VAPOR LIQUID EQUILIBRIA AND LIQUID LIQUID EQUILIBRIA IN THE OIL/FAT AND BIODIESEL INDUSTRIES: EXPERIMENTAL DATA, MODELLING AND SIMULATION

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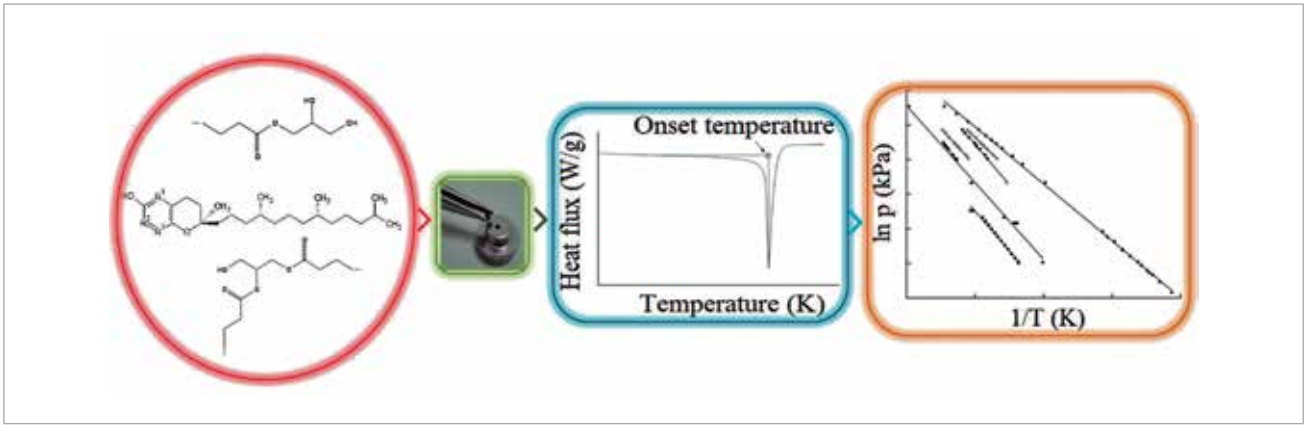

Figure 1. DSC tecnique applied for vapor pressure measurements. Toc graphic from article: Damaceno DS, Matricarde Falleiro RM, Krähenbühl MA, Meirelles AJA. 2014. Boiling Points of short-chain partial acylglycerols and tocopherols at low pressures by the differential scanning calorimetry technique. J. Chem.Eng. Data. **59**: *1515-1520*

Separation processes of the edible/oil and biodiesel involve multicomponent mixtures that consist of fatty acids, esters and alcohols, acylglycerols, glycerol, and also some minor compounds (nutraceuticals). In the case of edible oil/fat processing, the unit operations that are related to this project, include: steam stripping of fatty acids/odors for steam deacidification/ deodorization, with recovery of impurities as valuable side products, and solvent extraction as a new alternative for the deodorization process. In biodiesel production, the purification steps involve the separation of acylglycerols and glycerol from the methyl/ethyl esters. In these unit operations, some combination of phase equilibria between vapor-liquid and liquid-liquid phases takes place. Due to the inherent complexity of the mixtures involved, accurate and reliable predictive tools of phase equilibria and physical properties are very important for process design. With an increasing trend in the demand of edible oils/fats and biodiesel, correct prediction of the necessary properties (pure component and mixture) has become a concern. However, there is a lack of measured data in this research area that must be fulfilled in order to get suitable predictive models. The scope of this project can be divided as follows: Determination of novel vapor pressure data for partial acylglycerols by Differential Scanning Calorimetry; Determination of novel vapor liquid equilibrium data involving different classes of fatty compounds by Differential Scanning Calorimetry; Improvements in the Differential Scanning Calorimetry technique for the determination of vapor pressure and vapor liquid equilibrium data involving fatty compounds; Study of the viability of applying the solvent extraction process as an alternative for the deodorization step of edible oils. All experimental data will be used for testing and validating of modeling and simulation tools developed in the research group, and also for improving them when suitable.

SUMMARY OF RESULTS TO DATE AND PERSPECTIVES

The scope of this project is within vapor-liquid and liquid-liquid equilibria. In relation to vapor-liquid equilibria, the main efforts have been towards measurements of experimental data for physical properties and phase equilibria of pure fatty compounds and their mixtures using the Differential Scanning Calorimetry (DSC) technique, besides the improvement (optimization) of the technique itself. Up to data, novel boiling temperatures of pure short-chain mono- and diacylglycerols in the low-pressure range have been obtained, and these data were modeled using Antoine, Clapeyron and DIPPR equations. Also, the predictive group contribution equation of Ceriani et al. (2013) had its predictive capability checked by using these databank. DSC technique has been optimized for measuring vapor pressure of pure compounds in terms of its main variables, i.e., sample mass and heating rate. Further improvements will be achieved towards other variables that appear to be relevant in terms of accuracy of the DSC technique for measuring vapor-liquid equilibria of binary mixtures. Novel vapor-liquid equilibria have been obtained for mixtures involving vegetable oils by using other techniques. In relation to liquid-liquid equilibria, the work has focused in gathering experimental data for pseudoternary model systems composed by refined edible oil, odor compound and green solvent (ethyl lactate or ethanol). Odor compounds already investigated are aldehydes. Other classes of compounds will be evaluated. The main goal is to develop an alternative process for the industrial deodorization process used nowadays. Modelling and simulation tools applied in lipid technology have been updated and improved.

MAIN PUBLICATIONS

Belting PC, Gmehling J, Bölts R, Rarey J, Ceriani R, Chiavone-Filho O, Meirelles AJA. 2015. Measurement, correlation and prediction of isothermal vapor-liquid equilibria of different systems containing vegetable oils. *Fluid Phase Equilib.* **395**: 15-25.

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