Modeling systems relevant to the biodiesel production using the CPA equation of state. Part 2. Systems with supercritical CO2 - DTU Orbit (23/10/2019)

The CPA EoS is applied to binary mixtures of CO2 with fatty acids and their methyl- or ethyl-esters. The model, using one temperature independent binary interaction parameter, satisfactorily describes the phase behavior of such systems. Correlations of the binary interaction parameters with the number of esters’ or acids’ carbon atoms, or with the number of double bonds for compounds with the same number of carbon atoms, were developed in order to make predictions feasible in cases of lack of experimental data. Subsequently, the model was applied for predicting the phase behavior of ternary and multicomponent mixtures. The model rather satisfactorily predicts the vapor-liquid equilibrium of such systems.

In accordance with the first part of this series of articles [Tsivintzelis et al. 430 (2016) 75–92], since the binary parameters were optimized solely using experimental data for binary mixtures, CPA results for the ternary and multicomponent mixtures are pure predictions.

General information
Publication status: Published
Organisations: CERE – Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, KT Consortium
Corresponding author: Tsivintzelis, I.
Contributors: Tsivintzelis, I., Ali, S., Kontogeorgis, G. M.
Number of pages: 11
Publication date: 2020
Peer-reviewed: Yes

Publication information
Journal: Fluid Phase Equilibria
Volume: 504
Article number: 112337
ISSN (Print): 0378-3812
Ratings:
BFI (2020): BFI-level 2
Web of Science (2020): Indexed yes
Original language: English
Keywords: Biodiesel, CPA, Esters of fatty acids, Fatty acids, Phase equilibrium, Supercritical CO2
DOIs:
10.1016/j.fluid.2019.112337
Source: Scopus
Source ID: 85072759592
Research output: Contribution to journal › Journal article – Annual report year: 2020 › Research › peer-review