

High-pressure phase equilibrium calculations for carbon dioxide + cyclopentane binary system

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Abstract: The phase behavior of the carbon dioxide + cycloalkane mixtures usually receives low attention, though these systems are important for many industries, e.g. the carbon capture and storage. In this paper calculations results for the carbon dioxide + cyclopentane binary system are presented, based on SRK and PR cubic equations of state with classical van der Waals mixing rules.

A single set of binary parameters for each model was proposed to predict the global phase behavior of the system in a wide range of pressure and temperature. Albeit the thermodynamic models used are simple, they are able to represent fairly well the phase behavior of the system analyzed in this paper.

Keywords: Carbon dioxide • Cyclopentane • SRK • PR • High-pressures
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1. Introduction

In the last years many research focused on finding solutions for reducing the greenhouse gas effects, as over 80% of greenhouse gases are the carbon dioxide (CO₂) emissions produced by the fossil fuel powered plants and energy production facilities [1]. Substantial international cooperation is established to minimize these environmental concerns, without significantly increasing the costs. Among the solutions considered, the carbon capture and storage (CCS) is a promising way to reduce carbon emissions. The technologies used in CCS, if developed at scale, could allow the safe removal and permanent storage of CO₂ emissions from coal and gas

power stations as well as to remove and permanently store emissions from large industrial sources such as steel or cement factories [1,2].

In this context, to study the phase behavior of fluid mixtures of relevance for carbon capture and storage or enhanced oil recovery (EOR) is of fundamental importance. Among the systems of interest for CCS or EOR are the carbon dioxide + hydrocarbons binary mixtures [2,3]. While the carbon dioxide + n-alkanes series was extensively studied both experimentally and theoretically, and there are still unsolved issues [4], other carbon dioxide + hydrocarbon systems are less investigated [5-10]. Therefore, this paper is a beginning of a systematic study regarding other carbon dioxide

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+ hydrocarbons mixtures than CO₂ + n-alkanes. The purpose of the current research is to compare different thermodynamic models to represent the high-pressure phase behavior of carbon dioxide + cycloalkane systems. Previously, Jaubert et co-workers [11] showed that accurate predictions including the critical region can be obtained using the PPR78 predictive model [12-27] for the carbon dioxide + naphthenic compounds (cycloparaffins). Although in a recent paper by Cismondi *et al.* [4] the phase equilibria of carbon dioxide + n-alkanes series was successfully studied using a predictive correlation based on a three-parameter cubic equation of state, we started our investigation using two simpler models, namely Peng-Robinson (PR) [28] and Soave-Redlich-Kwong (SRK) [29] equations of state (EoSs). Particularly, this article focuses on the carbon dioxide + cyclopentane binary system phase behavior, as recently the cyclopentane hydrate has been studied as a thermal energy storage media [30]. The system is also important for other industries, e.g. cyclopentane is used in the manufacture of synthetic resins and rubber adhesives; it is the blowing agent in the manufacture of polyurethane insulating foam, as found in many domestic appliances such as refrigerators and freezers, replacing environmentally damaging alternatives such as CFC-11 and HCFC-141b [31]. More advanced technologies, such as computer hard drives and outerspace equipment employ multiply alkylated cyclopentane (MAC) lubricants because of their extremely low volatility [32].

The literature [5-10] review we performed revealed that only vapor-liquid equilibria data and critical points are available for the carbon dioxide + cyclopentane binary mixture at temperatures from 276.64 K to 493.11 K and pressures up to 122 bars. Thus, Eckert and Sandler [33] have published three isotherms (310.85, 318.15, and 333.15 K), Marathe and Sandler [34] have reported two isotherms (366.80 and 412.10 K) and densities at the same temperatures, and Shah *et al.* [35] have measured 15 isotherms and critical points. We found no experimental evidence about the type of phase diagram [36] of this system, according to the well-known classification of van Konynenburg and Scott [37] or to that up to date made by Privat and Jaubert [36], except for the critical points. Therefore, it can be assumed that the carbon dioxide + cyclopentane binary mixture is type I or II phase diagram [36,37]. Type I phase behavior is characterized by a continuous liquid = vapor (L = V) critical curve extending from the critical point of pure carbon dioxide to the critical point of pure cyclopentane, and there are no critical endpoints (CEP). Type II phase diagram is similar with type I, but in addition another liquid = liquid (L = L) critical curve appears, which

intersects in an upper critical endpoint (UCEP) with a three phase liquid-liquid-vapor (LLV) equilibrium line, which goes to lower temperatures.

The aim of this work is to represent correctly the global phase behavior of the system, even if with higher errors in bubble-point pressure [38]. The phase behavior of the carbon dioxide + cyclopentane binary system was modeled with the PR and SRK EoSs coupled with classical van der Waals mixing rules (two-parameter conventional mixing rule, 2PCMR), using a similar approach as in our previous papers [39-44]. The model results are compared with all available data.

2. Theoretical procedure

2.1. Modeling

One of the most popular methods used for the calculations (both correlations and predictions) of phase equilibrium in mixtures is the utilization of equations of state (EoS), as models of this type are the proper choice for describing the fluid phase behavior over a wide range of pressure [45-47]. Among the many cubic EoS derived from van der Waals equation of state, the models proposed by Soave and Peng and Robinson are widely used because of their simplicity and flexibility [11,47-49].

The original Peng–Robinson [28] is described by the following equation:

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

where the two constants, a and b, are:

$$a = 0.45724 \frac{R^2 T_c^2}{P_c} \alpha(T) \quad (2)$$

$$b = 0.077796 \frac{RT_c}{P_c} \quad (3)$$

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

$$m_{PR} = 0.37464 - 1.54226\omega - 0.26992\omega^2 \quad (5)$$

The Soave–Redlich–Kwong [29] equation of state is:

$$P = \frac{RT}{V-b} - \frac{a(T)}{V(V+b)} \quad (6)$$

where the two constants, a and b, are:

$$a = 0.42748 \frac{R^2 T_c^2}{P_c} \alpha(T) \quad (7)$$

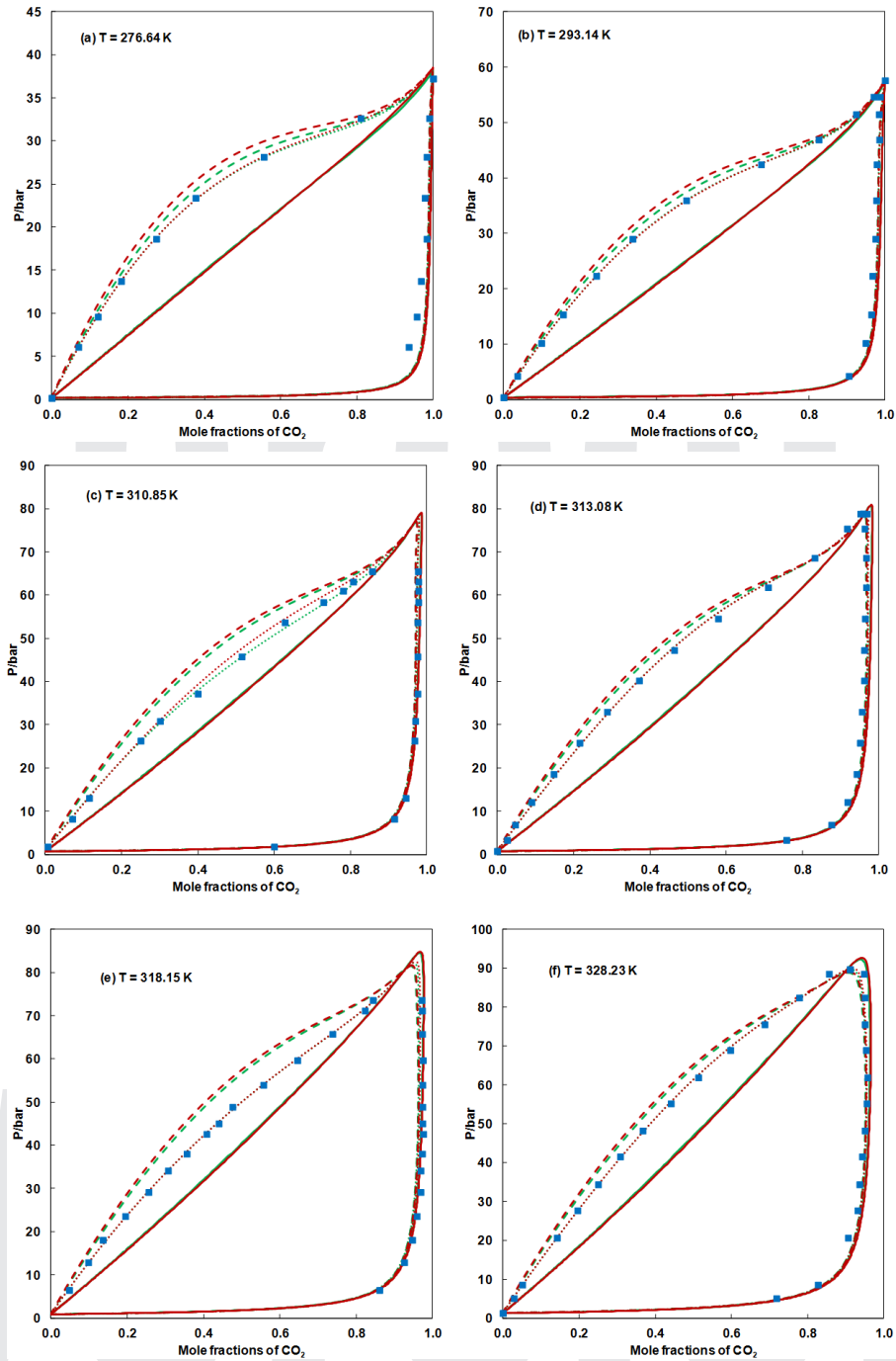


Figure 1. Comparison of literature data for the carbon dioxide + cyclopentane system and calculations by PR and SRK models: symbols, literature data at 276.64, 293.14, 310.85, 313.08, 318.15, and 328.23 K; dotted lines, correlations by PR (green) and SRK (red); dashed lines, calculations with average constant parameters by PR ($k_{12} = 0.1190, l_{12} = -0.0387$, green) and SRK ($k_{12} = 0.1290, l_{12} = -0.0421$, red); solid lines, predictions by PR ($k_{12} = 0.034, l_{12} = -0.001$, green) and SRK ($k_{12} = 0.030, l_{12} = -0.001$, red).

$$b = 0.08664 \frac{RT_c}{P_c} \quad (8)$$

$$m_{SRK} = 0.480 - 1.574\omega - 0.176\omega^2 \quad (10)$$

$$\alpha(T_R, \omega) = \left[1 + m_{SRK} (1 - T_R^{0.5}) \right]^2 \quad (9)$$

The two parameter conventional mixing rules are given by:

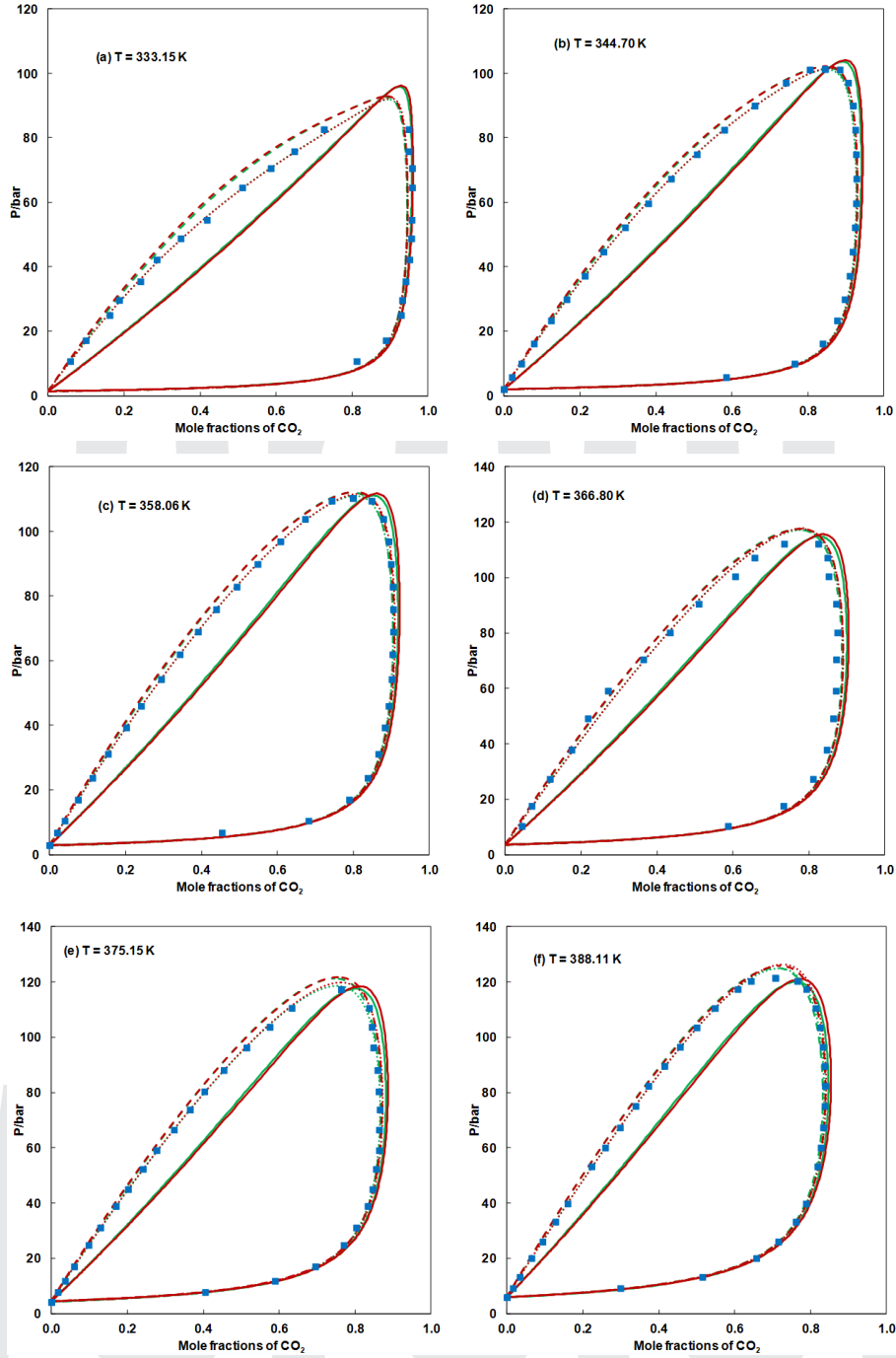


Figure 2. Comparison of literature data for the carbon dioxide + cyclopentane system and calculations by PR and SRK models: symbols, literature data at 333.15, 344.70, 358.06, 366.80, 375.15, and 388.11 K; dotted lines, correlations by PR (green) and SRK (red); dashed lines, calculations with average constant parameters by PR ($k_{12} = 0.1190$, $l_{12} = -0.0387$, green) and SRK ($k_{12} = 0.1290$, $l_{12} = -0.0421$, red); solid lines, predictions by PR ($k_{12} = 0.034$, $l_{12} = -0.001$, green) and SRK ($k_{12} = 0.030$, $l_{12} = -0.001$, red).

$$a = \sum_i \sum_j x_i x_j a_{ij} \quad (11)$$

$$b = \sum_i \sum_j x_i x_j b_{ij} \quad (12)$$

where

$$a_{ij} = \sqrt{a_i a_j} (1 - k_{ij}) \quad (13)$$

$$b_{ij} = \frac{b_i + b_j}{2} (1 - l_{ij}) \quad (14)$$

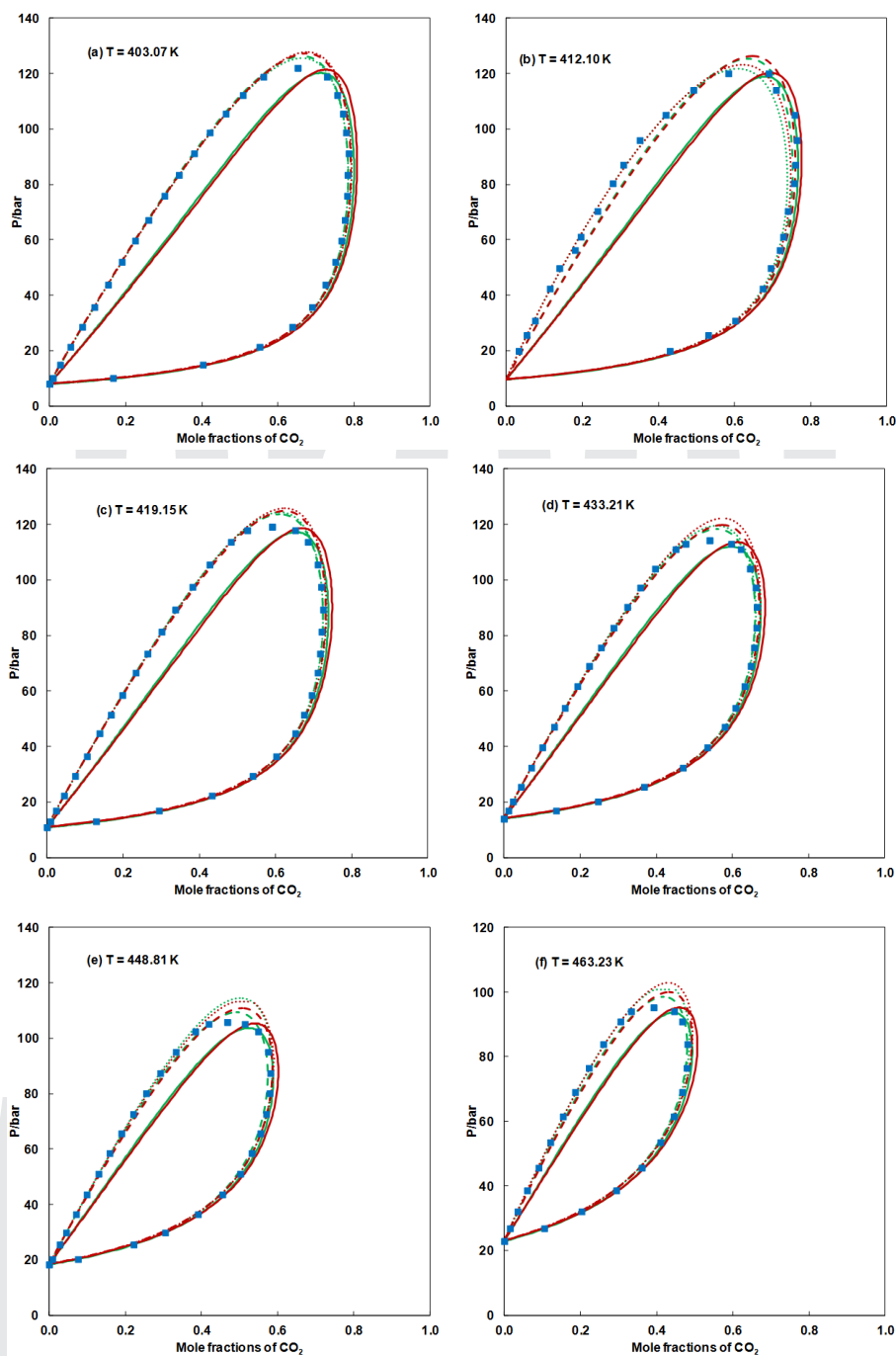


Figure 3. Comparison of literature data for the carbon dioxide + cyclopentane system and calculations by PR and SRK models: symbols, literature data at 403.07, 412.10, 419.15, 433.21, 448.81, and 463.23 K; dotted lines, correlations by PR (green) and SRK (red); dashed lines, calculations with average constant parameters by PR ($k_{12} = 0.1190$, $l_{12} = -0.0387$, green) and SRK ($k_{12} = 0.1290$, $l_{12} = -0.0421$, red); solid lines, predictions by PR ($k_{12} = 0.034$, $l_{12} = -0.001$, green) and SRK ($k_{12} = 0.030$, $l_{12} = -0.001$, red).

The calculations were made using the software packages PHEQ (Phase Equilibria Database and Calculations) [50] and GPEC (Global Phase Equilibrium Calculations) [51], developed in our laboratories.

3. Results and discussion

In this work all available isothermal vapor-liquid equilibrium data were firstly correlated with the PR and SRK EoSs coupled with classical van der Waals

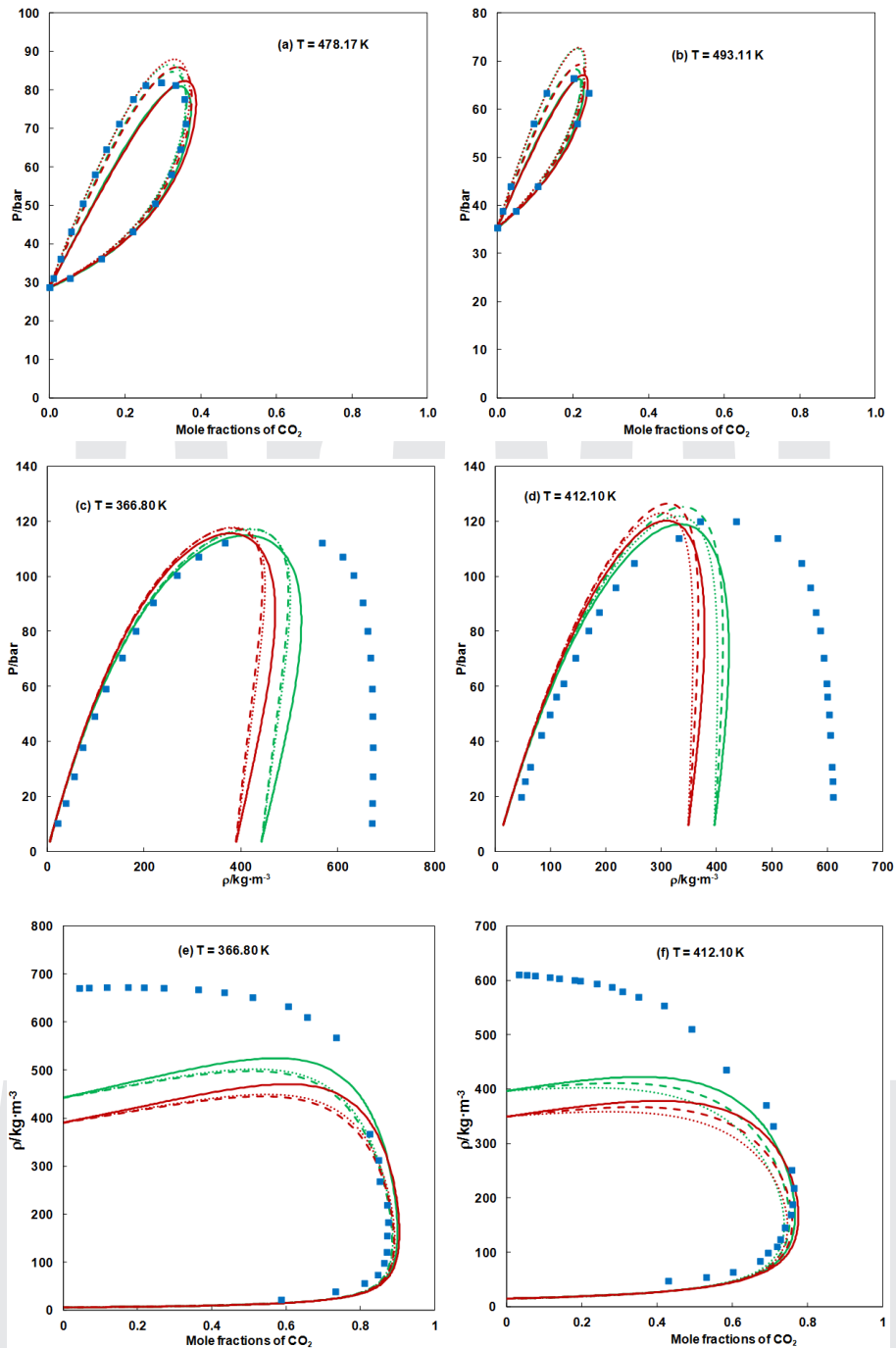


Figure 4. Comparison of literature data for the carbon dioxide + cyclopentane system and calculations by PR and SRK models: symbols, literature data at 366.80, 412.10, 478.17, and 493.11 K; dotted lines, correlations by PR (green) and SRK (red); dashed lines, calculations with average constant parameters by PR ($k_{12} = 0.1190$, $l_{12} = -0.0387$, green) and SRK ($k_{12} = 0.1290$, $l_{12} = -0.0421$, red); solid lines, predictions by PR ($k_{12} = 0.034$, $l_{12} = -0.001$, green) and SRK ($k_{12} = 0.030$, $l_{12} = -0.001$, red).

mixing rules (two-parameter conventional mixing rule, 2PCMR). Both equations have a similar behavior and, as temperature increases, the critical pressure is overestimated and the vapor phase is not very accurately described (Figs. 1-4, dotted dark red and

green lines). In Table 1 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

Table 1. Temperatures, optimized binary interaction parameters (k_{12} , l_{12}), number of experimental points, average absolute deviations in bubble point pressure (AADP, %), and average absolute deviations in the vapor phase compositions (AADY, %) for the carbon dioxide + cyclopentane binary system.

| Row | EoS | T/K | k_{12} | l_{12} | NEXP | AADP% | AADY% | Lit. |
|------|-----|--------|----------|----------|------|-------|-------|------|
| [5] | PR | 276.64 | 0.1078 | -0.0406 | 9 | 1.6 | 1.1 | 35 |
| [6] | SRK | | 0.1117 | -0.0401 | 9 | 1.0 | 1.1 | |
| [7] | PR | 293.14 | 0.1110 | -0.0354 | 12 | 0.8 | 0.5 | 35 |
| [8] | SRK | | 0.1129 | -0.0375 | 12 | 0.6 | 0.6 | |
| [9] | PR | 310.85 | 0.0790 | -0.0438 | 12 | 2.9 | 1.1 | 33 |
| [10] | SRK | | 0.1057 | -0.0225 | 12 | 3.7 | 0.9 | |
| [11] | PR | 313.08 | 0.1209 | -0.0137 | 15 | 3.4 | 0.8 | 35 |
| [12] | SRK | | 0.1240 | -0.0152 | 15 | 3.5 | 0.9 | |
| [13] | PR | 318.15 | 0.0812 | -0.0422 | 15 | 1.4 | 1.0 | 33 |
| [14] | SRK | | 0.0859 | -0.0416 | 15 | 1.4 | 0.8 | |
| [15] | PR | 328.23 | 0.1124 | -0.0212 | 15 | 1.3 | 0.8 | 35 |
| [16] | SRK | | 0.1189 | -0.0203 | 15 | 1.3 | 0.8 | |
| [17] | PR | 333.15 | 0.0904 | -0.0534 | 12 | 1.4 | 1.2 | 33 |
| [18] | SRK | | 0.0966 | -0.0535 | 12 | 1.4 | 1.0 | |
| [19] | PR | 344.70 | 0.1059 | -0.0434 | 17 | 0.7 | 0.8 | 35 |
| [20] | SRK | | 0.1148 | -0.0422 | 17 | 0.7 | 0.8 | |
| [21] | PR | 366.80 | 0.1128 | -0.0299 | 12 | 4.9 | 1.7 | 34 |
| [22] | SRK | | 0.1230 | -0.0290 | 12 | 4.9 | 2.1 | |
| [23] | PR | 358.06 | 0.1073 | -0.0387 | 18 | 0.3 | 1.0 | 35 |
| [24] | SRK | | 0.1178 | -0.0368 | 18 | 0.3 | 1.0 | |
| [25] | PR | 375.15 | 0.1027 | -0.0437 | 18 | 1.0 | 0.4 | 35 |
| [26] | SRK | | 0.1144 | -0.0421 | 18 | 1.1 | 0.6 | |
| [27] | PR | 388.11 | 0.1131 | -0.0295 | 19 | 0.5 | 0.5 | 35 |
| [28] | SRK | | 0.1254 | -0.0281 | 19 | 0.6 | 0.7 | |
| [29] | PR | 403.07 | 0.1159 | -0.0397 | 18 | 0.3 | 0.4 | 35 |
| [30] | SRK | | 0.1306 | -0.0387 | 18 | 0.5 | 0.9 | |
| [31] | PR | 412.10 | 0.1140 | -0.0911 | 14 | 1.5 | 1.2 | 34 |
| [32] | SRK | | 0.1288 | -0.0957 | 14 | 1.6 | 0.9 | |
| [33] | PR | 419.15 | 0.122 | -0.0347 | 18 | 0.5 | 0.3 | 35 |
| [34] | SRK | | 0.1343 | -0.0391 | 18 | 0.7 | 0.8 | |
| [35] | PR | 433.21 | 0.1261 | -0.0345 | 18 | 0.5 | 0.4 | 35 |
| [36] | SRK | | 0.1432 | -0.0351 | 18 | 0.8 | 0.8 | |
| [37] | PR | 448.81 | 0.1507 | -0.0138 | 16 | 0.7 | 0.6 | 35 |
| [38] | SRK | | 0.1503 | -0.0381 | 16 | 0.9 | 0.7 | |
| [39] | PR | 463.23 | 0.1466 | -0.0356 | 13 | 0.4 | 0.5 | 35 |
| [40] | SRK | | 0.1615 | -0.0482 | 13 | 0.6 | 0.6 | |
| [41] | PR | 478.17 | 0.1487 | -0.0564 | 11 | 0.4 | 0.7 | 35 |
| [42] | SRK | | 0.1659 | -0.0705 | 11 | 0.5 | 0.7 | |
| [43] | PR | 493.11 | 0.2114 | -0.0328 | 6 | 0.2 | 0.6 | 35 |
| [44] | SRK | | 0.2144 | -0.0680 | 6 | 0.1 | 0.6 | |

Table 2. Critical data and acentric factor [52] for carbon dioxide and cyclopentane.

| Component | T_c /K | P_c /bar | w |
|--------------------------------|----------|------------|-------|
| CO ₂ | 304.21 | 73.83 | 0.224 |
| C ₅ H ₁₀ | 511.70 | 45.10 | 0.195 |

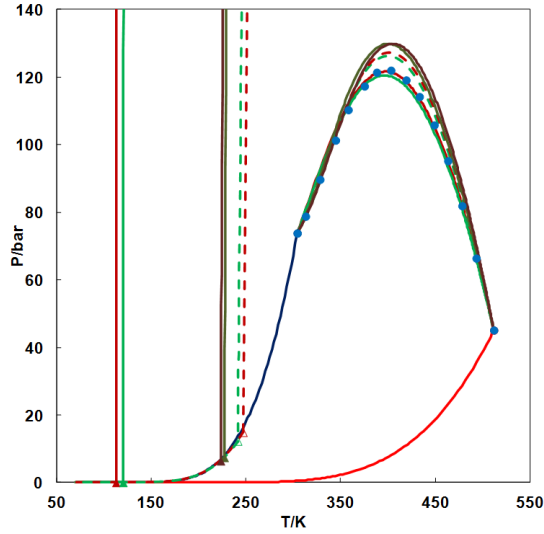


Figure 5. P - T fluid phase diagram of carbon dioxide + cyclopentane binary system: blue full circle (●), experimental critical curve; dark blue full circle (●) and red full circle (●), experimental critical points of pure components; dark blue and red solid lines (—, —), calculated vapor pressure curves of pure components; green and dark red triangles (▲, ▲), calculated UCEP and green and dark red dashed lines (---, ---), calculated critical curves and LLV lines respectively with average constant parameters by PR ($k_{12} = 0.1190$, $l_{12} = -0.0387$) and SRK ($k_{12} = 0.1290$, $l_{12} = -0.0421$); green and dark red full triangles (▲, ▲), calculated UCEP and green and dark red solid lines (—, —), calculated critical curves and LLV lines respectively by PR ($k_{12} = 0.034$, $l_{12} = -0.001$) and SRK ($k_{12} = 0.030$, $l_{12} = -0.001$); dark green and brown full triangles (▲, ▲), calculated UCEP and dark green and brown solid lines (—, —), calculated critical curves and LLV lines respectively by PR and SRK ($k_{12} = 0.123$, $l_{12} = 0$);

(AADY%). The AADP, respectively AADY are calculated by the equations:

$$AADP(\%) = \frac{1}{N_{\text{exp}}} \sum_{i=1}^{N_{\text{exp}}} \left| \frac{P_i^{\text{exp}} - P_i^{\text{calc}}}{P_i^{\text{exp}}} \right| \times 100 \quad (15)$$

$$AADY(\%) = \frac{1}{N_{\text{exp}}} \sum_{i=1}^{N_{\text{exp}}} |Y_i^{\text{exp}} - Y_i^{\text{calc}}| \times 100 \quad (16)$$

It can be seen that most errors in bubble-point pressures are less than 1.5% and the few exceptional cases with the highest errors are the fitting results for the experimental data measured by Eckert and Sandler [33]

at 310.85 K, Shah *et al.* [35] at 313.08 K and Marathe and Sandler [34] at 366.80 K.

The overall average absolute deviations in bubble-point pressures is 1.2% for PR/2 PCMR and 1.3% for SRK/2PCMR and the overall corresponding average absolute deviations in the vapor-phase compositions are 0.8% and 0.9% respectively. The critical values of the pure carbon dioxide and cyclopentane together with the acentric factors used in the calculations are presented in Table 2.

It should be also remarked that a degree of scatter is observed when the experimental data are plotted together. For instance, when comparing graphically the experimental data measured at 313.08 K [35] with those determined at 318.15 K [33], it can be noticed that they intersect. Although the phase behavior of carbon dioxide + cyclopentane binary mixture seems properly represented by fitting the experimental data, the global phase diagram, meaning the projection of the critical locus in the P - T diagram, is not always correctly showed. As previously mentioned, this system should be type I or type II phase behavior, according to the classification of van Konyneburg and Scott [36,37]. Nevertheless, the optimum values of binary interaction parameters for some temperatures lead to a type III phase behavior or to azeotropic/heterogeneous endpoints for which there is no physical evidence [9]. However, averaged values of the optimum binary interaction parameters were used to calculate the global diagram for the carbon dioxide + cyclopentane system (Fig. 5, dashed dark red and green lines). These parameters ($k_{12} = 0.1190$, $l_{12} = -0.0387$ for PR, $k_{12} = 0.1290$, $l_{12} = -0.0421$ for SRK respectively) predict type II phase behavior. It can be easily observed the overestimation of the critical pressure maximum as well as the appearance of the upper critical endpoint at about 250 K for both equations. The average values of the optimum binary interaction parameters were also used to recalculate the isothermal literature data (Figures 1-4, dashed dark red and green lines). Both equations behave similarly, but at low temperatures the results for the liquid phase by PR are better than SRK (Fig. 1). Overall, the predictions with the averaged parameters are reasonably well, even the errors are bigger in bubble-point pressures (4.5% for PR/2PCMR and 5.5% for SRK/2PCMR).

Finally, based on previous results [4,38-44] with mixtures containing carbon dioxide and alcohols, or alkanes, the PR and SRK EoSs coupled with classical van der Waals mixing rules (two parameter conventional, 2PCMR) were also used in a semi predictive approach to model the phase behavior of carbon dioxide + cyclopentane system. For each equation of state,

one set of parameters temperature independent that guarantee a good representation of the critical line was used to predict the phase behavior [38-44], i.e., critical curves, LLV line, isothermal VLE, and densities.

The parameter sets were obtained by a trial and error method in order to represent well the experimental critical pressure maximum (CPM) and to avoid the appearance of an upper critical endpoint (UCEP) at lower temperatures. Thus, the sets of binary interaction parameters are ($k_{12} = 0.030$, $l_{12} = -0.001$) for SRK and ($k_{12} = 0.034$, $l_{12} = -0.001$) for PR EoS respectively.

As expected, the calculations (which are called predictions in the figure captions) with the new two sets of parameters are less accurate for the liquid phase (Figs. 1-4). It can be observed that both correlations and predictions are satisfactory only for the saturated vapor densities (Fig. 4c-4f). It should remark that Privat [53] also used a unique set of parameters ($k_{12} = 0.123$, $l_{12} = 0.0$) temperature independent to model the carbon dioxide + cyclopentane binary system with the PPR78 model obtaining accurate results. This set of parameters was also used to calculate the phase behavior for the carbon dioxide + cyclopentane system with SRK and PR models coupled with classical van der Waals mixing rules (Fig. 5). The overall average absolute deviations in bubble-point pressures are in this case 5.3% for PR EoS and 6.2% for SRK.

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4. Conclusion

The phase equilibrium data of the carbon dioxide + cyclopentane binary mixtures was modeled with PR and SRK thermodynamic models with classical van der Waals mixing rules. Both correlations and a semi predictive approach were used to represent the phase behavior of the system. The predictions have the advantage to represent correctly the topology of phase diagram, but with larger errors in the description of the liquid phase.

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