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Consistent thermodynamic properties of lipids systems

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Physical and thermodynamic properties of pure components and their mixtures are the basic requirement for process design, simulation, and optimization. In the case of lipids, our previous works[1-3] have indicated a lack of experimental data for pure components and also for their mixtures. To contribute in this area, experimental data were obtained using the Differential Scanning Calorimetry (DSC) technique for isobaric vapor-liquid equilibrium (VLE) of two binary mixtures at two different pressures (1.2 and 2.5 KPa): system 1 [monoacylglycerol (monocaprylin) + fatty acid (palmitic acid)] and system 2 [monoacylglycerol (monocaprylin) + fatty ester (methyl stearate)]. System 1 is relevant in the purification steps of the deodorizer distillates while system 2 is relevant in the purification steps of biodiesel and bioglycerin. A non-ideal behavior is revealed for both systems at the two different pressures, with azeotrope behavior observed. Available thermodynamic consistency tests for TPx data were applied before performing parameter regressions for Wilson, NRTL, UNIQUAC and original UNIFAC models. The relevance of enlarging experimental databank of lipids systems data in order to improve the performance of predictive thermodynamic models was confirmed in this work by analyzing the calculated values of original UNIFAC model. For solid-liquid equilibrium (SLE) data, new consistency tests have been developed [2]. Some of the developed tests were based in the quality tests proposed for VLE data by Kang et al. [4] and a methodology that combines solute activity coefficients in the liquid phase at infinite dilution and a theoretically based term to account for the non-ideality in dilute solutions are discussed. In this work, case studies considering the methodology proposed for SLE thermodynamic consistency tests and data from open literature and databases such as NIST-TDE®, DIPPR® and DECHEMA® are presented. The SLE consistency test and data evaluation is performed in a software containing option for data analysis, model analysis and parameter regression.

References

- [1] L.P. Cunico, A.S. Hukkerikar, R. Ceriani, B. Sarup, R. Gani, Molecular structure-based methods of property prediction in application to lipids: A review and refinement, *Fluid Phase Equilib.*, 2013, 357, 2-18.
- [2] L.P. Cunico, R. Ceriani, B. Sarup, J.P. O'Connell, R. Gani, Data, analysis and modeling of physical properties for process design of systems involving lipids, *Fluid Phase Equilib.*, 2014, 362, 318-327.
- [3] R. Ceriani, R. Gani, Y.A. Liu, Prediction of vapor pressure and heats of vaporization of edible oil/fat compounds by group contribution, *Fluid Phase Equilib.*, 2013, 337, 53-59.
- [4] J.W. Kang, V. Diky, R.D. Chirico, J.W. Magee, C.D. Muzny, I. Abdulagatov, A.F. Kazakov, M. Frenkel, Quality assessment algorithm for vapor-liquid equilibrium data, *J. Chem. Eng. Data*, 2010, 55, 3631-3640.