Thermodynamic Property Needs for the Oleochemical Industry

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The oleochemical industry cover mainly the food and pharmaceutical reactions but production of fuels (biodiesel) and other speciality chemical production processes also handle oleochemicals (in other words, lipids). The core of process synthesis and design depend on availability of properties data and/or reliable thermodynamic models for the chemicals involved. Limited availability of consistent physical and thermodynamic properties of lipids compounds and their mixtures lead to difficulties with the use of process simulators for process synthesis and design, since all the models to be used require apriori estimated parameters from experimental data.

Lipids applications such as bio-diesel, edible applications, and production of other important chemical compounds from the fatty acids include a series of processes such as: fat splitting, esterification, epoxidation, hydrogenation, amidation, sulfonation, ethoxilation, etc [1]. Each of these processes involves several types of unit operations. The lipids hydrolysis process (high pressure, high temperature conditions – Colgate Emery) [2], which is an old process, still applied worldwide nowadays, involves several phase equilibria: first a liquid-liquid equilibrium is involved for the fat splitting column where the main components are: unreacted triglycerides, fatty acids, glycerol and water. Further, the process consist in separating the two liquid phases (fatty acids-water, and glycerol-water) by distillation. This involves the vapour-liquid equilibria of the mixture species (fatty acids-water, glycerol-water). Further, if separation of fatty acids mixture into high purity individual components is considered, several methods can be applied: fractional distillation/steam stripping within vacuum condition [3] or fractional crystallization with or without using a solvent [1]. For this process/separations several phase equilibria are involved: VLE equilibria of fatty acids and water, if we are talking about steam stripping, and several SLE equilibria (fatty acid-fatty acid, or fatty acid-solved), in the case of fractional crystallization. In order to be able to design these type of processes, involving different types of phase equilibria, one need to have knowledge about and to be able to predict the behaviour of these type of systems.

A database and a properties library have been developed for chemical product and process design. The database includes 45500 compounds, and according to the compound type (e.g.: normal fluids, polar non-associating compounds, multifunctional group compounds, polymers, electrolytes, etc) different properties are given according to group contribution approach for primary properties (e.g.: acentric factor, critical properties, triple point temperature and pressure, normal boiling point, liquid volume, ideal gas enthalpy, ideal gas Gibbs energy, ideal gas entropy, solubility parameters, van der Waals surface area and volume, dipole moment, etc.), temperature dependent properties (solid density, liquid density, vapour pressure, heat of vaporization, solid heat capacity, liquid and vapour viscosity, liquid and vapour thermal conductivity, etc.), and mixture properties (e.g.: binary and ternary data for VLE, LLE and SLE, infinite dilution activity coefficients, enthalpies of mixing, etc.).

For this, available property and thermodynamic models needs to be fine-tuned for this type of compounds. Regarding the use of models for mixtures properties, such as phase equilibria, available binary interactions parameters for predictive models are not sufficiently good to describe

them. New parameters for UNIFAC original model have been calculated for lipids compounds. In order to be able to use all this data and models for process design and simulation, development of a lipids database is required. Our developed lipids database, SPEED LIPIDS Database, together with our chemicals database, includes all this options: one part of the database is dedicated to the pure compounds and it includes: 330 pure compounds and 27 models to describe the pure compound properties (e.g.: single values properties – critical properties, heat of formation; temperature dependent properties: vapour pressure, liquid heat capacity, liquid density, liquid viscosity, and surface tension, etc.). Safe extrapolation of pure compound properties is enabled. The other part of the database is dedicated to phase equilibria for the mixtures and it is composed from 4500 measure data points for 332 different phase equilibrium data-sets (92 VLE, 91 LLE, 70 SLE and 79 solubility data). For all the available VLE and SLE data sets, consistency tests are performed. It is seen that many mixture data published related to lipids do not pass these tests: only 3% of the data sets have quality factors over 0.5 (where the quality factor varies between 0 – minimum, and 1 – maximum) [4].

The database has the following features: property data consistency test; optimization based data regression to estimate the model parameters; knowledge representation and search engine for database use knowledge representation and search engine for database; computer aided modelling tool to quickly and efficiently develop the necessary property prediction models; and ability to integrated with process simulation tools. The application of the developed properties models will be illustrated through case studies involving different lipid compound processing steps. It allows a better and easier utilization of available thermodynamic models.

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