ABSTRACT

Lipids Phase Equilibria Modeling Applied to Process Design and Analysis

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Industrial use of lipids increased as a result of fast development in bio-based economies. Besides food products applications, lipids are used in other industries such as biodiesel, edible oil, personal care, oleochemicals and others. The lipid-based industries expansion leads to new design and development challenges.
Accurate and consistent prediction of lipids pure compounds properties, as well as, lipids mixture properties and phase equilibria are very important when process synthesis, design, optimization, along with energy, economic and environmental impact analysis are performed through model-based tools. The main drawback is the lack of widely available experimental data for such compounds and mixtures. Use of predictive models for lipids systems, such as group contribution (GC) models, which do not require substantial experimental data, can provide a fast and reliable estimation of needed properties so that processes handling lipids can be synthesized, designed, analysed and optimized reliably.
The aim of this work was to develop a systematic identification method for data analysis and phase equilibria modelling for lipids systems, and further to use the results within process modelling, design and analysis for lipid processes. The developed method offers support for a fast assessment and solution of data selection, and parameter estimation for Group Contribution (GC) type of models. The method was applied to identify new parameters especially dedicated to lipids systems for Original UNIFAC model, using the Lipids Database to provide phase equilibria experimental data and models for pure component properties. The lipid binary group interaction parameters set is extended by using KT-UNIFAC parameters, and allows a broader application, making feasible the synthesis, design and analysis of lipid related processes. An example is represented by the Shea oil solvent fractionation for producing Shea stearin, which used as a cocoa butter replacement in confectionary products. The process is presented and analysed in four steps: (1) process data collection, (2) process model development and consistency check, (3) process design and performance analysis (e.g.: energy, economic and environmental analysis), (4) process hot-spots identification and retrofit solutions. The use of the Lipids Database with the new lipid-based parameters for Original UNIFAC model allows a fast implementation and evaluation of the process.