Experimental Determination and Modeling of Bubble and Dew Points in the System $CO_2 + CHF_3$

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Bubble point (L + V → L) and dew point (L + V → V) pressures were measured for the binary system $CO_2 + CHF_3$, using Cailletet equipment. The measurements were carried out for the whole mole fraction range and for temperatures from 263 K up to the mixture critical points. The experimental data were used to determine binary interaction parameters for the Peng−Robinson equation of state with a Stryjek and Vera modification (PRSV) and a Margules-type binary interaction parameter.

Introduction

In the presence of water and at specific conditions, CO_2 forms clathrates, also known as gas hydrates. The hydrate of CO_2 has several potential applications, for instance, desalination of seawater to produce potable water or storage of emitted CO_2 into depleted reservoirs (sequestration). Compounds that facilitate hydrate formation[1] can be added to the system to make the process more attractive. Previous work showed that small amounts of CHF_3 promote hydrate formation in systems with CO_2 by forming a mixed hydrate.[2]

Supercritical CO_2 and CHF_3 are also potential solvents in extraction processes.[3,4] These processes are characterized by high mass transfer rates that improve solute extraction. Where process efficiency and selectivity are important, a mixture of $CO_2 + CHF_3$ could be beneficial.[5]

Assessment of these applications for mixtures of CO_2 and CHF_3 requires a good understanding of the phase behavior of this system.[6] Experimental data of these systems can also be used to adjust parameters for model predictions.[7]

This work presents experimentally determined bubble (L + V → L) and dew point (L + V → V) pressures in the system $CO_2 + CHF_3$ for a wide range of overall compositions and for temperatures from 263 K up to the mixture critical point. The measured data are used to derive binary interaction parameters for the Peng−Robinson equation of state with a modification according to Stryjek−Vera (PRSV). Calculated values are compared with the experimental data.

Experimental

The measurements were performed in a so-called Cailletet apparatus. The Cailletet apparatus is basically a half-open glass tube with an inner and outer diameter of (3 and 8) mm, respectively. The binary mixtures were prepared by a synthetic method; i.e., at fixed temperature and prespecified pressures, known volumes of CO_2 and CHF_3 were dosed into the Cailletet tube. Then, the number of moles and compositions were calculated using the ideal gas law or a virial equation depending on the pressure.[2,8,9] Having filled the tube with a sample, the open end is submerged in mercury. The mercury seals the sample and also transmits

Table 1. Pure Component Properties Used in This Work

compound	T_C /K	p_C /MPa	ω	κ_1[a]
CO_2	304.21	7.382	0.225	0.04258
CHF_3	299.30	4.860	0.260	0.01896

[a] Determined in this work.

Table 2. Margules-Type Binary Interaction Parameters $(1 - x_1k_{12} - x_2k_{21})$ for the System CO_2 (1) + CHF_3 (2)

k_{12}	0.009
k_{21}	−0.001

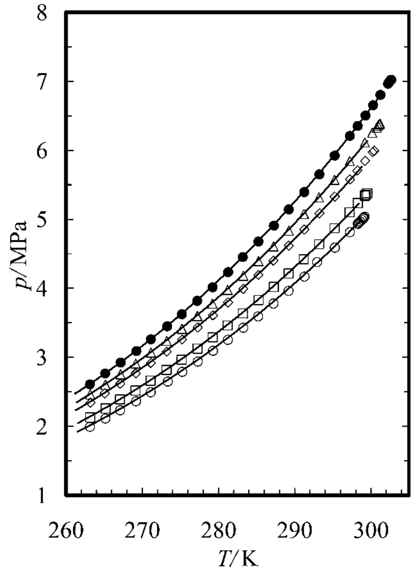

Figure 1. p, T projection for experimental (markers) and calculated (−) bubble points (L + V → L) in the system CO_2 (1) + CHF_3 (2) at overall CHF_3 composition: ●, 0.105; Δ, 0.353; ◇, 0.5; □, 0.75; ○, 0.894.

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Table 3. Bubble Point Conditions (L + V → L) for the System CO_2 (1) + CHF_3 (2) for Several Isopleths

$x_2 = 0.105$		$x_2 = 0.250$		$x_2 = 0.353$		$x_2 = 0.500$		$x_2 = 0.655$		$x_2 = 0.752$		$x_2 = 0.895$	
T/K	p/MPa	T/K	p/MPa	T/K	p/MPa	T/K	p/MPa	T/K	p/MPa	T/K	p/MPa	T/K	p/MPa
263.15	2.608	263.19	2.533	263.18	2.463	263.21	2.342	263.19	2.214	263.16	2.129	263.15	1.992
265.15	2.763	265.12	2.668	265.16	2.603	265.09	2.477	265.15	2.339	265.20	2.259	265.18	2.112
267.19	2.923	267.14	2.828	267.17	2.753	267.13	2.617	267.17	2.474	267.09	2.389	267.11	2.232
269.23	3.088	269.11	2.983	269.16	2.908	269.16	2.767	269.17	2.614	269.12	2.519	269.19	2.362
271.14	3.258	271.21	3.153	271.16	3.068	271.14	2.917	271.18	2.764	271.10	2.659	271.13	2.492
273.26	3.448	273.20	3.328	273.21	3.238	273.21	3.082	273.21	2.914	273.20	2.814	273.38	2.647
275.20	3.623	275.20	3.503	275.21	3.413	275.25	3.257	275.26	3.079	275.18	2.964	275.25	2.787
277.23	3.818	277.26	3.698	277.23	3.598	277.28	3.432	277.23	3.239	277.25	3.124	277.28	2.937
279.25	4.013	279.21	3.883	279.20	3.778	279.27	3.607	279.23	3.413	279.24	3.289	279.29	3.092
281.28	4.233	281.22	4.093	281.21	3.978	281.27	3.795	281.19	3.583	281.21	3.459	281.23	3.252
283.21	4.451	283.22	4.298	283.26	4.183	283.26	3.990	283.23	3.768	283.20	3.634	283.26	3.427
285.24	4.676	285.24	4.518	285.26	4.393	285.22	4.190	285.23	3.963	285.27	3.829	285.21	3.592
287.28	4.906	287.20	4.738	287.20	4.608	287.21	4.400	287.19	4.163	287.26	4.019	287.23	3.777
289.22	5.141	289.15	4.973	289.21	4.838	289.23	4.615	289.25	4.373	289.21	4.214	289.19	3.962
291.25	5.391	291.20	5.218	291.21	5.078	291.25	4.850	291.19	4.583	291.18	4.419	291.28	4.167
293.24	5.651	293.17	5.468	293.18	5.318	293.25	5.085	293.27	4.813	293.22	4.639	292.94	4.377
295.25	5.921	295.15	5.728	295.19	5.573	295.25	5.327	295.23	5.043	295.22	4.869	295.27	4.587
297.24	6.206	297.23	6.008	297.23	5.843	297.23	5.577	297.28	5.293	297.21	5.104	297.24	4.812
298.26	6.351	299.22	6.288	299.20	6.113	298.22	5.707	298.26	5.413	298.28	5.234	298.28	4.932
299.28	6.501	300.18	6.433	300.18	6.253	299.23	5.847	299.21	5.533	299.21	5.339	298.43	4.947
300.29	6.651	301.59^{a}	6.638^{b}	300.74	6.328	300.21	5.972	299.43	5.558	299.33	5.354	298.61	4.967
301.25	6.801			300.93	6.358	300.43^{a}	5.992^{b}	299.57	5.578	299.50^{a}	5.374^{b}	298.80	4.992
302.26	6.961			301.11	6.378			299.73	5.599			298.96	5.012
302.41	6.991			301.19^{a}	6.388^{b}			299.84^{a}	5.614^{b}			299.06	5.022
302.61	7.021											299.17^{a}	5.037^{b}
302.67^{a}	7.021^{b}												

^{a} Critical temperature. ^{b} Critical pressure.

Table 4. Dew Point Conditions (L + V → V) for the System CO_2 (1) + CHF_3 (2) for Several Isopleths

$x_2 = 0.105$		$x_2 = 0.353$		$x_2 = 0.500$		$x_2 = 0.655$		$x_2 = 0.752$		$x_2 = 0.895$		$x_2 = 1$	
T/K	p/MPa	T/K	p/MPa	T/K	p/MPa	T/K	p/MPa	T/K	p/MPa	T/K	p/MPa	T/K	p/MPa
263.13	2.592	263.15	2.393	263.13	2.282	263.14	2.154	263.15	2.066	263.17	1.969	263.18	1.878
265.19	2.746	265.19	2.527	265.17	2.417	265.21	2.284	265.20	2.201	265.22	2.084	265.12	1.988
267.12	2.901	267.14	2.672	267.17	2.552	267.10	2.413	267.11	2.320	267.12	2.198	267.16	2.108
269.08	3.061	269.13	2.822	269.21	2.697	269.17	2.552	269.12	2.454	269.16	2.328	269.14	2.228
271.19	3.241	271.12	2.982	271.17	2.841	271.20	2.702	271.10	2.593	271.15	2.463	271.18	2.358
273.27	3.426	273.23	3.156	273.28	2.990	273.27	2.862	273.24	2.752	273.22	2.607	273.19	2.488
275.27	3.615	275.22	3.331	275.21	3.155	275.25	3.012	275.41	2.896	275.21	2.747	275.18	2.623
277.26	3.805	277.23	3.511	277.21	3.350	277.22	3.172	277.25	3.050	277.27	2.902	277.26	2.773
279.23	4.000	279.26	3.700	279.26	3.544	279.20	3.342	279.19	3.220	279.28	3.056	279.25	2.923
281.24	4.210	281.22	3.895	281.24	3.729	281.18	3.516	281.19	3.399	281.26	3.221	281.24	3.078
283.29	4.430	283.23	4.100	283.31	3.929	283.21	3.706	283.20	3.579	283.21	3.386	283.23	3.233
285.24	4.650	285.18	4.310	285.25	4.124	285.24	3.901	285.21	3.763	285.22	3.556	285.16	3.398
287.20	4.873	287.24	4.529	287.28	4.339	287.27	4.106	287.21	3.953	287.26	3.746	287.19	3.573
289.25	5.124	289.26	4.754	289.23	4.554	289.22	4.315	289.22	4.157	289.26	3.941	289.22	3.763
291.17	5.364	291.24	4.994	291.26	4.779	291.28	4.535	291.19	4.362	291.28	4.139	291.19	3.943
293.28	5.639	293.24	5.249	293.25	5.019	293.22	4.755	293.22	4.582	293.24	4.343	293.24	4.148
295.29	5.909	295.22	5.514	295.19	5.269	295.23	4.994	295.23	4.821	295.26	4.563	295.20	4.353
297.27	6.189	297.19	5.784	297.26	5.534	297.18	5.239	297.27	5.071	297.25	4.793	297.23	4.573
299.30	6.479	299.18	6.068	299.25	5.814	299.25	5.514	298.28	5.195	298.29	4.918	298.29	4.693
301.21	6.784	300.20	6.218	300.26	5.964	299.62	5.568	298.61	5.234	298.86	4.987	298.99^{a}	4.788^{b}
302.27	6.953	300.96	6.343	300.38	5.984	299.75	5.588	298.95	5.279	299.02	5.007		
302.57	7.008	301.06	6.368			299.83	5.598	299.10	5.294	299.16	5.027		
								299.26	5.314				
								299.44	5.349				

^{a} Critical temperature. ^{b} Critical pressure.

the pressure. Pressure is produced through a dead-weight gauge with an uncertainty of ± 0.005 MPa. The exerted pressure could range from (0.35 to as high as 15) MPa. The Cailletet tube is immersed in ethanol which maintains the sample temperature. With this arrangement, the temperature range that can be studied extends from (255 to 355) K. However, at higher temperatures up to 455 K, the Cailletet tube is immersed in silicon oil. The temperature outside the tube is measured using a PT-100 platinum resistance thermometer. The uncertainty of the PT-100 thermometer is better than ± 0.02 K. Within the tube, the sample is optimally mixed using a magnetic stirrer. Normally, the system reaches equilibrium after a few minutes.

The bubble point (L + V → L) is measured by gradually raising the pressure at constant temperature. The bubble point is recorded at the pressure where the gas bubble disappears. Similarly, the dew point (L + V → V) is measured by gradually reducing the pressure at a constant temperature. The dew point is recorded at the pressure where the last droplet of liquid disappears. The temperatures ranged from 263 K up to the mixture critical point. The critical point (L = V) is recorded at the conditions where the vapor and liquid

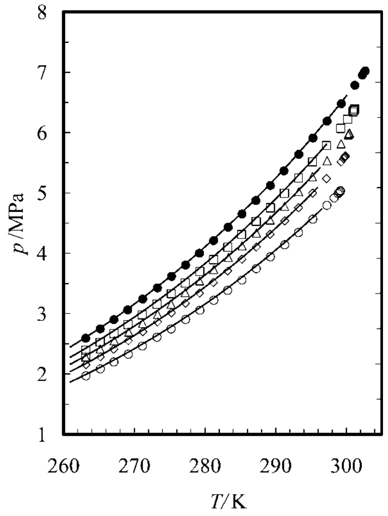

Figure 2. p, T projection for experimental (markers) and calculated (—) dew points (L + V → V) in the system CO_2 (1) + CHF_3 (2) at overall CHF_3 composition: ●, 0.105; □, 0.353; △, 0.5; ◇, 0.656; ○, 0.894.

phase become identical (visual observation). The repeatability of the measurements in terms of variance (σ^2/MPa^2) was $2.67 \cdot 10^{-4}$.

In the experiments, CO_2 with purity better than 99.95 % was used. The supplier for CO_2 was Messer-Griesheim. For CHF_3, the supplier was Air Products with a claimed purity of 99.5 %. No further purification was performed.

Modeling

To model the experimentally determined bubble and dew point conditions in the system $CO_2 + CHF_3$, the Peng–Robinson (PR)[10] equation of state (EoS) as modified by Stryjek and Vera (PRSV)[11,12] is used. The PRSV and PR EoS differ in the temperature-dependent term for the attraction parameter. The PRSV EoS is expressed by

$$p = \frac{RT}{v-b} - \frac{a}{v^2 + 2bv - b^2} \tag{1}$$

with

$$b = 0.077796\frac{RT_C}{p_C} \tag{2}$$

$$a = 0.457235\frac{R^2T_C^2}{p_C}\alpha \tag{3}$$

where p/MPa is the pressure; v/m$^3\cdot$kmol^{-1} is the molar volume; T/K is the temperature; R/MPa$\cdot$m$^3\cdot$kmol$^{-1}\cdot$K^{-1} is the universal gas constant; a/MPa$\cdot$m$^6\cdot$kmol^{-2} is the attraction parameter; and b/m$^3\cdot$kmol^{-1} is the molar covolume. In eqs 2 and 3, the subscript C stands for the critical properties. In eq 3, the parameter α is defined by

$$\alpha = [1 + \kappa(1 - T_r^{0.5})]^2 \tag{4}$$

with

$$\kappa = \kappa_0 + \kappa_1(1 + T_r^{0.5})(0.7 - T_r) \tag{5}$$

$$\kappa_0 = 0.378893 + 1.4897153\omega - 0.17131848\omega^2 + 0.0196554\omega^3 \tag{6}$$

In eq 5, the parameter κ_1 is component-specific, which is determined by matching experimental data and model calculations from pure component vapor pressure data from the triple point up to the critical point. If κ_1 is set to zero, the classical Soave-type expression for the PR EoS will be recovered. However, inclusion of κ_1 improves the accuracy of the PRSV EoS in calculating the vapor pressure of pure compounds, especially from low temperatures up to reduced temperatures of around 0.7.[11] This approach yields accurate pure component attractive parameters and consequently mixture attractive parameters to be used in the equilibrium calculations. In this work, smoothed data reported by ASHRAE[13] for CO_2 and CHF_3 were used to determine the κ_1 parameters. The optimized κ_1 parameters for CO_2 and CHF_3 along with other necessary pure component properties are summarized in Table 1.

For calculating mixture properties, the conventional van der Waals mixing rules with a Margules-type binary interaction parameter[12] are used

$$b = \sum\nolimits_j x_j b_j \tag{7}$$

$$a = \sum\nolimits_i \sum\nolimits_j x_i x_j a_{ij}(1 - x_i k_{ij} - x_j k_{ji}) \tag{8}$$

where $a_{ij} = \sqrt{a_{ii}a_{jj}}$ and k_{ij} and k_{ji} are two adjustable parameters. The binary interaction parameters $k_{11} = k_{22} = 0$ and k_{12} and k_{21} ($k_{12} \neq k_{21}$) are determined by regression of the experimental data reported in this work.

Results

Experimental Section. Once a mixture was prepared at a specified overall composition, bubble point (L + V → L) pressures were measured at prespecified temperatures in the region 263 K up to the mixture critical point. The measured data are collected in Table 3. Similar experiments were performed for measuring dew point (L + V → V) pressures for the various overall compositions. The dew point (L + V → V) pressures at different isopleths are given in Table 4. The mixture critical points (L = V) are reported in Tables 3 and 4 and were measured as part of the bubble and dew point curves. Further, the measurements are visualized in Figures 1and 2. For clarity, some isopleths were skipped.The bubble and dew point curves of each overall composition almost coincide because CO_2 and CHF_3 have close boiling points. Also, their critical conditions are very close. Despite this similarity, mixtures of these components do not show azeotropic behavior. Almost ideal behavior was observed.

To check the consistency of the measurements, the pressure–temperature data at different overall compositions were fitted to polynomials (with average correlating coefficient better than 0.9995). Then, at specified round values of the temperature in the region from (265 to 295) K pressures of the isotherms were interpolated. The data of different isotherms are reported in Table 5 for bubble point pressures and in Table 6 for dew point pressures. The interpolated data were also depicted in Figures 3 and 4, showing almost linear relations between bubble and dew point pressures with CHF_3 composition.

Modeling Section. The experimentally determined bubble points, as given in Table 3 for the system CO_2 (1) + CHF_3 (2) for several isopleths, were used to determine the binary interaction parameters k_{12} and k_{21}: see Table 2. Using a nonlinear regression package,[14] the following objective function was minimized

Table 5. Interpolated Bubble Point Pressures (L + V → L) for Several Isotherms in the System CO_2 (1) + CHF_3 (2)

	p/MPa								
T/K	$x_2 = 0$	$x_2 = 0.105$	$x_2 = 0.250$	$x_2 = 0.353$	$x_2 = 0.500$	$x_2 = 0.655$	$x_2 = 0.753$	$x_2 = 0.895$	$x_2 = 1$
265	2.776	2.717	2.682	2.602	2.497	2.341	2.269	2.089	1.993
270	3.191	3.125	3.074	2.984	2.862	2.687	2.604	2.404	2.295
275	3.644	3.572	3.507	3.404	3.265	3.069	2.972	2.752	2.626
280	4.142	4.063	3.986	3.868	3.711	3.491	3.379	3.137	2.991
285	4.691	4.603	4.514	4.379	4.202	3.956	3.827	3.563	3.396
290	5.296	5.198	5.094	4.942	4.742	4.468	4.322	4.033	3.847
295	5.963	5.852	5.731	5.561	5.334	5.031	4.868	4.550	4.350

Table 6. Interpolated Dew Point Pressures (L + V → V) for Several Isotherms in the System CO_2 (1) + CHF_3 (2)

	p/MPa							
T/K	$x_2 = 0$	$x_2 = 0.105$	$x_2 = 0.353$	$x_2 = 0.500$	$x_2 = 0.655$	$x_2 = 0.752$	$x_2 = 0.895$	$x_2 = 1$
265	2.776	2.705	2.526	2.376	2.288	2.190	2.071	1.993
270	3.190	3.110	2.903	2.724	2.630	2.519	2.384	2.295
275	3.644	3.557	3.319	3.123	3.009	2.887	2.730	2.626
280	4.142	4.048	3.782	3.572	3.430	3.295	3.113	2.991
285	4.691	4.589	4.294	4.069	3.896	3.747	3.538	3.396
290	5.296	5.183	4.862	4.613	4.413	4.247	4.010	3.847
295	5.963	5.834	5.489	5.204	4.986	4.797	4.531	4.350

$$\Delta = \sum_{j}^{np} \left| \frac{p_{\text{calcd},j} - p_{\text{exptl},j}}{p_{\text{exptl},j}} \right| \qquad (9)$$

where Δ is the objective function; *np* is the total number of data points; and the subscripts calcd and exptl stand for calculated and experimental pressures.

If one takes $k_{12} = k_{21}$, the conventional binary interaction parameter, which is a function of temperature, will be recovered. With this arrangement, it is likely to accurately correlate the bubble and dew points of the system CO_2 + CHF_3. However, this work was part of our main research interest, i.e., formation of CO_2 hydrate in the presence of CHF_3. Because the PR EoS with conventional mixing rules is not adequate for systems containing associating water, polar CHF_3, and quadrapolar CO_2, for the consistency in the modeling, we decided to use a more complex binary interaction parameter. This explains the use of van der Waals mixing rules with a compositional dependence for binary interaction parameters. However, in this case, the mixing rule is not quadratic and does not obey the exact expression for mixture second virial coefficients at low densities.

The calculated and experimental bubble point pressures are in good agreement, as shown in Figure 1. For the dew point pressures, the agreement between the calculated and experimental data is fairly good, except close to the critical points where the PRSV EoS with the Margules-type binary interaction parameter fails. This failure is attributed to the nonquadratic behavior of the mixing rule after employing a Margules-type compositional-dependent binary interaction parameter to the van der Waals mixing rule.

The PRSV EoS was also used to predict the interpolated bubble and dew point pressures at different isotherms. In Figures 3 and 4 it is shown that the agreement between experimental data and calculations is satisfactory for the whole composition range and temperatures varying from (265 to 295) K.

Conclusions

The binary system CO_2 + CHF_3 shows a narrow phase envelope; i.e., bubble (L + V → L) and dew point (L + V → V) pressures are very close at constant overall composition. The system shows almost ideal behavior, e.g., a phenomenon like azeotropy is absent.

The PRSV EoS gives good results for the bubble and dew points of the system CO_2 + CHF_3 in the whole mole fraction

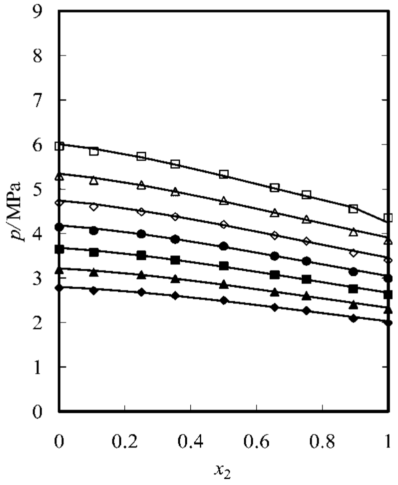

Figure 3. *p*, *x* cross section for interpolated (markers) and calculated (—) bubble points (L + V → L) in the system CO_2 (1) + CHF_3 (2) at various temperatures: ♦, 265 K; ▲, 270 K; ■, 275; ●, 280 K; ◇, 285 K; Δ, 290 K; □, 295 K.

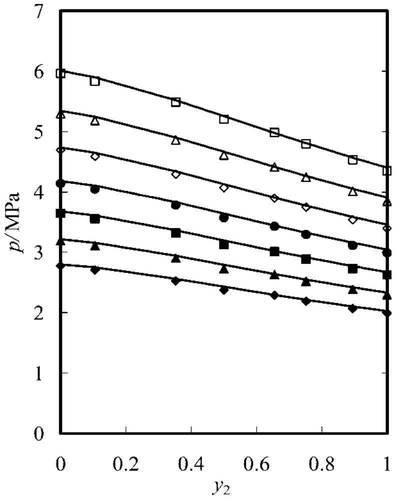

Figure 4. *p*, *x* cross section for interpolated (markers) and calculated (—) dew points (L + V → V) in the system CO_2 (1) + CHF_3 (2) at various temperatures: ♦, 265 K; ▲, 270 K; ■, 275 K; ●, 280 K; ◇, 285 K; Δ, 290 K; □, 295 K.

range and far from the system critical point. However, near the system critical point, the PRSV EoS fails. The binary interaction parameters for the PRSV EoS have been determined from fitting to the data reported in this study. The values for binary interaction parameters indicate that there is a weak interaction between CHF_3 and CO_2 molecules.

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