LABORATORY FOR CHEMICAL TECHNOLOGY
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Coach	**Supervisor(s)**	**Funding**
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CFD simulation of a novel photocatalytic reactor for dilute flow VOC abatement

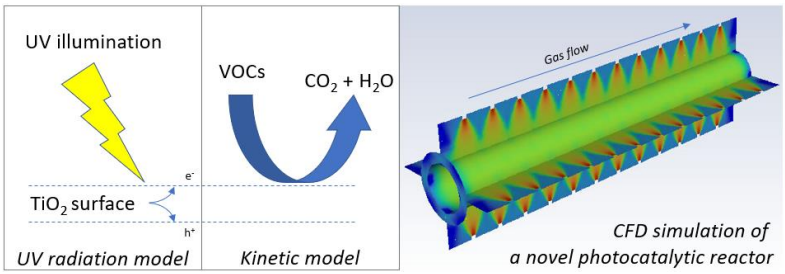
Aim

Developing a Computational Fluid Dynamics (CFD) model to simulate a novel photocatalysis reactor equipped with modern UV LED lights and state-of-the-art TiO_2 as a photocatalyst material.

Justification

Clean air is vital for our well-being. However, human activities contribute significantly to air contamination, which includes Volatile Organic Compounds (VOCs) and gaseous compounds like ozone, nitrogen oxides, and ammonia. Basic abatement techniques such as adsorption, thermal oxidation, and membrane separation are not suitable for treating dilute streams with concentrations below 1000 ppm of VOCs which are typically found in indoor air. To address this, methods like photocatalysis, catalytic oxidation, and plasma catalysis can be used.

The COP-CAT project is a multidisciplinary research project that investigates the use of alternative technologies, such as plasma and (photo)catalysis, to treat VOCs in indoor air. The project involves researchers from different fields and research groups at the university. One of the major innovative elements in the project is the multiscale simulation of an in-plasma or post-plasma reactor combined with a (photo)catalytic reactor. Modelling the reactor hydrodynamics (reactor scale) and the reaction kinetics (molecular scale) will provide numerical data. These numerical results will be supported by experimental data obtained by other researchers through in-situ monitoring of the experimental photocatalytic setup. A novel photocatalytic reactor will be simulated using the combination of a UV radiation model, a reaction model, and an appropriate CFD model. Currently, a first version of the CFD model linking the UV radiation and the reaction model has been prepared, and further extensions are needed to improve the quality of the modelling. The work is being carried out in collaboration with the LumiLab group, Department of Solid-State Sciences, Faculty of Sciences, UGent.



Program

- ✓ Literature study on the use of CFD model to simulate a gas-phase photocatalytic reactor.
- ✓ Performing CFD simulations of the photocatalytic reactor combining the extended UV radiation model, the reaction model, and the CFD model.

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