COMPARISON OF DIFFERENT APPROACHES TO PREDICT THE EQUILIBRIUM OF VEGETABLE OILS IN SUPERCRITICAL CO_2

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In this study two different approaches to calculate the equilibrium of different mixtures of vegetable oils in supercritical CO2 were compared: on the one hand a mathematical procedure used commercial ASPEN+ software package to process equilibrium data according to the classical cubic equations of state (EOS) and on the other hand the group contribution equation of state (GCEOS).
As first step the binary equilibriums between CO2 and the pseudocomponents used to describe the vegetable oil were modelled and compared with bibliographical data to calculate the binary interaction parameters, kij, in the case of the ASPEN+ model and the group parameters, k*ij, k'ij y aij, when GCEOS was used. Once the parameters were obtained in both methods, the ternary diagram of the mixture could be achieved for different temperatures and pressures.
The calculations performed with the ASPEN+ software fit fairly well with the experimental results published for a wide variety of vegetable oils, whereas GC-EOS provides a better agreement of global phase equilibrium diagrams within a wide range of pressures and temperatures despite requiring more parameters to predict the equilibrium.
The importance of the approaches described in this study to predict the equilibrium of complex mixtures can be established in the use of pseudo-components, which provide a suitable way to study real processes such as deacidification of oils.