Systematic identification method for data analysis and phase equilibria modelling for lipids systems - DTU Orbit (17/08/2019)

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Industrial use of lipids has been increasing as a consequence of increased developments related to biobased economies. In addition to applications in food-products, lipids are used by many industrial sectors, for example, biodiesel, edible oil, health, and personal care. Phase equilibria predictions for chemical systems with lipids play a major role in process–product modelling, simulation and design. Due to the large number of lipid-compounds involved, predictive methods like group contribution based methods are particularly suitable for estimation of pure compound and mixture properties that may not be available. Limited experimental data availability and poor performances of currently available group contribution based methods is therefore an obstacle for obtaining the necessary information regarding phase equilibria of chemical systems with lipids. In this paper, a systematic identification-regression method (to be called identification method) for phase equilibrium modelling, where, based on the available experimentally measured phase equilibrium data, the selected model parameters are estimated in a hierarchical and efficient manner, is presented. The aim of the method is to improve the quality of phase equilibria prediction for the selected group contribution based methods. By applying the identification method, a new set of binary group interaction parameters regressed from vapour-liquid equilibrium data for chemical systems with lipids is presented for the Original UNIFAC model, together with regression statistics and model performance. An extended and updated version of the in-house SPEED Lipids database, which is used for the needed pure compound properties and phase equilibria data, is also presented.

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