

Book of Abstracts

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Measurements and Modeling of the Solubility of Naturally Occurring Phenolics

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Phenolic compounds are well known for their biological activity and, due to their reactivity, are important starting materials for the synthesis of complex molecules. These compounds can be obtained either by chemical synthesis or by extraction from different biological media. Thus, solubility in aqueous systems, organic and supercritical solvents are fundamental for a better design of reaction, separation and purification processes involving these molecules.

For phenolics not many phase equilibria data are available. Usually, when data are reported, only a limited range of thermodynamic conditions is presented, and for many of the more complex phenolics data are extremely scarce or unavailable.

In our laboratory we have been implementing a systematic study on the solubility of different hydroxybenzoic, phenylpropenoic and more complex phenolics in water and several organic solvents. Solubilities were determined using the analytical shake-flask method for generating the saturated solutions, followed by compositional analysis by Uv-vis spectrophotometry, HPLC and/or gravimetry [1,2]. A synthetic method based on the use of differential scanning calorimetry (DSC) for determining solubilities has also been investigated.

For better understanding the solubilization process, melting properties (T_{fus} and $\Delta_{fus}H$) were determined by DSC and aqueous acid dissociation constants by potentiometric titration [1, 2].

Modeling was performed with the Cubic-plus-Association (CPA) equation of state, where a predictive methodology for obtaining the pure component parameters solely from the chemical structure is proposed. In this, the cubic parameters are obtained from correlations involving T_c , P_c and the van der Waals volume, while the association term parameters depend on the nature and position of each associating group [1,2].

Results showed that a good description of the solubility of phenolics using a single, small and temperature independent binary interaction parameter can be obtained in different solvents.

References

- [1] F.L. Mota, A.J. Queimada, S.P. Pinho, E.A.Macedo, Ind. Eng. Chem. Res. 47 (2008) 5182-5189.
[2] A.J. Queimada, F.L. Mota, S.P. Pinho, E.A. Macedo, J. Phys. Chem. B 113 (2009) 3469-3476.