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Session 8b: Biochemical Systems
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Invited Lecture: **E. Gomes de Azevedo**

Session 8b: Biochemical Systems

Modelling Amino Acid Solubility in Several Aqueous Alkanol Solutions with the PC-SAFT EoS

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Since their isolation in the 19th century, the physical and chemical properties of amino acids became a very important studied subject, no only because of their value as basic elements in all forms of life, but also for their industrial importance, particularly for food, chemical, medical, pharmaceutical and cosmetics industries.

Solid-liquid equilibrium is one of those properties, which is essential for the design, optimization and scale-up of the separation processes. Although it is possible to find in the literature a considerable number of both experimental and modelling works concerning amino acid studies in pure water, that is not the case for aqueous amino acid solutions with an alcohol. For these, there is still a great lack of information.

On the other hand, thermodynamic models have not been widely used in biotechnological industry as is the case for the chemical industry, but it is becoming more important due to the increasing demand for computer aided process design and optimisation [1]. An overview of the thermodynamic models, such as g^E models or equations of state already applied was given recently [2-5], and it was possible to conclude that despite the relative success obtained with the foregoing models, they exhibit several limitations. Therefore, the work development in this field is still a growing challenge.

The results produced using the g^E models are quite acceptable. Our group explored the potentialities of the excess solubility approach combined with conventional thermodynamic models, namely g^E models such as the NRTL, the modified NRTL, the modified UNIQUAC and also with the model presented by Gude et al. [6,7] to represent the solubility of amino acids in water-alcohol systems and satisfactory results were obtained [3]. However, the equations of state become a very attractive alternative. Since experimental data are often scarce, from a practical and critical point of view, an equation of state is more robust for predictions beyond the region where model parameters were estimated [8,9]. Therefore, the recently developed PC-SAFT EoS [8,10] was applied to model the solubilities of glycine, DL-alanine, L-serine, L-threonine and L-isoleucine in pure water, pure alcohols (ethanol, 1-propanol and 2-propanol) and in mixed solvent systems. The amino acids were considered as non-associative molecules and the three pure component parameters were fitted to the densities, activity and osmotic coefficients, vapour pressures, and water activity of their aqueous solutions. Only one temperature independent binary parameter is

required for each amino acid/solvent pair. The model could accurately describe the solubility of the amino acids in water, but the correlation for the solubility in pure alcohols was not so satisfactory. The solubilities in the ternary systems were predicted using the pure component and binary parameters without fitting any additional parameters and the results were reasonable. Fitting the binary parameter for the pair amino acid/alcohol to the solubility in the mixed solvent system instead, the description of the solubility in the ternary systems was clearly improved and the results were in fair agreement with the experimental data for all mixture compositions. This EoS was also used by Fuchs et al. [4] to model the solubility of glycine and DL-alanine in aqueous and alcohol solutions. A critical comparison between two works will be shown, and some conclusions drawn.

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