Karlsruher Institut für Technologie

Institut für Mikroverfahrenstechnik,
Prof. Dr.-Ing. habil. Roland Dittmeyer

in Kooperation mit dem Lichttechnischen Institut,
Prof. Dr. rer. nat. U. Lemmer

**Master Thesis**

# Entwicklung und Simulation der optischen Komponenten eines Photoreaktors mit hoher Flussdichte zur Umsetzung von $CO_2$ im Labormaßstab
# Development and simulation of optical components of a lab-scale high flux photo reactor for $CO_2$ conversion

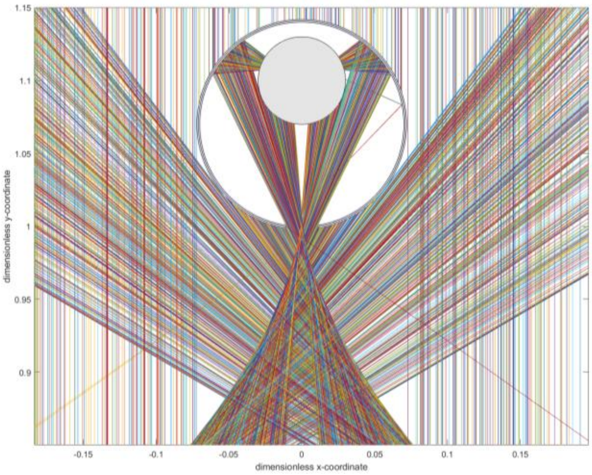
## Background

According to the report of the Intergovernmental Panel on Climate Change (IPCC)[1] published in October 2015, net global anthropogenic $CO_2$ emissions must reach zero by 2050 if man-made global warming is to be kept *'well below 2.0 °C*', as set out in the Paris Agreement[2] in 2015. According to the possible positive scenarios recorded by the IPCC, achieving a $CO_2$-neutral global economy by 2050 is only possible if significant quantities of $CO_2$ are removed from the atmosphere and bound in the long term. This requirement represents an unprecedented challenge for people of all societies on all continents and for many branches of world's economy. Especially changes in the energy and mobility sector and in energy-intensive industries such as the chemical industry will be drastic.

Therefore, at the Institute of Micro Process Engineering (IMVT) at the Karlsruhe Institute of Technology (KIT), as well as at numerous other research institutions worldwide, processes for chemical $CO_2$ fixation and/or use are examined. Current examples of IMVT's engagement in this field are the ongoing works in the 'Energy Lab 2.0'[3] or the Kopernikus project P2X[4], in which $CO_2$ is converted into hydrocarbons together with water and renewable electrical energy. In addition to these works, pioneering research at the IMVT is investigating the direct use of sunlight in processes that catalytically convert $CO_2$ with water to hydrocarbons. In addition to the development of suitable photo-catalyst systems, the development of a photo-reactor, in which light is efficiently concentrated and appropriately coupled into the reaction volume, is a decisive task, to which the thesis should contribute.

The manifold challenges in the development of an efficient photochemical process are addressed at the IMVT within the framework of national and international cooperations. The development of catalyst systems is e.g. promoted in cooperation with the Geoffrey Alan Ozin Group at the University of Toronto[5] (UoT) in Canada. The development of the optical system of a photo reactor will take place within the framework of a cooperation between IMVT and LTI.

**Tasks / Planned Works**




Ray path diagram of an exemplary 2D ray tracing simulation in MATLAB®

The student is supposed to develop an optical system for a photo-reactor in the context of his thesis supported by raytracing simulations using LightTools® and MATLAB®. A cluster infrastructure will be provided for the required calculations. The aim of the development is a high photonic efficiency of the system, a homogeneous illumination of the reaction volume with a high concentration of incident light and a high thermal efficiency. The key points here will be the concentration of the incident light and the distribution of the light in the reaction space under simultaneous minimization of heat radiation losses.

Main aspects of the work are:

- Familiarisation with the simulation software
- Development of a basic understanding of radiation transport and optics
- Development of a design proposal for the concentration and distribution of incident light on the outer surface of the reactor
- Development of a design proposal for the effective minimization of heat losses / radiation losses

Additional fields of activity are:

- Development of a concept for the transport of light in catalyst support
- Simplifying / generalizing description of the problem, e.g. via dimensional analyses
- Assistance in prototype design (in cooperation with IMVT's microfabrication engineers).
- Support in the construction of a test rig in which the results of the development can be validated experimentally
- Experimental validation

The results of the investigations must be documented in written form (60 pages excluding appendix) and presented in a seminar lecture at the IMVT (30 minutes).

**Framework / Requirements**

The thesis will be conducted in the environment of the cooperation between IMVT and LTI and will be supervised by a supervisor at each institute for the respective areas (reaction engineering at IMVT and optical systems at LTI). Furthermore, during a planned visit of Prof. Geoffrey Ozin in February 2019, the current status of the concepts will be discussed and possibly important boundary conditions of the catalyst system will be exchanged.
The status of the work will be discussed continuously with the supervisors at LTI and IMVT as well as in the two-week group meetings of the group "Catalytically Active Layers" at IMVT. After 50% of the processing time a half time lecture is expected. After two and four months of the processing time, discussions with Prof.

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Roland Dittmeyer are planned in which the progress of the work will be discussed. Knowledge of chemical reaction technology and the basics of heat transfer are required. Experience with simulation software (e.g. for raytracing) and MATLAB is desired.

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| Begin: | XX.XX.2019 |
| Professors: | Prof. R. Dittmeyer (IMVT) & Prof. U. Lemmer (LTI) |
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**Sources**


1. Allen, M. *et al.* Global Warming of 1.5 °C. Intergovernmental Panel on Climate Change (IPCC) (2018).
2. Paris Agreement. United Nations (2015).
3. Karlsruhe Institut of Technology. Energy Lab 2.0. Available at https://www.elab2.kit.edu/index.php (2018).
4. Federal Ministry of Education and Research. The P2X Kopernikus project. Available at https://www.kopernikus-projekte.de/en/projects/power2x (2018).
5. University of Toronto. Solar Fuels Cluster. Available at http://www.solarfuels.utoronto.ca/ (2018).