## Accepted Manuscript

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PII: S0896-8446(18)30210-9

DOI: https://doi.org/doi:10.1016/j.supflu.2018.06.012

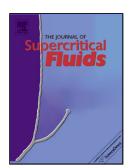
Reference: SUPFLU 4304

To appear in: J. of Supercritical Fluids

Received date: 30-3-2018 Revised date: 12-6-2018 Accepted date: 13-6-2018

Please cite this article as: Héctor Quinteros-Lama, Fgraveelix Llovell, Global phase behaviour in carbon dioxide plus *n*-alkanes binary mixtures, <![CDATA[The Journal of Supercritical Fluids]]> (2018), https://doi.org/10.1016/j.supflu.2018.06.012

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Global phase behaviour in carbon dioxide plus n-alkanes binary mixtures

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Abstract

The family of carbon dioxide  $(CO_2)$  plus linear alkanes is one of the most common type of mixtures found in supercritical CO<sub>2</sub> separation and extraction. Consequently, an accurate thermodynamic representation is a key

element for a proper process design. In this contribution, the PPC-SAFT equation of state is applied to the

construction of the serial-prediction-domain global phase diagram (spd-GPD) of the CO<sub>2</sub> plus n-alkanes series

to carefully analyse the presence of different thermodynamic phenomena. The goal is to address the capability

of the equation to predict the global behaviour of these mixtures, with emphasis in accurately reproducing their

mechanisms and topology. The results obtained reveal quantitative agreement with the available experimental

data, including a complete description of the emergence of different phenomena as a function of the hydrocarbon

chain length, such as azeotropy, double retrograde behaviour, critical transitions, mass and molar density

inversions and critical pressure step points.

Keywords: Carbon dioxide; Alkanes; Equation of state (EoS); Global Phase Diagram (GPD); Critical

transitions; double retrograde behaviour; PPC-SAFT

1. Introduction

The use of carbon dioxide (CO<sub>2</sub>) as a supercritical fluid for a variety of applications related to extraction

processes has become one of the most versatile technologies in the industry. Carbon dioxide is chosen because it is readily available, cheap, non-toxic and non-flammable, resulting into an ideal solvent to be used in this

kind of processes. In addition, its relatively low critical temperature and pressure allow reaching supercritical

conditions with a modest energy investment.

One of the most important applications of this compound is the use of supercritical CO<sub>2</sub> for the enhanced oil

recovery (EOR) process. Nowadays, natural and industrial sources of CO2 are used to enhance production of oil

from older wells by injecting CO<sub>2</sub> into appropriate underground formations. Carbon dioxide is used selectively,

primarily in wells which will benefit not only from repressurisation, but also from a reduction in viscosity of the

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Preprint submitted to The Journal of Supercritical Fluids

11th June 2018

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