

Modeling of Biodiesel Multicomponent Systems with the Cubic-Plus-Association (CPA) Equation of State

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Biodiesel is now being seen as a promising and sustainable short-term alternative fuel, as the continuous increase in crude oil prices, scarce resources of fossil energies and environmental concerns limit the use of petroleum based fuels. The transesterification of vegetable oils and animal fats is the most used method to produce biodiesel and commonly used alcohols are methanol or ethanol although higher chain alcohols have also been suggested. During its production, that takes place in a multiphase reactor, the oil reacts with an alcohol, usually in presence of a catalyst, to form fatty acid esters (biodiesel) and glycerol. A better understanding and prediction of the phase equilibria of the multicomponent systems that are present in the transesterification reactor are required for the design and optimization of the reactor if the reaction rate, selectivity and yield are to be improved. Although their importance in the biodiesel production process, phase equilibria data for the products of the transesterification unit only recently became available and new experimental measurements will be presented in this work. In previous works, we have shown that the CPA EoS can be successfully applied to model systems of interest for the biodiesel production such as the water solubility in fatty acid esters and biodiesels and the liquid-liquid equilibria of fatty acids and water. The good results obtained so far are quite encouraging for using the CPA-EoS towards the description of the phase equilibria of multicomponent systems existing in the biodiesel production process. Particularly, the good predictive performance of the CPA EoS for the description of the liquid-liquid equilibria of ternary or multicomponent mixtures containing alcohols, glycerol, water, FAME's and oils, will be shown.

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