Solid-liquid equilibrium of fatty derivatives: Mixtures of tripalmitin + fatty alcohols

Maximo, G.J; Costa, M.C.; Meirelles, A.J.A.

EXTRAE – Laboratório de Extração, Termodinâmica Aplicada e Equilíbrio, Department of Food Engineering, Faculty of Food Engineering, University of Campinas, Brazil.

Vegetable oils present several nutraceutical and functional compounds whose physical chemical properties lead to the design of chemical products with added value. In this way, the purification and extraction of these components from fats and oils are relevant processes in the oilchemistry industry and biorefinery. In fact, the growing demand for biofuels will probably promote the production of these biocompounds, extracted from the same sources. Triacylglycerols and fatty alcohols are chemicals found in vegetable oils used in the formulation of cosmetic, pharmaceutical or food products, for example. Although information about phase transitions of these compounds and mixtures of them is frequently required for design and optimization of processes involving such substances, these data are yet scarce in the literature. In the present study, the phase diagrams of two binary systems formed by tripalmitin (1,2,3-propanetriyl ester) + 1-hexadecanol and tripalmitin + 1-octadecanol were evaluated by Differential Scanning Calorimetry (DSC) as well as some properties of pure compounds (temperature and enthalpy of melting transition) and phase transitions of their mixtures. The experimental data were compared with predicted data by solving the phase equilibrium equations using a computer-aided procedure. The liquid phase activity coefficients were calculated using two approaches: i) the Margules-two-suffix equation and ii) the group contribution UNIFAC-Dortmund model (UNIversal Functional-group Activity Coefficient). The experimental data and phase diagrams allowed the evaluation of the behavior of the solid-liquid equilibrium of the mentioned mixtures. The prediction showed that the approaches used for modeling of the systems' equilibrium were well applied, resulting in an accurate prediction of the *liquidus* line with low deviation from experimental data. The observation of the results suggested that future investigations on triacylglycerols + fatty alcohols are promising and highlights the relevance for the development of an integrated biochemicals complex.

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