measured and then, the carbon monoxide is introduced step by step, to increase the overall compositions of CO. Then, for each step at equilibrium condition, at least 5-10 samples of both vapour and liquid phases are withdrawn using the ROLSITM sampler and analysed to check for the measurement repeatability. The thermodynamic equilibrium in the system is assumed when the total pressure remains unchanged during a period of 10 min under efficient stirring while temperature is constant.

3. Thermodynamic modelling

Six thermodynamic approaches have been used to model the new equilibrium data:

- The first thermodynamic approach is based on the Peng-Robinson equation of state [6] combined with the classical mixing rules. The binary interaction parameters (BIPs) were fitted to literature data presented in Table 1. The binary interaction parameter was found to follow the temperature dependency described below:

$$k_{ij} = -2.98999 \times 10^{-2} - 1.38667 \times 10^{-4} \times (T/K)$$

- The second model is the *Enhanced* Predictive-PR78 (E-PPR78) equation of state as described by Xu et al. [25] and was used without further adjustment.

- The third approach is the Peng-Robinson equation of state combined with the Wong-Sandler [26] mixing rules + the NRTL local composition model [27] (PR-EoS/WS-NRTL). The binary interaction parameters listed in **Table 4** were fitted to literature data presented in **Table 1**. To improve the calculation of the vapour pressure of carbon dioxide, the *Mathias-Copeman* (*MC*) alpha function [28] with three adjustable parameters was also used for this compound :

$$
\begin{cases}
if \; T < T_C, \;\; \alpha(T) = \left[1 + c_1\left(1 - \sqrt{\frac{T}{T_C}}\right) + c_2\left(1 - \sqrt{\frac{T}{T_C}}\right)^2 + c_3\left(1 - \sqrt{\frac{T}{T_C}}\right)^3\right]^2 \\
otherwise \;\; \alpha(T) = \left[1 + c_1\left(1 - \sqrt{\frac{T}{T_C}}\right)\right]^2
\end{cases}
$$

Table 4. Adjusted parameters of the PR-WS/NRTL model

Parameters	Values
k_{ij}	0.161
α	0.119
τ_{CO2-CO}/RT	1.508
τ_{CO-CO2}/RT	-0.468
c_1	0.71381
c_2	-0.4422
c_3	2.4364

- The fourth, fifth and sixth models are based on Multi-Fluid Helmholtz Energy Approximation equations of state. In the work, the original GERG-EoS [13], EoS-CG [14] and EoS-CG with the departure function proposed by Souza et al. [29] were also used.

The critical temperature (T_c), critical pressure (P_c), critical density and acentric factor (ω), for each pure compound are provided in **Table 5**.

Table 5. Critical Properties of Pure Compounds

Compound	P_c / MPa	T_c / K	ρ_c / mol.m^{-3}	ω	Reference
CO	3.494	132.86	10850	0.0497	[30]
CO_2	7.3773	304.1282	10624.9	0.2236	[31]

4. Results and discussions

VLE data were measured for binary mixtures of CO + CO_2 at (253.15, 261.45, 273.00, 283.05, 293.05, 298.15) K. Details of the obtained results including pressure, temperature and CO composition in liquid and gas phases at each point are tabulated in **Table 6**. Vapour pressures were measured at five temperatures from 253.15 to 298.15 K for CO2. For each point, the experimental value was compared with the calculated one using the Span and Wagner equation of state for pure CO_2 [32]. The absolute relative deviation observed between experimental and calculated values is less than than 0.15%.Also, the generated data in this work, data available in the literature, and VLE curves predicted using the models investigated in this study have been compared in **Figures 3** to **5**. Except for the data points measured at 261.45 Kliterature data were available for comparison purpose. **Figure 3** depicts the literature data, and models predictions for four isotherms between 218.15 to 243.15 K. A reasonable agreement is seen between most data points measured by Kaminishi et al. (1968) [19], Souza et al. (2018) [23], Christiansen et al. (1974) [20] and Shen (1991) [21]. The only exceptions were some of the bubble points measured by Christiansen et al. (1974) [20] and some of the dew points measured by Shen (1991) [21] at 243.15 K. The bubble point pressures measured by Christiansen et al. (1974) [20] at this isotherm, are systematically higher than other references.

In **Figure 4**, experimental data measured in this work are compared against literature data. At 253.15 K, the obtained results of this study agree well with the reported data by Westman et al. (2018) [24], and Kaminishi et al. (1968) [19]. For the experimental data at 273.15 K, despite the consistency of the literature data with the results of this work for the measured bubble points, some deviations are observed between experimental results obtained for the dew curve in different studies. Among the experimental data shown in **Figure 4**, significant differences were noticed between the bubble points reported by Blanco et al. (2014) [22] and all other

experimental data. Similar differences were identified at higher temperatures, as shown in **Figure 5**, where isotherms of (283.15, 293.15 and 298.15) K were investigated. As shown in this figure, at 283.15 K and 298.15 K, a reasonably good agreement is observed between results of this study and those obtained by Westman et al. (2018) [24] and Christiansen et al. (1974) [20] (only dew points at 283.15 K).

Among the different thermodynamic models tested in this study, the GERG-EoS is the one that is predicting bubble points with the largest deviation from the experimental results (except for data measured by Blanco et al. (2014) [22]). For dew curves, at low pressure, the model predictions agreed reasonably well with the experimental data. However, as pressure increases the GERG-EoS is unable to estimate the dew curve precisely, and deviations are significant. The E-PPR78-EoS can reproduce the phase behaviour accurately in the CO_2 rich region. However larger deviation from experimental data are seen closer to the critical point of the mixtures. A similar conclusion can be reached for the PR78-EoS with the adjusted binary interaction parameters.
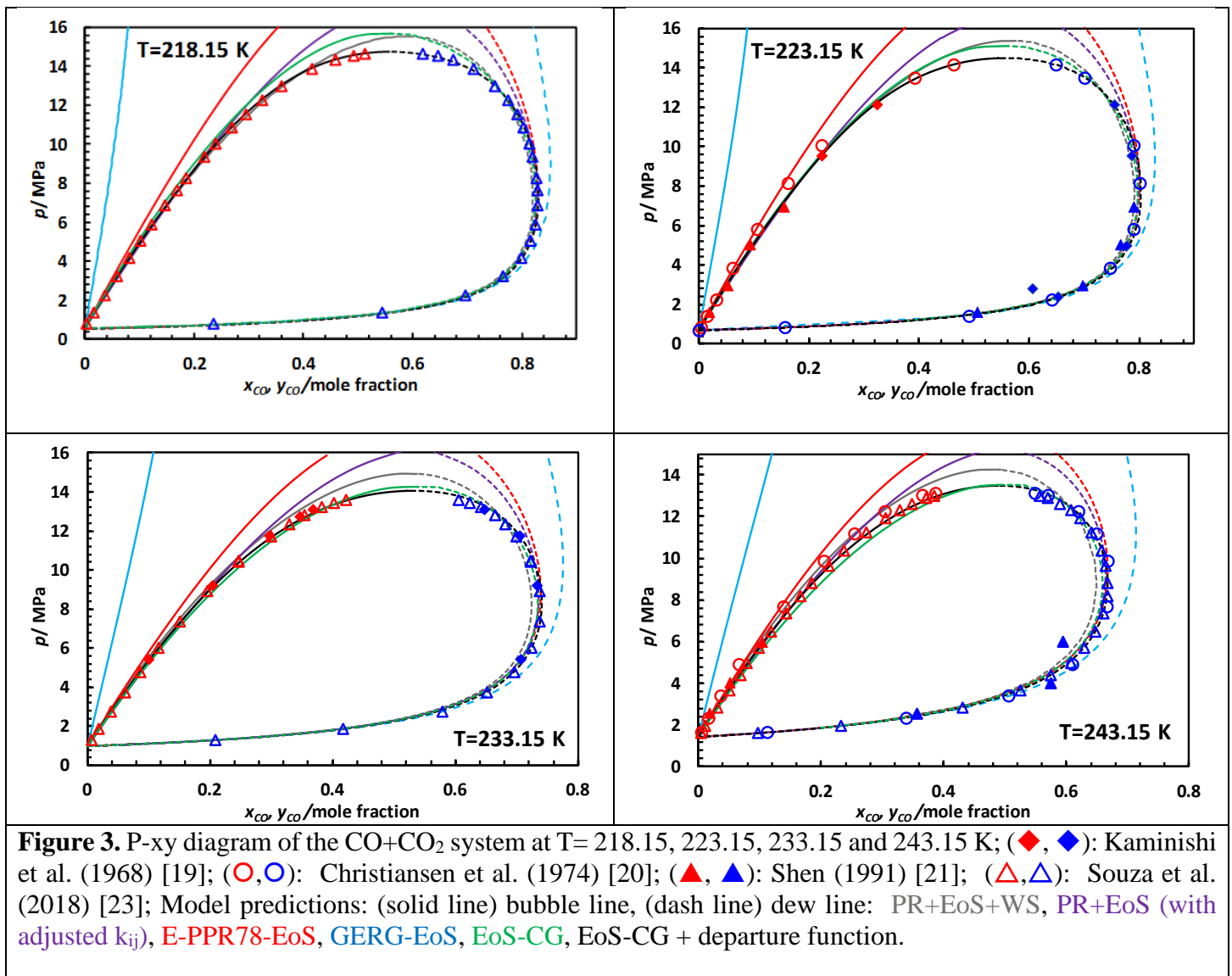
Among the other predictive tools examined in this study, predictions of EoS-CG with the departure function proposed by Souza et al. (2018) [23] are in a very good agreement with their experimental data, the data measured in this work, and the results obtained by Kaminishi et al. (1968) [19], Christiansen et al. (1974) [20] (only dew curves). This model also shows a good agreement with only one of the isotherms (223 K) investigated by Shen (1991) [21]. A notable deviation is seen when the model predictions are compared with data reported by Shen at 243.15 and 263.15 K. For these isotherms, some of Shen's data points have a significant deviation from the VLE measurements conducted in this work, and those performed by Christiansen et al. (1974) [20] and Souza et al. (2018) [23]. As seen in these three figures (**Figure 5**), EoS-CG with the departure function enables more accurate description of the phase behaviour than the original EoS-GC.

Analysing the performance the PR+EoS and PR+EoS+WS models show that the PR+EoS+WS can predict the equilibrium curves more accurately in comparison to other cubic models tested in this work. However in the vicinity of the critical points, the predicted values from this model are showing large deviations from the experimental data. In this region, the EoS-CG with departure function show much lower deviations.

Table 6. Experimental Vapour–liquid equilibrium data for CO (1) - CO$_2$ (2) mixtures at temperature T, pressure P, vapour mole fraction of CO y, and liquid mole fraction of CO x. *.

T/ K	P/ MPa	y	x	σ$_y$	σ$_x$	N$_y$	N$_x$
253.15	1.969	0.000	0.000	-	-	-	-
253.65	4.920	-	0.066	-	0.02%	-	23
253.15	5.988	-	0.093	-	0.02%	-	15
253.15	7.429	-	0.132	-	0.06%	-	22
253.15	8.887	-	0.176	-	0.07%	-	17
253.15	10.122	-	0.218	-	0.04%	-	23
253.15	11.385	-	0.276	-	0.11%	-	20
253.15	11.887	-	0.305	-	0.09%	-	20
261.55	2.528	0.000	0.000	-	-	-	-
261.45	2.927	0.058	0.008	0.09%	0.02%	20	17
261.45	3.800	0.253	0.028	0.02%	0.01%	21	18
261.45	4.547	0.320	0.046	0.17%	0.02%	17	14
261.45	5.493	0.404	0.068	0.13%	0.04%	22	14
261.55	7.073	0.472	0.110	0.07%	0.04%	23	23
261.55	7.897	0.485	0.135	0.09%	0.03%	23	15
261.55	8.949	0.481	0.167	0.13%	0.07%	23	23
261.55	10.328	0.464	0.217	0.25%	0.08%	18	23
261.55	11.332	-	0.272	-	0.05%	-	14
273.00	4.137	0.090	0.014	0.06%	0.01%	12	15
273.00	5.137	0.211	0.039	0.03%	0.02%	14	21
273.00	6.526	0.298	0.075	0.06%	0.02%	23	17
273.00	7.619	0.335	0.105	0.33%	0.04%	17	16
273.00	8.587	0.362	0.138	0.13%	0.04%	23	23
273.00	9.273	0.372	0.161	0.11%	0.03%	22	23
273.00	9.842	0.368	0.184	0.13%	0.03%	23	21
273.00	10.173	0.361	0.201	0.10%	0.03%	23	23
273.00	10.728	0.329	0.247	0.10%	0.07%	23	15
283.05	4.495	0.000	0.000	-	-	-	-
283.05	4.870	0.038	0.008	0.05%	0.01%	22	19
283.05	5.557	0.111	0.025	0.08%	0.03%	20	21
283.05	6.295	0.166	0.044	0.09%	0.04%	20	22
283.05	6.977	0.199	0.064	0.20%	0.02%	20	17
283.05	7.632	0.231	0.084	0.04%	0.02%	20	23
283.05	8.674	0.255	0.119	0.14%	0.04%	20	15
283.15	9.320	-	0.148	-	-	-	13
283.05	9.735	0.235	-	0.12%	-	23	
293.05	5.726	0.000	0.000	-	-	-	-
293.05	5.991	0.024	0.007	0.02%	0.01%	21	22
293.05	6.233	0.045	0.013	0.01%	0.02%	22	21
293.05	6.678	0.075	0.026	0.06%	0.01%	22	22
293.05	7.350	0.112	0.046	0.03%	0.04%	23	22
293.05	8.067	0.136	0.070	0.03%	0.01%	23	22
293.05	8.618	0.137	0.099	0.03%	0.01%	23	22
298.15	6.434	0.000	0.000	-	-	-	-
298.15	6.550	0.008	0.003	0.01%	0.01%	22	22
298.15	6.905	0.032	0.013	0.01%	0.01%	22	19
298.15	7.244	0.050	0.023	0.03%	0.02%	18	12
298.15	7.623	0.066	0.036	0.02%	0.01%	22	23
298.15	7.950	0.073	0.050	0.02%	0.02%	23	12

* Standard uncertainties of measurements: *u*, are *u(T)* = 0.1 K, *u(P)* = 0.005 MPa, for CO2 *u(x,y)* =0.008 and for CO *u(x,y)* =0.008. σ: Standard deviation between samples; N: number of samples.
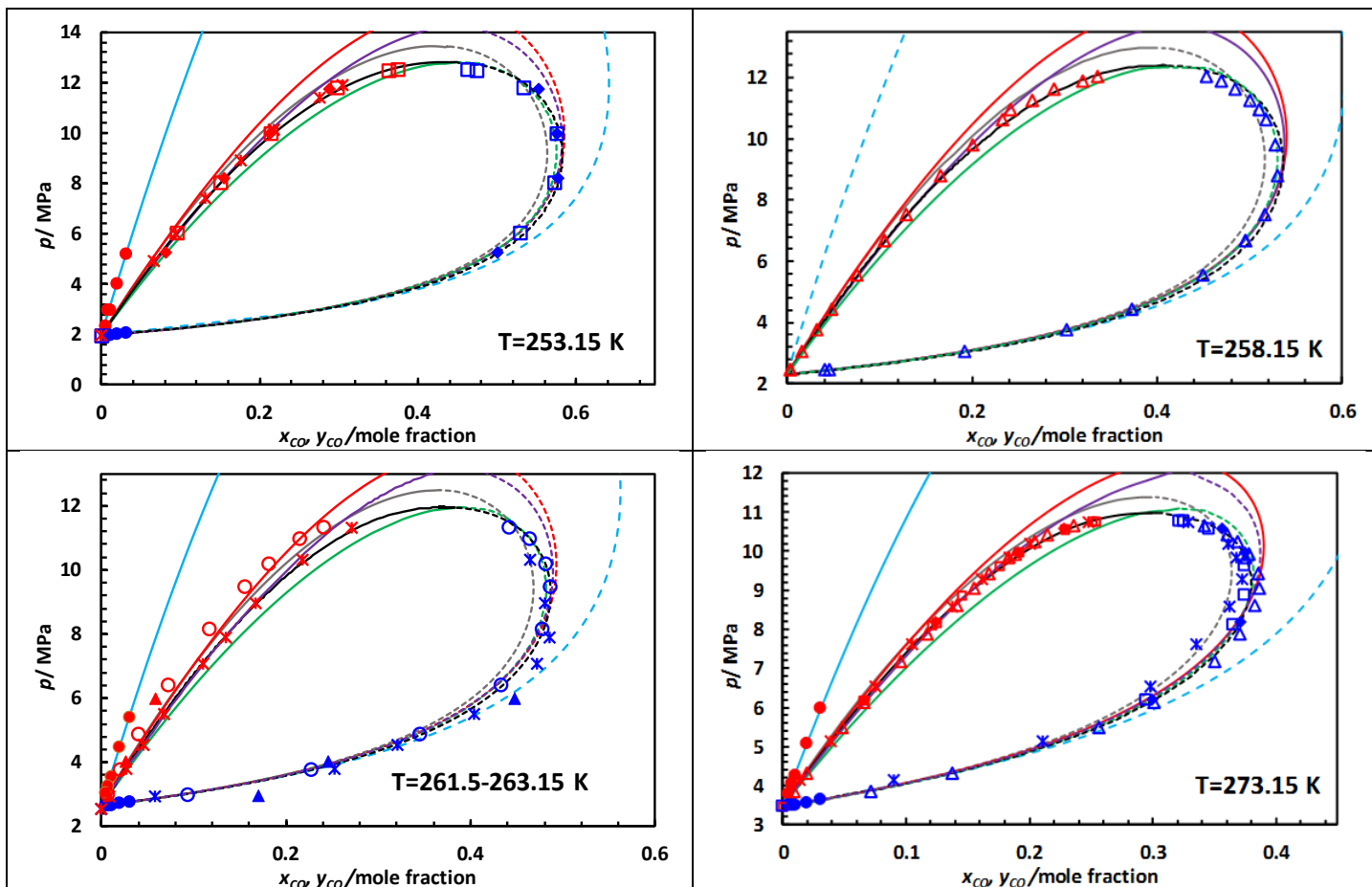

Figure 3. P-xy diagram of the CO+CO_2 system at T= 218.15, 223.15, 233.15 and 243.15 K; (◆, ◆): Kaminishi et al. (1968) [19]; (○,○): Christiansen et al. (1974) [20]; (▲, ▲): Shen (1991) [21]; (△,△): Souza et al. (2018) [23]; Model predictions: (solid line) bubble line, (dash line) dew line: PR+EoS+WS, PR+EoS (with adjusted k_{ij}), E-PPR78-EoS, GERG-EoS, EoS-CG, EoS-CG + departure function.
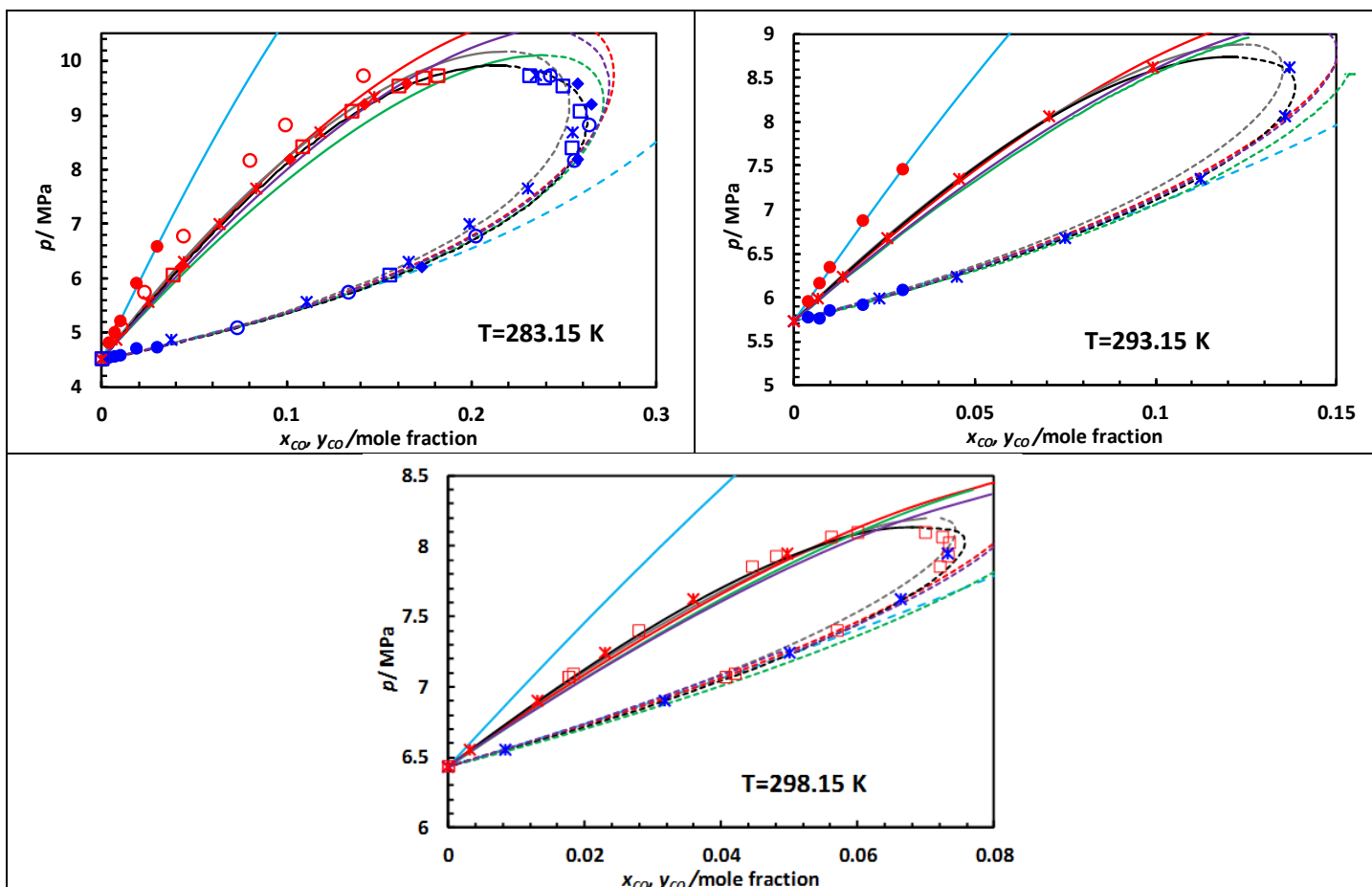
Figure 4. P-xy diagram of the CO+CO₂ system at T= 253.15, 258.15, 261.45/263.15 and 273.15 K; (✳, ✳): This work; (◆, ◆): Kaminishi et al. (1968) [19]; (○,○): Christiansen et al. (1974) [20]; (▲, ▲): Shen (1991) [21]; (●, ●): Blanco et al. (2014) [22]; (△,△): Souza et al. (2018) [23]; (□, □): Westman et al. (2018) [24]; Model predictions: (solid line) bubble line, (dash line) dew line: PR+EoS+WS, PR+EoS (with adjusted k_ij), E-PPR78-EoS, GERG-EoS, EoS-CG, EoS-CG + departure function.

Figure 5. P-xy diagram of the CO+CO₂ system at T= 283.15, 293.15 and 298.15 K; (✱, ✱): This work; (◆, ◆): Kaminishi et al. (1968) [19]; (○,○): Christiansen et al. (1974) [20]; (●, ●): Blanco et al. (2014) [22]; (△,△): Souza et al. (2018) [23]; (▢, ▢): Westman et al. (2018) [24]; Model predictions: (solid line) bubble line, (dash line) dew line: PR+EoS+WS, PR+EoS (with adjusted k_{ij}), E-PPR78-EoS, GERG-EoS, EoS-CG, EoS-CG + departure function.

5. Conclusions

New VLE data for binary mixtures of CO+CO2 were obtained using the static-analytic method at six isotherms of (253.15, 261.45, 273.00, 283.05, 293.05, 298.15) K and the pressures up to 12 MPa. The experimentally measured VLE data were then compared against the available data in the literature, and predictions of the PR-EoS, GERG-EoS and EoS-CG. Results of the experimental research in this work was found to be in a sound agreement with some of the VLE

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data published in the open literature. Moreover, for all isotherms, a reasonable agreement between experimental results and predicted VLE data from the EoS-CG with departure function and PR-EoS+WS are observed.

6. Acknowledgements

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