

# Determination of Reaction Rates by Raman Spectroscopy in Continuous Plug Flow Capillary Reactors with In-situ Extraction

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Reaction rates are a fundamental part of process engineering, which represents the relationship between the amount of substance per volume and time. However, mass transfer limitations have an important influence on the reaction rate, the conversion rate and product formation [1]. Unfortunately, distinguishing between the contributions of the reaction rate and the mass transfer in two-phase liquid-liquid reaction systems is a challenge since the homogeneous reaction in one of the phases and the extraction via mass transfer in the other phase occur simultaneously and are intimately linked. However, accurate determination of the individual effects is crucial for predicting the overall performance of the two-phase liquid-liquid reaction system across various conditions [2]. Numerous efforts have been made to consider the influence of mass transfer effects on the reaction rate due to its importance.

The (double) stirred cell is a common method to investigate the reaction rate in liquid-liquid reaction systems. Despite its versatility and easy usability, the reaction rate cannot be determined independently as, even with strong mixing, the convective mass transfer in the phases cannot be neglected. To overcome this disadvantage, droplets with a Sauter diameter down to 2.5  $\mu\text{m}$  are used in a rotor-stator spinning disk reactor. Due to the extreme small dimensions and high surface to volume ratio the mass transfer can be neglected [3]. But, due to high shear forces and a difficult isothermal temperature management, this setup is not suitable for all liquid-liquid reaction systems.

In our work, we contribute the new method of combining a capillary microreactor with Raman spectroscopy. By injecting a liquid-liquid reaction system into a capillary, a plug flow with alternating phases is formed. Due to the flow profile, vortices form within the plug and lead to a very high degree of mixing in the plugs. In combination with the high surface-to-volume ratio typical for microfluidic devices, the influence of the mass transfer can be neglected. In addition, the high surface-to-volume ratio enables an isothermal reaction even for strong endo- or exothermal reactions. The use of Raman spectroscopy allows for a fast in-situ analysis across a wide temperature and pressure range without disturbing the flow regime. Furthermore, the combination of a capillary microreactor and Raman spectroscopy has a low sample consumption. To demonstrate the functionality of the new method, we show measured data of a liquid-liquid reaction system compared to the literature data.

## References

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