Modelling of physical and thermodynamic properties in systems containing edible oils and biodiesel - DTU Orbit (09/11/2017)

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The knowledge of physical and thermodynamic properties of pure components and their mixtures is a basic requirement for performing tasks related to process design, simulation, and optimization and also for performing chemical product design using computer aided molecular/mixture design (CAMD) tools. With an increasing trend in the production rates of edible oils, fats and other lipids, accurate prediction of the necessary properties (pure component and mixture) has become a major concern and issue. The mixtures handled consist of large complex chemicals such as fatty esters, acids alcohols, glycerides, sterols, etc., with or without the presence of water. Because of the lack of measured data, it is necessary to have available truly predictive but reliable models requiring very little data for their development. A systematic numerical analysis to identify the needs of phase equilibria and related properties in process design and analysis for the production of edible oils and related products has been done and from this analysis the requirements of a database with respect to model development has been established. In total, 333 different phase equilibrium systems (91 VLE, 91 LLE, 70 SLE), 80 solubility systems, and around 4500 data points on phase equilibria has been found in addition to 8 pure component properties for 290 lipids. The consistency of the available VLE data has been checked with six tests (Van Ness, Herington or Area, Point or Differential, Infinite Dilution, Pure component and EOS), using a general and robust approach developed by Thermodynamics Research Center (TRC) of the National Institute of Standards and Technology (NIST). It was found that most of the data failed, at least one of these tests. Nevertheless, using data-quality factors, all data have been used to regress parameters of UNIFAC model. This procedure has also been repeated for SLE-data, where new thermodynamic consistency tests are proposed. The performance of molecular models (UNIQUAC, UNIFAC, and NRTL) as well as GC+ approach based UNIFAC-CI method is discussed and compared for phase equilibria calculations. For lipids systems, a special set of group-interaction parameters have been determined to make the GC-based models more predictive. These results are then used to obtain interaction parameters for the PC-SAFT to add further predictive power.

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