# Measurement and Calculation of Multicomponent Diffusion Coefficients in Liquids

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Diffusion is a physical phenomenon which occurrs in every natural or industrial process involving mass transfer. It can play an important role as the rate determining step. Therefore, the determination of diffusivities in liquids is of great interest for the calculation of mass transfer processes. Most studies about diffusion concentrate on measuring and predicting diffusivities in binary mixtures. Research on this topic has advanced, also due to a fair database of experimentally determined binary diffusivities. However, real processes mostly deal with mixtures involving more than two components. In these cases, both the experimental and theoretical investigations of diffusion are much more complex. Therefore, few multicomponent diffusion data are found in the literature. There are two well established theories describing diffusion. The more commonly used is Fick's Law. This theory was developed in the 19th century, in analogy to Fourier's description of heat transfer. However, Maxwell and Stefan developed a physically consistent theory describing diffusion. Contrary to Fick's Law, the multicomponent Maxwell-Stefan diffusivities can be related to the binary case.

Existing methods for the prediction of multicomponent diffusivities cannot be validated, due to the lack of ternary diffusion data. To overcome this limitation, holographic interferometry is used to investigate multicomponent diffusivities within the whole concentration space of non-ideal ternary systems. These measurements include more than 100 data points. Experimental Fickian diffusivities are transformed into Maxwell-Stefan diffusivities. The required thermodynamic data are taken from binary VLE-experiments applying excess enthalpy models such as Wilson, UNIQUAC, or NRTL. The methods for measuring Fickian diffusivities are well established. However, there is a lack of proven rules for the selection of appropriate thermodynamic data sets needed for the calculation of Maxwell-Stefan diffusivities from experimental ternary Fickian diffusivities. The influence of different thermodynamic data sets on this calculation is shown, and criteria for the selection of appropriate parameters are given.