Thermodynamic modeling of solid-liquid equilibrium of fatty alcohol and fatty ester mixtures

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The increasing demand for biofuels has generated further opportunities for replacing petrochemicals by products derived from renewable sources, such as bioethanol and sugar based products or chemicals derived from fats and oils. Some of these compounds are the fatty alcohols presented in the fermentation broth in the ethanol production processes. These fatty alcohols are high-value by-products which can be used in the pharmaceutical and cosmetic industries.

The purification of by-products of the biofuel production depends on information on the phase equilibrium of systems containing these compounds. For fatty alcohols, the main purification operation is the crystallization, which requires knowledge of the solid-liquid equilibrium. On the other hand, fatty esters are the main constituents of biodiesel, and the knowledge of the solid-liquid equilibrium is necessary to assess flow properties at low temperatures.

In this work a thermodynamic modeling of the solid-liquid equilibrium of mixtures of fatty alcohols and of fatty esters is presented. The thermodynamic framework comprises the description of dense phase non-idealities through excess Gibbs energy models. In many cases the compounds are miscible in solid phase, and this phase has been modeled as a solid solution – except in those cases for which there is experimental evidence of partial miscibility.

The developed model has allowed a good description of the liquidus line (i.e., the temperature of the onset of formation of the solid phase). The description of the solid composition equilibrium is satisfactory, considering the inherent uncertainty of these data. Computer programs were generated in FORTRAN language, and can be readily used and/or extended for mixtures of related compounds.

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