Phase Equilibria Prediction for Systems Containing Lipids

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455103 Phase Equilibria Prediction for Systems Containing Lipids

Monday, November 14, 2016
Grand Ballroom B (Hilton San Francisco Union Square)

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In recent years, utilization of fats and oils has started to shift towards the bio-industry making them one of the most important renewable materials for the future chemical industry, and leading to oils and fats industry expansion along with a scale reorientation from local to large-scale industry [1]. Such developments have led to new challenges regarding the design and development of better performing processes and products. Despite the advances in property modelling and process design techniques available via different computer-aided methods and tools for the chemical and petrochemical industries, the oleochemical industry is not able to exploit this knowledge due to a lack of experimental data and property models within commercial software applications and the ability to describe accurately the phase behaviour of systems with lipids. Over the past years, new methods and models for predicting single properties and temperature dependent properties (e.g. critical properties [2], viscosity [3], heat capacity [4], heat of vaporization [4], [5], vapour pressure [5]) have been reported. Likewise, another important modelling task is phase equilibria prediction which is directly related to process synthesis, modelling and simulation. An important aspect in phase equilibria prediction is represented by quality of the data used for regression of model parameters. In previous work, Cunico et al. [5] applied several consistency tests for VLE data sets involving lipids that are available in open literature and their results show that only 3% of the analysed data sets have quality factors over 0.5 (where the quality factor varies between 0 – minimum, and 1 – maximum) [5].

In this work, our available extended CAPEC Lipids Database and CAPEC Lipids Mixtures Database is used for revising the Original UNIFAC model group contribution parameters for lipids by proposing new values, aimed to offer a better prediction of phase equilibria calculation (vapour-liquid equilibrium VLE, solid-liquid equilibrium, SLE). The regression of the new parameters is done using carefully selected VLE data sets, screened out for possible erroneous data. VLE data selection is performed based on the quality factor given by the different consistency tests available in ThermoData Engine (TDE) from NIST. More than 60 VLE data sets consisting of over 600 data points, available in CAPEC LIPIDS Mixture Database, are used for the regression of the 54 binary interaction parameters corresponding to 10 groups for Original UNIFAC model. Note that only 10 groups are needed to represent all the lipids data sets. However, to allow a better performance of the model for this type of systems, two new groups were introduced: one group is describing the behaviour of hydroxyl within mono and diglycerides (OHacyl) and another one is describing the glycerol molecule (GLY). The parameters are tested and evaluated on VLE and SLE data and by using a cross validation method. Compared to original UNIFAC, the performance of the new parameters for the lipids systems present a substantial improvement in phase equilibria predictions.

Keywords: Lipids, phase equilibria, original UNIFAC

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