Multicomponent diffusion coefficients in liquids from a fully automated microfluidic setup using Raman-microspectroscopy

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Experimental data on diffusion in fluids are valuable input for modeling and design of chemical processes. Still, experimental data are often lacking since conventional diffusion experiments are time- and material-consuming. Material consumption is a particular critical issue for screening of new systems containing expensive components of limited availability.

In this work, we present a measurement setup for time- and material-efficient determination of multicomponent diffusion coefficients in liquids. The measurement setup consists of an inverse confocal Raman-microscope and a microchannel. Thereby, the setup combines the advantages of microfluidics and Raman-microspectroscopy: Small microfluidic dimensions inherently reduce both sample consumption and measurement time, since diffusion lengths are short; Raman-microspectroscopy allows for rapid simultaneous in-situ quantification of all components with a high spatial resolution.

The chosen microchannel geometry and experimental parameters ensure stable steady-state flow of two liquid phases next to each other. Mass transfer occurs only perpendicular to the flow direction. At different retention times of the fluids in the channel, Raman spectra are collected along the channel cross-section. Spectral analyses yield spatially resolved concentration profiles. From the concentration profiles, the mutual diffusion coefficients are determined by least-squares fitting of diffusion process model. The experimental setup has already been successfully applied in measuring multicomponent diffusion coefficients [1]. The results show that the presented setup allows rapid and reliable determination of diffusion data using small sample volumes.

However, until now, one experiment provides diffusion coefficients for only one mean mixture composition. Each experiment requires about 30 minutes for preparation and about another 30 minutes for start-up, in which time and material are lost. Additionally, samples are prepared manually by weight in a time-consuming and error-prone step. In fact, these steps mainly determine the overall time and accuracy for diffusion measurements.

Here, we present the automation of the microfluidics diffusion setup to further reduce experimental time and effort. In the automated setup, independent syringe pumps feed pure components into a micro-mixer to prepare mixture samples by volume before entering the microchannel. By changing the volumetric flow rates of the syringe pumps during the experiment, diffusion coefficients can be measured for multiple mixture compositions in one experiment. This procedure avoids tedious manual sample preparation and only needs one start-up period for several mixture compositions.

The results show that the presented setup saves time and sample volume for the measurement of diffusion data needed for process modeling and design.

References

[1] C. Peters, L. Wolff, S. Haase, J. Thien, T. Brands, H.-J. Koß, A. Bardow: *Multicomponent diffusion coefficients from microfluidics using Raman microspectroscopy*. Lab on a Chip **17**, 2768-2776 (2017).