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Experimental Vapor-Liquid Equilibria for the Carbon Dioxide + Octane, and Carbon Dioxide + Decane Systems from 313 to 373 K

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ABSTRACT

The study of systems containing carbon dioxide + hydrocarbon is important for the enhanced oil recovery, at the chemical, and petrochemical industries. We are focused on the application of supercritical carbon dioxide to extract sulfur compounds from fuels. In the development of an extraction process are involved multicomponent mixtures. For the modeling of these systems the interaction parameters are required for all the binary pairs presented. Unfortunately, the determination of these interaction parameters requires of high accurate experimental data over a wide range of temperatures. Binary systems involving carbon dioxide + sulfur compound, and carbon dioxide + sulfur compound + alkane have been already reported in the literature [1,2]. This work is focused in the study of the phase behavior of the carbon dioxide + alkane mixtures as complement of the previous papers [1,2].

Vapor-liquid equilibria for the carbon dioxide + octane, and carbon dioxide + decane systems were measured at temperatures from 313 to 373 K. The experimental data were obtained using an apparatus based on the static-analytic method [3]. Data from the literature [4,5] were compare with the results obtained in this work. Good agreement was found. Vapor-liquid equilibrium data were correlated with the Peng-Robinson equation of state. Partition coefficients were calculated from the equilibrium compositions.

EXPERIMENTAL METHOD AND APPARATUS

Measurements were made in an apparatus based on the static-analytic method [1,2] previously described by Elizalde-Solis et al (figure 1). The equilibrium cell can be used up to 60 MPa and 523.15 K. This apparatus allows studying systems in one, two or three phases. A detailed description of the apparatus is found at reference [3].

A gas chromatograph (HP 6890) with a thermal conductivity detector TCD and a 4-ft by 1/8-in-diameter column packed (Porapak Q) was used for analysis. The carrier gas was helium at a flow rate of 30 ml/min. Pressure was measured using a thermoregulated Druck transducer model PDCR. This was calibrated against a Desgranges & Huot dead weight gauge (Model 5304 Class S2, $\pm 0.005\%$ F.S. precision up to 138 MPa). Temperature was measured using two platinum probes Pt100 (Specitec, France) immersed in thermometric wells at the top and bottom of the cell body [3]. They were connected to a digital indicator (F250, USA, accuracy ± 0.03 K). Platinum probes were calibrated against a 25- Ω reference probe (model 162CE of ± 0.005 K certified accuracy) connected to an Automatic Systems F300S calibration system.

The purities of the compounds used in this work were 99+% for octane and decane, both supplied by Aldrich Chemical Co. Inc. Certified purities of carbon dioxide and helium were 99.995% and 99.998%, respectively. Air Products-Infra supplied both gases. These compounds were used without any further purification, except for careful degassing of octane and decane.

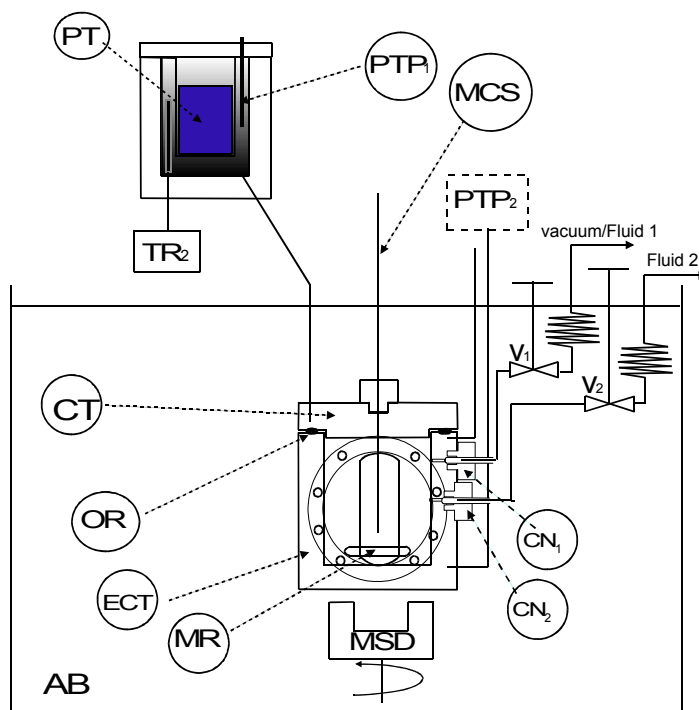


Figure. 1. Flow diagram of the equilibrium cell: AB air bath; CT titanium cap; CNi connecting nuts; ECT titanium equilibrium cell; MCS movable capillary sampler; MR magnetic rod; MSD magnetic stirring device; OR O-ring; PT pressure transducer; PTPi platinum temperature probe; TRi thermal regulator i, and Vi shut-off valve i.

First the alkane was introduced into the equilibrium cell, and then it was degassed under vacuum and vigorously stirred with the magnetic rod. After 20 minutes of degassing, the system was closed, and then reopened to introduce CO_2 into the measuring cell using an Isco syringe pump (100DM) until the desired pressure was achieved. Once the pressure and temperature in the cell were kept constant the measurements were carried out taking small amount of each phase by a ROLSI sampler [6] and then sending them to the chromatograph to obtain the phase compositions. When finished, the pressure inside the cell was modified by adding or removing CO_2 .

EXPERIMENTAL RESULTS

Experimental VLE data for CO₂ + octane mixture was determined at 322.39, 348.25 and 372.53 K. The data at ~348 K is presented in figure 2 together with those reported by Weng and Lee [5] at similar temperature. There is a very good agreement between both sets of data, even at conditions near the critical point of the mixture where the system takes more time to stabilize. The vapor phase composition for the CO₂ + Octane mixture at ~348 K is shown in figure 3.

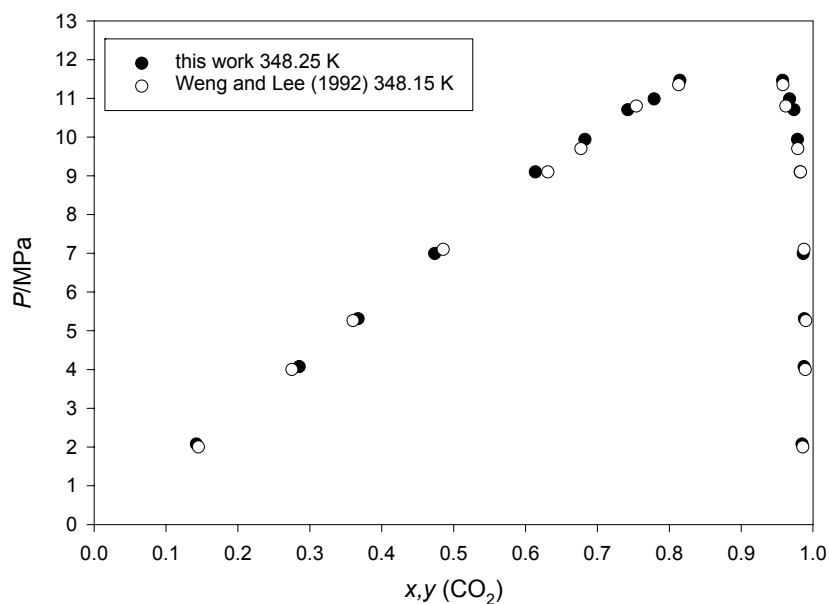


Figure 2. Vapor-liquid equilibria for CO₂ + octane

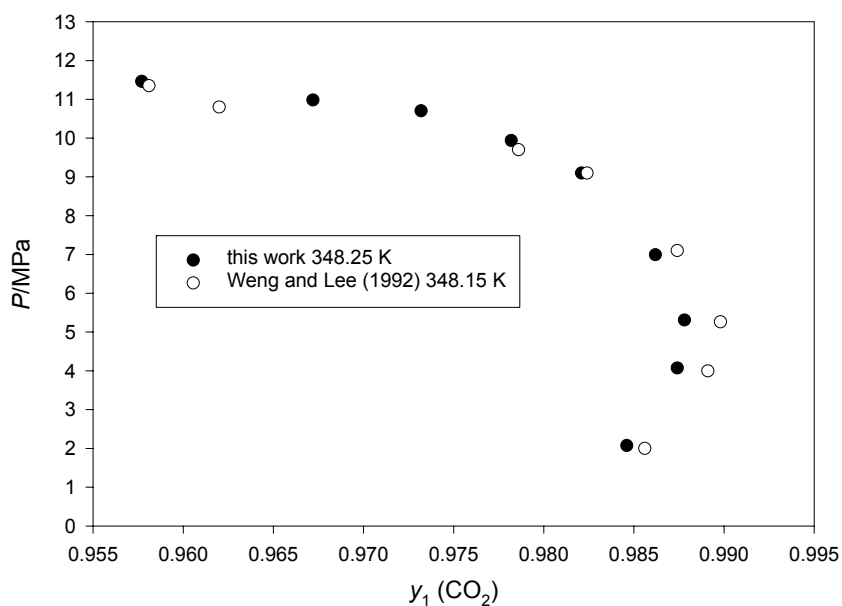


Figure 3. Vapor phase composition for the CO₂ + octane

The VLE data for CO₂ + decane was obtained at temperatures of 319.11, 344.74 and 372.94 K. The data reported at ~344 K is shown in figure 4. The data reported by Shaver et al at the same conditions is plotted as reference showing a good agreement with the data reported in this work.

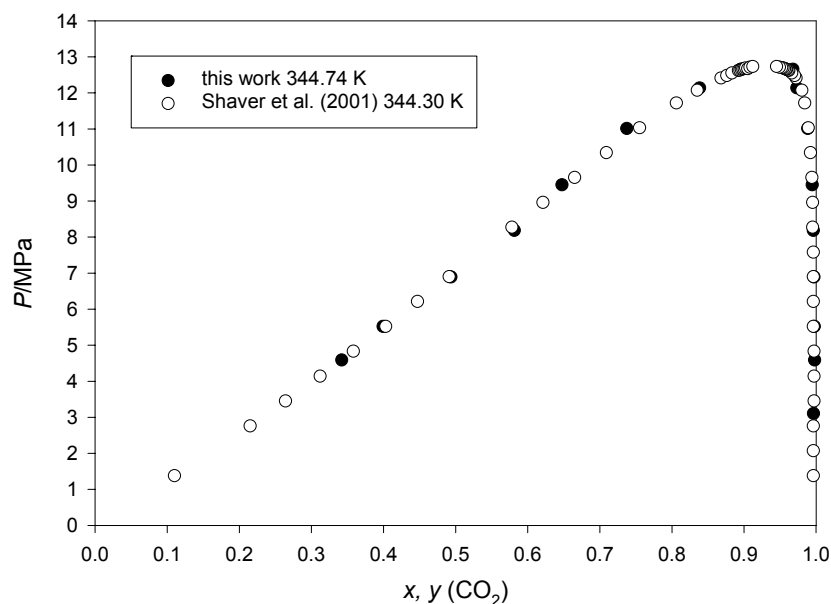


Figure 4. Vapor-liquid equilibria for CO₂ + decane

The data for the phase equilibria was correlated with the Peng-Robinson equation of state with classical mixing rules, the binary interaction parameter was fitted to the VLE data, no temperature dependence was tested. The AAD obtained for the CO₂ + octane were 0.31% for the vapor composition and 4.80% for the pressure. While for the CO₂ + decane system the obtained AAD were 0.29% and 2.67% for vapor composition and pressure, respectively. The binary interaction parameters obtained were 0.1208 for the CO₂ + octane mixture, and 0.1034 for the CO₂ + decane mixture.

The partition coefficients for both systems are presented in figure 5 at the same temperature that the reported for figure 2 and 4. As can be observed in this figure the partitions coefficient for both systems have almost the same behavior.

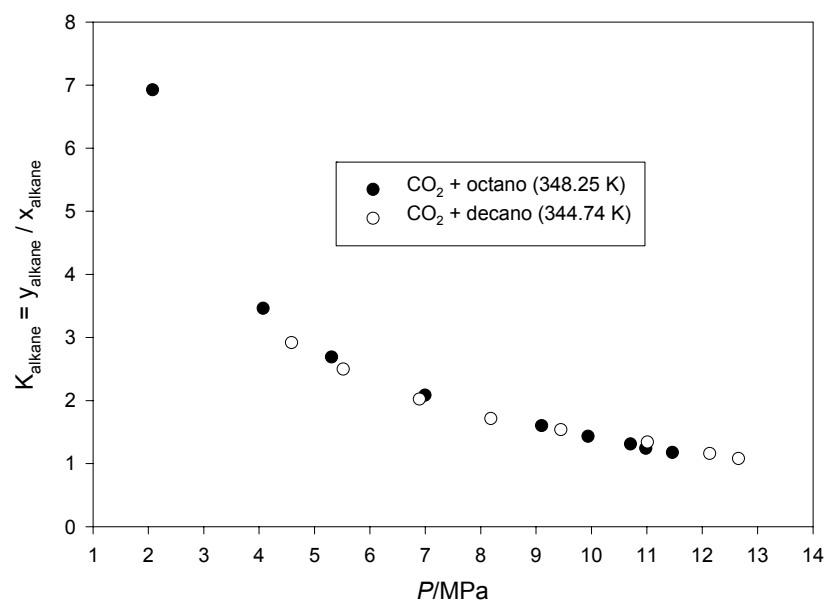


Figure 5. K_{alkane} values for system $\text{CO}_2 + \text{octane}$ and $\text{CO}_2 + \text{decane}$.

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