

NMR Spectroscopic Method for Estimating Activity Coefficients of Target Components in Poorly Specified Mixtures

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Poorly specified mixtures, of which the composition is only partially known, are common in bioprocess engineering but also important in many other fields of process engineering. Dealing with such mixtures in process design is challenging. A typical separation task in such cases is that a target component, of which the concentration is known, has to be removed from a liquid mixture of which the composition is not or only partially known. In the present work, a method was developed to predict the activity of the target component in that situation. It is based on an NMR spectroscopic analysis that yields information on the nature and concentration of chemical groups in the mixture. The determination of species concentrations is, however, not required. Using the NMR spectroscopic data on the groups in the mixture, the activity coefficient of the target component can be predicted by the UNIFAC group contribution method. The new method is tested using a large variety of model mixtures as examples, which are inspired by fermentation broths and of the type target component + side components + water. The ability of the new method to predict effects like the influence of the nature and concentration of the side components or the concentration of the target component on the activity of the target component is systematically investigated. Surprisingly good agreement is found even for complex mixtures. The new method has broad applications and can be developed further in several directions.