Prediction of the Interfacial Tension of Binary Systems of Water + Hydrocarbon (A Formal Thermodynamic Model Together with the UNIFAC Model)

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Interfacial tension is a very important thermophysical property from both fundamental and practical points of view because of its role in mass transfer phenomena in which the liquid-liquid interface is involved. In fact, it is well known that this property influences many industrial processes: formation or breaking of emulsions, liquid extraction, enhanced oil recovery using water and/or surfactants, etc.

This work presents the extension of a method used previously to predict mixture surface tension [1] which uses a formal thermodynamic model based on the iso-molar Gibbs energy for both a bulk liquid phase and an interface, without considering explicitly if the interface is formed by two liquids or liquid and vapor phases. Also, as in the previous work, the UNIFAC predictive model is used. Using the calculation method here developed, we obtain values for the interfacial tension of a given water + hydrocarbon mixture together with the concentration (solubility) of the hydrocarbon in the water-rich liquid phase. The UNIFAC binary interaction parameters used in the calculations are all reported in the open literature, and correspond to those obtained from liquid-liquid equilibrium data.

The results of the prediction of the interfacial tension obtained in this work were used to compare with experimental results for eight different binary systems from the open literature, and those obtained in our laboratory which are included in a separate work to be presented in this event, for the following binary systems: water (2-methylpentane; 3-methylpentane; 2,3-dimethylpentane; 2,3,4-trimethylpentane; and 2,2,4-trimethylpentane) covering the temperature interval 303 to 343.15 K. The comparison between experimental and predicted interfacial tension values for the binaries above mentioned showed an average relative error of less than 1 %.

[1] L. Ramírez-Verduzco, A. Romero-Martínez, and A. Trejo. *A Model to Predict the Surface Tension and Surface Concentration of Binary Systems*, Proceedings of the Fourteenth Symposium on Thermophysical Properties, NIST-University of Colorado. Boulder, CO, USA, June 2000.