SOLUBILITY OF AMINO ACIDS BY GROUP-CONTRIBUTION METHOD

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Crystallization and precipitation are widely used for the separation of proteins. Therefore, the study of the solubility of amino acids, peptides, and proteins is of fundamental importance for the design of separation units.

The correlation and prediction of the solubilities of amino acids are the basis for further progress in this area. However, the successful representation of the solubilities depends on the ability to correlate and predict the activity coefficients of the amino acids in solution. In this way, several models have been proposed in the last few years: Nass (1988) has assumed the activity coefficients of amino acids to be a product of two terms due to chemical reaction equilibrium and physical interactions using for this the Wilson equation. Although the results are satisfactory, they are limited to a few amino acids; Chen et al. (1989) combined electroestatic and physical interactions (NRTL model) without considering the chemical equilibrium, which they recognize to be very important for same ranges of pH; Gupta and Heidemann (1990) have considered only short range interactions using the UNIFAC model, but the results were very poor. Orella and Kirwan (1991) tried to correlate solubility data of amino acids in mixtures with alcohols using an excess solubility approach based on three different models: Margules, Wilson and NRTL. The best approach is the one related to Wilson equation, with deviations smaller than 15%.

The major disadvantage of the referred models comes from the fact that they can't be used for prediction purposes and therefore are of limited application.

In this work a generalized thermodynamic model has been developed based on the UNIFAC method; new groups have been defined according to the group-contribution concept, and chemical equilibrium is taken into account simultaneously with the physical equilibrium.

Results are shown and a comparison with the previous models is given.