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Industrial use of lipids increased as a consequence of the rapid development in bio-based economies. In addition to food products applications, lipids are used by many other industrial sectors, like biodiesel, edible oil, health, personal care, oleochemicals to name a few. The lipid-based industry expansion led to new challenges regarding the design and development of better performing processes and products. Despite the advances in the currently available property modellings and product-process design techniques via different computer-aided methods and tools for the chemical and petrochemical industries, the lipid-based industry has not exploited this knowledge. Availability of pure compounds and mixture models is of high importance as they are the core of all methods and tools for process-product design. It is very difficult to provide a complete set of experimental data for developing pure compound and mixtures thermodynamic models to cover all of the lipid compounds. These issues justify the effort made to develop thermodynamic models that are able to predict the properties of lipid components and their mixtures from a minimum amount of experimental data. The models should also be able to be implemented within different tools, in order to achieve reduced time and cost when designing lipid related products and processes.

In this work, a systematic identification method for data analysis and phase equilibria modelling for lipid systems was developed. The aim of the method is to offer support for fast assessment and solution of the data selection and binary interaction parameter estimation for group contribution based models problem. The developed method covers the following aspects: (1) inclusion of a detailed algorithm for data selection, which complements personal judgment and available expertise; (2) use of an efficient calculation sequence, which can be further exploited for planning experimental data collection in order to fill in the gaps within the binary interaction matrix; (3) the regression problem formulation and solution for each regression step. The method utilised the Lipids Database, which provided the pure compound information, and the data for lipid mixtures. The method was applied for different UNIFAC model variants, and the new lipid-based parameters were validated and tested for predictive abilities. This thesis shows that for the VLE description, the lipid-based parameters for all the UNIFAC variants provide the best performances when compared with published parameters for the same models. The extrapolation of the lipid-based parameter to SLE description show similar performances as the published parameters.

The Lipids Database containing the new parameters for Original UNIFAC model was used to study the solvent fractionation process of Shea oil. The process design, modelling and analysis were performed using well-known methods and tools. The analysis results of the base case provided the opportunity to bring improvements to the process economics. The process retrofit involved heat integration and led to a decrease in utility consumption by 50%. The use of the Lipids Database with the new lipid-based parameters for Original UNIFAC allowed a faster implementation and evaluation of the process. This highlights the importance of having such a database with necessary thermodynamic models for developing and improving processes within lipid-based industry.