Computer-Aided Modeling of Lipid Processing Technology

Vegetable oils and fats have an important role in human nutrition and in the chemical industry since they are a source of energy, fat-soluble vitamins, and now also in the production of renewable sources of energy. Nowadays, as the consumer preferences for natural products and healthier foods increase along with growing interest in biofuels, the oleochemical industry faces in the upcoming years major challenges in terms of design and development of better products and more sustainable processes to make them. Computer-aided methods and tools for process synthesis, modeling and simulation are widely used for design, analysis, and optimization of processes in the chemical and petrochemical industries. These computer-aided tools have helped the chemical industry to evolve beyond commodities toward specialty chemicals and ‘consumer oriented chemicals based products’. Unfortunately, this is not the case for the edible oil and biodiesel industries. The oleochemical industry lags behind the chemical industry in terms of thermophysical property modeling and development of computational tools suitable for the design/analysis, and optimization of lipid-related processes. The aim of this work was to develop systematic computer-aided methods (property models) and tools (database) related to the prediction of the necessary physical properties suitable for design and analysis of processes employing lipid technologies. The methods and tools include: the development of a lipid-database (CAPEC_Lipids_Database) of collected experimental data from the open literature, data from industry, and, generated data from validated predictive property models; as well as the development of a database user-interface and an external version of this database, for use in commercial process simulators, for fast adoption-analysis of property prediction models and for fast development of process models not available in process simulators. This was achieved by first identifying and classifying the lipid compounds found in the edible oil and biodiesel industries. Then creating a list of the thermophysical properties needed for model-based design and analysis of edible oil and biodiesel processes. Next, collection of the available experimental data from different sources for the identified lipid compounds. Finally, selecting and adopting the appropriate models to predict the necessary properties, to fill-out the lipid-database and to make it suitable for application with other computer-aided tools (such as commercial process simulators). The developed computer-aided methods (property models) and tools (CAPEC_Lipids_Database) have been linked to the proposed methodology for the design/analysis of lipid-related processes. In this PhD thesis, the analysis, in terms of their design variables and their impact in the process behavior, of three lipid-related processes has been performed: the solvent recovery section of the extraction of crude soybean oil, the deodorization of palm oil, and the deacidification of soybean oil.