Combining Microfluidics and Raman Microspectroscopy: Efficient Measurement of Multicomponent Diffusion and Liquid-Liquid Equilibria

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Liquid-liquid equilibria and diffusion coefficients are important data for chemical engineering processes such solvent extraction. However, experimental data are often lacking since conventional experiments are time and material consuming. This is particularly problematic for screening of new systems containing expensive components of limited availability. In this work, we present a novel measurement setup for time- and material-efficient determination of liquid-liquid equilibria and diffusion coefficients. The measurement setup consists of an inverse confocal Raman microscope and a microchannel. Thus, the setup combines advantages of microfluidics and Raman microspectroscopy: Small microfluidics dimensions inherently reduce sample consumption and lead to short measurement time as mass transport distances for equilibration of liquid phases and diffusion processes are short; Raman microspectroscopy allows for rapid simultaneous in-situ quantification of all components with a high spatial resolution. The same setup can measure liquid equilibria and diffusion coefficients. In both kinds of measurements, the chosen microchannel geometry and experimental parameters ensure stable flow of two liquid phases next to each other in steady state. Mass transfer only occurs perpendicular to the flow direction. Raman spectra are collected spatially resolved across the channel cross-section at different retention times of the fluids in the channel. Results of spectral analyses are spatially resolved concentration profiles. From the concentration profiles, either the liquid-liquid equilibrium of immiscible liquid phases or the mutual diffusion coefficient of miscible liquid components are determined. Ternary liquid-liquid equilibria and diffusion coefficients have successfully been determined for the system cyclohexane-toluene-methanol to validate the setup. The results show that the presented setup saves time and sample volume for the measurement of data needed for process analysis and design.