Bachelor-/Masterthesis, Research Internship (Chem.Eng.):

Simulation and Experimental Application of Actinometry

Scope of the Project:
The main goal of the project “Photon Fluxes in microstructured photoreactors” is the development of general design and application rules to optimize photochemical process concepts. For this purpose, different reactor setups are investigated by conducting photochemical reactions with well-known properties in the reaction volume to calculate the available photon flux from the conversion over irradiation time. This technique is called actinometry. Combined with radiometric measurements, the whole radiation field can be characterized to give general advice on significant parameters to optimize the efficiency of numerous specific photoreactions. Contribution to the parameter field are e.g. the type of the light source, reactor geometry and material or residence times and starting concentrations.

Current Scientific Work:
In the research group of Prof. Ziegenbalg, basic experimental methods for the evaluation of photochemical processes in continuously operated standard microreactor setups have been developed. Some elementary reactor concepts were characterized by convenient figures of merit allowing an unbiased and meaningful comparison. Nevertheless, some self-made and especially commercially available or industrially relevant scale reactors cannot be characterized due to limitations of the standard measurement methods. E.g. the limited solubility of main actinometry components requires new experimental procedures. One approach is to conduct actinometry in pulsed mode: a distinct volume of reactant is surrounded by solvent that resolves potentially precipitated species before it affects the result remarkably by remaining in the capillary or shadowing the progressing reaction.

Your Profile and Possible Working Packages:
Experimental data have already been published, but the deviance of the continuous and the pulsed method cannot be explained satisfactorily yet (see figure 1).[1] To overcome this challenge, the actinometer pulse shall be simulated according to already conducted residence time measurements. After that, the photochemical reaction shall be implemented to gain insight on the influence of the pulsed mode in whole as well as the effect of different concentrations and pulse lengths of the actinometer. For verification, assumptions made for simulation shall be proven by newly conducted experiments to show the congruence of simulation and experiment.

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Figure 1: Correlation of continuous and pulsed mode within the same photoreactor setup.