

Bachelor/Masterthesis, Research Internship:

CFD-simulations for photochemical reactors used for photocatalytic systems

Scope of the Project:

In recent years, heterogeneous photocatalytic reactions gain more and more attention. Usually, these reactions are applied in organic synthesis on lab and industrial scale by using semiconductors such as TiO2 as photocatalyst. In terms of photochemical reaction engineering this special reaction type raises some new challenges to the reactor design. Compared to homogeneous systems not two but three components (Substrate, photon and catalyst) have to be brought into contact. This means that a high suspension quality as well as a high adaption to the light source characteristics is mandatory in order to reach high conversions or selectivities.

The QuinoLight project is a cooperative work between the research group Ziegenbalg, the research institute of the DECHEMA and the research group Marschall from Bayreuth university. Utilizing the photocatalytic synthesis of quinoline, the project's objective is the development and optimization of reactors for photocatalytic systems by application of 3D-printing.

Current scientific work and possible working packages:

Current approaches at the ICIW focus on the development and manufacturing of irradiated stirred tank reactors and flowthrough reactors. Thanks to the technology of 3D-printing virtually no limitations for the reactor design exist. However this is associated with a high number of possible reactor prototypes. To reduce the experimental effort, a preselection has to be conducted. In this context CFD-simulations can be a powerful tool to identify beneficial reactor geometries. For the stirred tank reactor the influence of the stirrer geometry as well as of installations like buffles has to be investigated. In flowthrough reactors fluid guidance is important to activate or deactivate axial mixing in the irradiated zone. Therefore, a new reactor concept has to be developed using CAD-software. Finally, test reactions have to be conducted to correlate the simulation results to experimental findings.



LED Flow direction

Peristaltic Pumr

Figure 1: CFD-simulations for photochemical flowthrough reactors.

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Figure 2: Experimental setup utilizing a 3D-printed flowthrough reactor.