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That

The work entitled: **"Solubility of bioinsecticides in supercritical CO2. Experimental measurement and modeling with the GC-EOS"** (EQ-121), by **Nicolás Gañán, Hernán Mazzei, Leonardo Ortega and Alfonsina Andreatta,** has been presented in the *XI Iberoamerican Conference on Phase Equilibria and Fluid Properties for Process Design*, which took place in Córdoba (Argentina) in October 22-25, 2018

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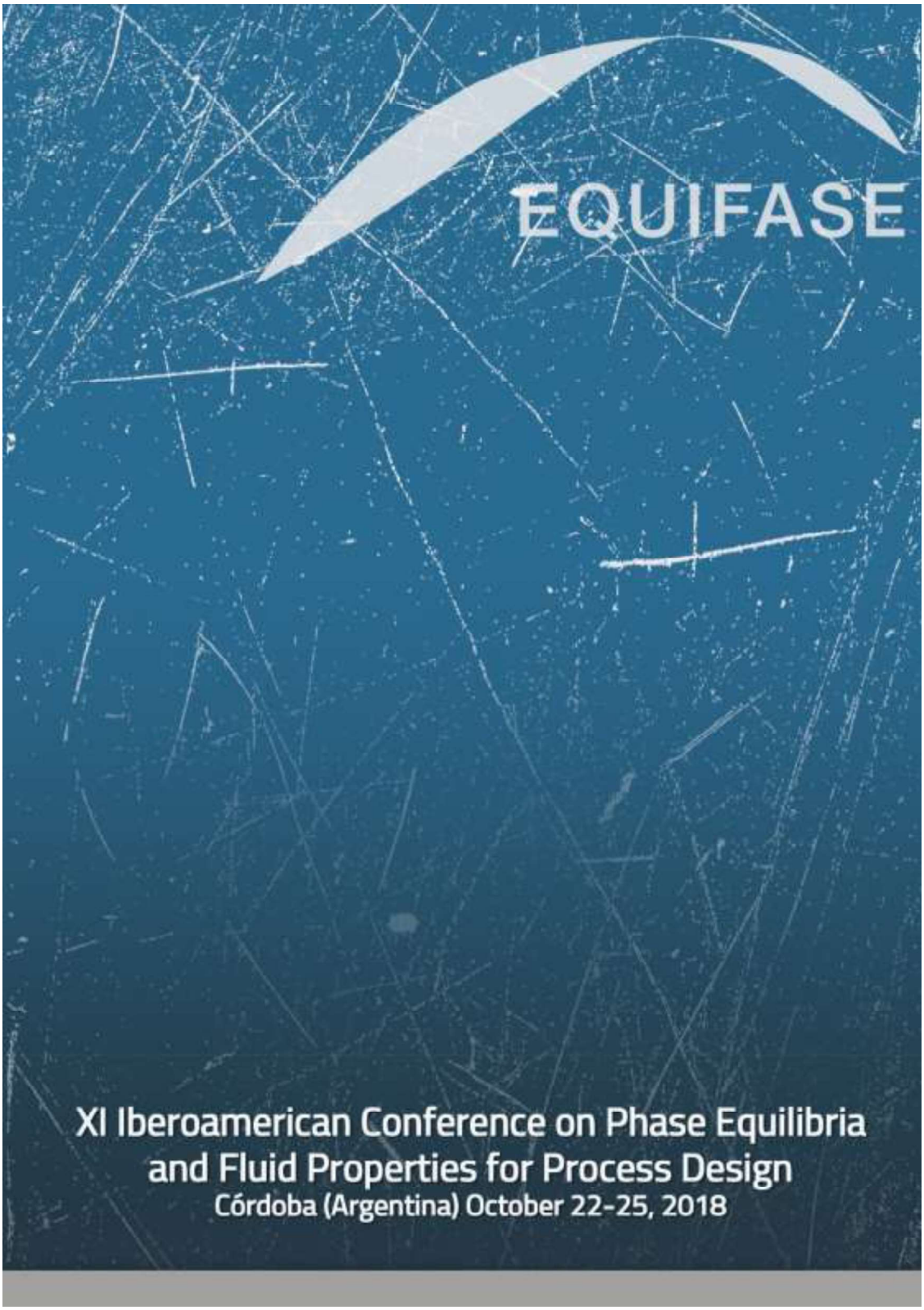
EQUIFASE
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2019

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Solubility of bioinsecticides in supercritical CO_2. Experimental measurement and modeling with the GC-EOS

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Keywords: supercritical CO_2, pulegone, thymoquinone, 1-octen-3-ol, GC-EOS.

Introduction

The knowledge of the solubility of natural compounds in supercritical CO_2 ($scCO_2$), as well as the development of suitable models for its description and/or prediction, is a key parameter in supercritical-based processes, as it determines the amount of fluid required or the highest concentration that can be obtained in the fluid phase in an impregnation, extraction, fractionation or particle formation system. In this work, the solubility of three natural volatile compounds with insecticidal activity (*R*-(+)-pulegone, thymoquinone and 1-octen-3-ol) is measured and modeled using the group contribution equation of state (GC-EOS). Goñi et al. [1] have studied the $scCO_2$-assisted impregnation of low density polyethylene films with thymoquinone and *R*-(+)-pulegone, for developing active packaging materials, showing the importance of the fluid phase concentration on impregnation yield and kinetics. Moreover, Sovová et al. [2] have investigated the $scCO_2$ extraction of thymoquinone from *Monarda didyma* and *Monarda fistulosa*. Fractionation with $scCO_2$ has been proposed as an alternative methodology to reduce the content of pulegone in mint essential oils, as well as to recover bioactive compounds from dementholized mint oils [3]. Therefore, the solubility of these compounds in $scCO_2$ at typical process conditions is presented with the objective of providing useful data for the design and optimization of supercritical processes.

Experimental methods and model

Materials. *R*-(+)-pulegone (≥ 97 %), thymoquinone (≥ 99 %) and 1-octen-3-ol (≥ 98 %) were purchased from Sigma-Aldrich (Steinheim, Germany). Industrial extra-dry carbon dioxide (water content ≤ 10 ppm v/v) was supplied by Linde (Argentina).

Experimental procedure. The binary solubility of the selected compounds was measured in a high pressure cell using a dynamic or "gas-saturated" method, following the procedure described in a previous work [3]. Measurements were performed at 45, 55 and 65°C and within a pressure range of 8-12 MPa, corresponding to typical process conditions. CO_2 flow rate was set in the range of 0.05-0.10 g/min to ensure saturation conditions. Solubility was calculated combining gravimetric determination of the recovered solute and volumetric measurements of circulated CO_2.

Modeling. Experimental solubility data were compared with predictive calculations performed using the Group Contribution Equation of State (GC-EOS) [4]. The model parameters were taken from the literature according to the latest revisions and updates [5].

Results and Discussion

Figure 1(a-c) shows the experimental solubility of *R*-(+)-pulegone, thymoquinone and 1-octen-3-ol, as well as the GC-EOS predictions, at different pressure and temperature conditions.

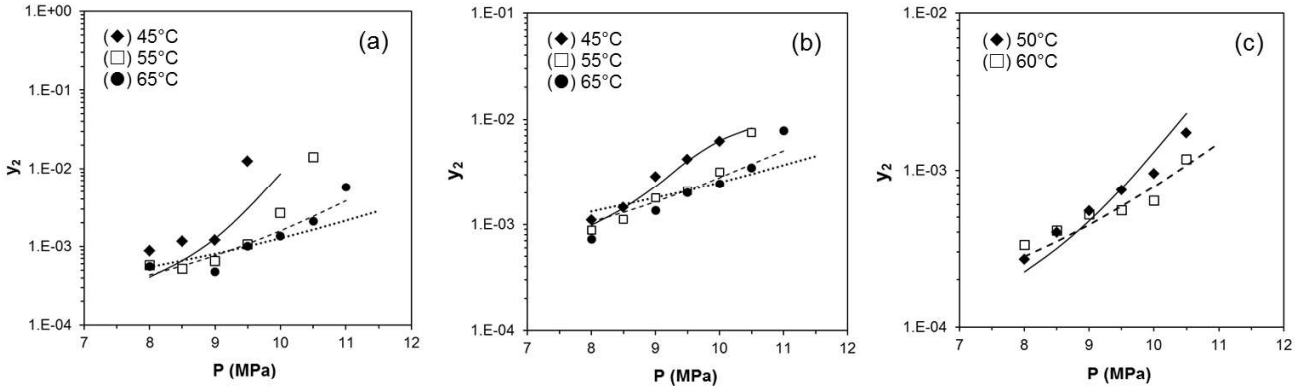

Figure 1. Solubility (mole fraction) of: (a) *R*-(+)-pulegone, (b) 1-octen-3-ol, and (c) thymoquinone in $scCO_2$. Dots: experimental measurements; lines: GC-EOS predictions.

The typical behavior of volatile compounds can be observed, with solubility in the supercritical phase increasing with pressure at a given temperature. It can also be seen that the two-phase region extends to higher pressure values when increasing temperature. The GC-EOS model provided satisfactory qualitative and quantitative predictions of the solubility behavior, with average relative deviations (AARD%) of (27-44) % (for pulegone), (7-31) % (for 1-octen-3-ol) and (14-21) % (for thymoquinone).

Conclusions

The experimental method provided a fast determination of the solubility of three bioinsecticides in $scCO_2$ at common supercritical process operation conditions, up to complete miscibility conditions. Thermodynamic modeling was applied to validate the method. There was an adequate correlation between the experimental data and the predictive calculations performed with the GC-EOS model, which allowed a correct representation of the dependence of the solubilities on pressure and temperature, using a single set of pure group and binary interaction parameters taken from literature and fitted from other experimental data. The proposed method exhibited also high measurement accuracy for pressures below complete miscibility. This information is useful for the design and optimization of supercritical processes such as extraction from plant materials, fractionation of extracts and impregnation of bioinsecticides in polymeric matrices for delivery purposes.

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