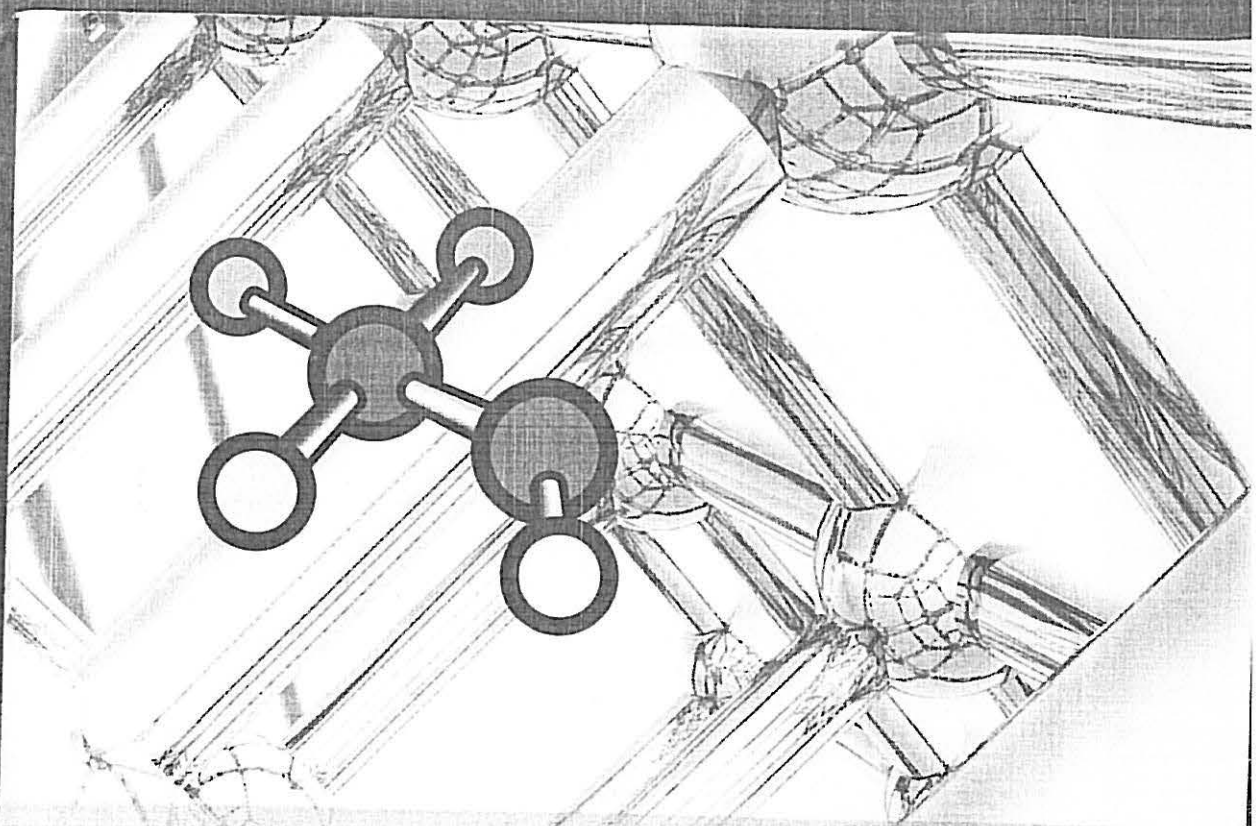

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11 a 13 de Junho de 2008

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SPQ

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PHASE EQUILIBRIA OF SOME PHENOLIC COMPOUNDS: EXPERIMENTAL AND MODELLING

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Several phenolic compounds are important for the food, chemical and pharmaceutical industries, some of them presenting complex chemical structures with different and multiple functional group substitutions.

To describe the phase equilibria of these complex chemicals, models able to take into account different intermolecular interactions, such as association, are required. To evaluate, improve or develop models an extensive database of experimental data is required.

In this work, solubilities were measured for some phenolic compounds in the temperature range 288 - 323 K, by the shake-flask method coupled with quantitative spectrophotometric analysis. Besides solubility, melting data and acid dissociation constants were also determined, providing a broader knowledge about the solubilization process of these molecules.

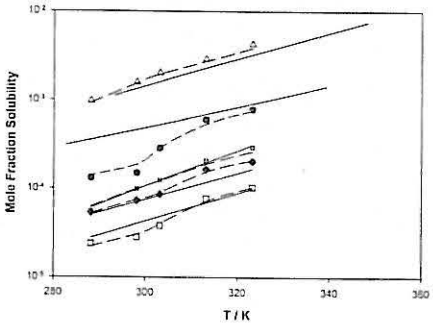

Figure 1. Experimental aqueous solubility data (●, salicylic acid; Δ, gallic acid; □, trans-cinnamic acid; crossed circles, caffeic acid; ♦, ferulic acid) and modelling results by CPA (solid line) and UNIQUAC (dotted line).

These new measurements and other literature data were combined to develop a methodology to model the phase equilibria of phenolic compounds using the Cubic-plus-Association (CPA) equation of state [1]. The modified UNIQUAC model [2] was also evaluated using the measured data. Both CPA and the modified UNIQUAC model showed to be appropriate tools to represent the solubility of these molecules.

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[1] F.L. Mota, A.J. Queimada, S.P. Pinho E.A. Macedo. *Ind.Eng.Chem. Res.* (accepted).
[2] M. Peres,E.A. Macedo, *Fluid Phase Equilibria* 123 (1996) 71.