CFD Investigation of a Photocatalytic Multi-Tube Reactor for Indoor Air Purification

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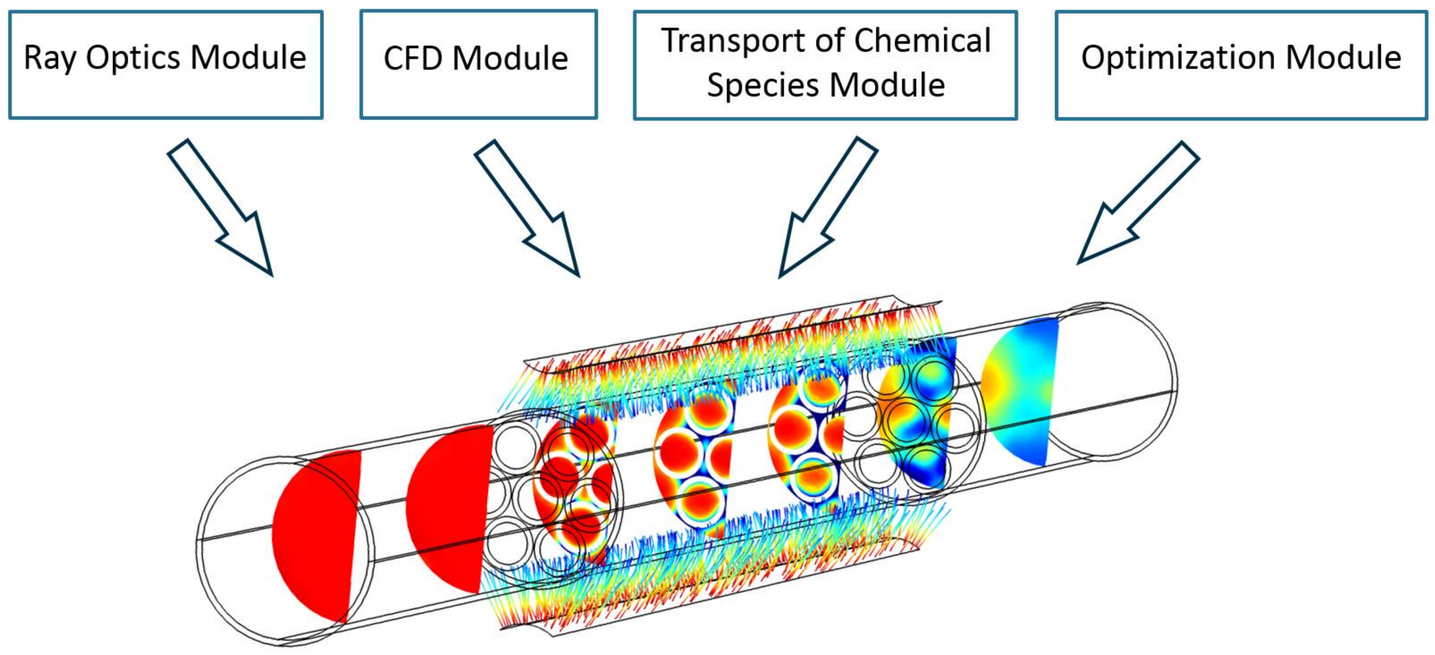
Introduction: Photocatalytic oxidation (PCO) is an interesting, cost-effective and efficient approach for indoor air pollution abatement. However, there is still a substantial gap to be filled between lab-scale investigation of suitable photocatalysts and applied PCO technology for air purification. Efficient operation of a PCO reactor requires insights in mass transfer rates, i.e. convective and diffusive transport towards the catalytic surface, irradiance and the kinetics of adsorption, desorption and photocatalytic reaction.

Computational Methods: Finite element modeling (FEM) is a numerical method for solving complex physics and is a very attractive approach for the analysis of a PCO reactor performance through integrated simulations of fluid dynamics (CFD), irradiance distribution (Ray Optics) and kinetics of desorption, adsorption and reaction at the catalytic surface (Transport of Chemical species).



References:
1. Verbruggen S.W. et al., Analytic versus CFD approach for kinetic modeling of gas phase photocatalysis, Chem. Eng. J. 262, 1–8 (2015).
2. Verbruggen, S.W. et al., CFD Modeling of Transient Adsorption/Desorption Behavior in a Gas Phase Photocatalytic Fiber Reactor, Chem. Eng. J. 292, 42–50 (2016).
3. van Walsem, J. et al., CFD investigation of a multi-tube photocatalytic reactor in non-steady-state conditions, Chem. Eng. J. 304, 808–816 (2016).

Results: The optical model was able to accurately predict the irradiance on the catalytic surface within the reactor. Consequently, the radiation field model was used to define an irradiance dependent reaction rate constant in a coupled Multiphysics model. An optimization routine was deployed to estimate the intrinsic adsorption, desorption and photocatalytic reaction rate constants on the TiO_2-surface, using 4 experimentally determined, transient outlet concentrations of acetaldehyde (figure 1). Additionally, a successful validation test was performed in an air-tight climate chamber at much higher flow rates, higher irradiance and realistic indoor pollutant concentrations to emphasize the reliability and accuracy of the intrinsic parameters for adsorption, desorption and photocatalytic reaction, as shown in figure 2.

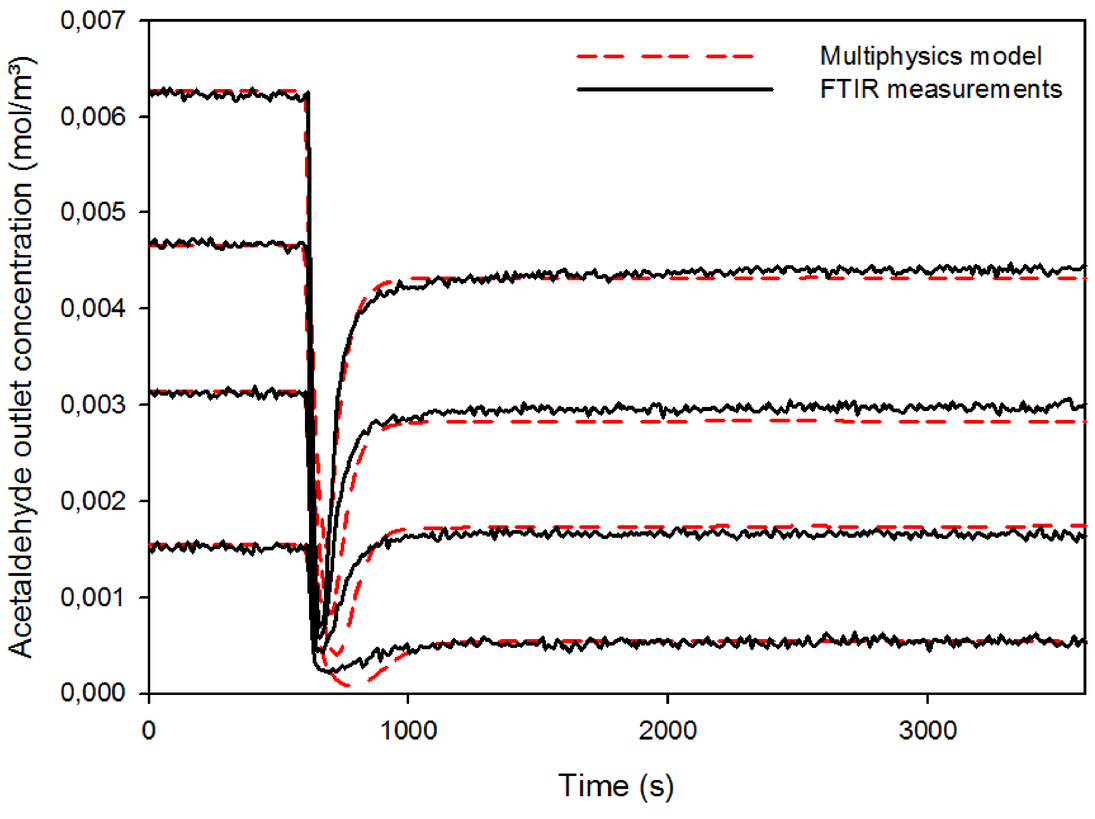


Figure 1: CFD simulations (dotted lines) based on FTIR measurements of acetaldehyde (solid lines) at 4 different bulk concentrations.

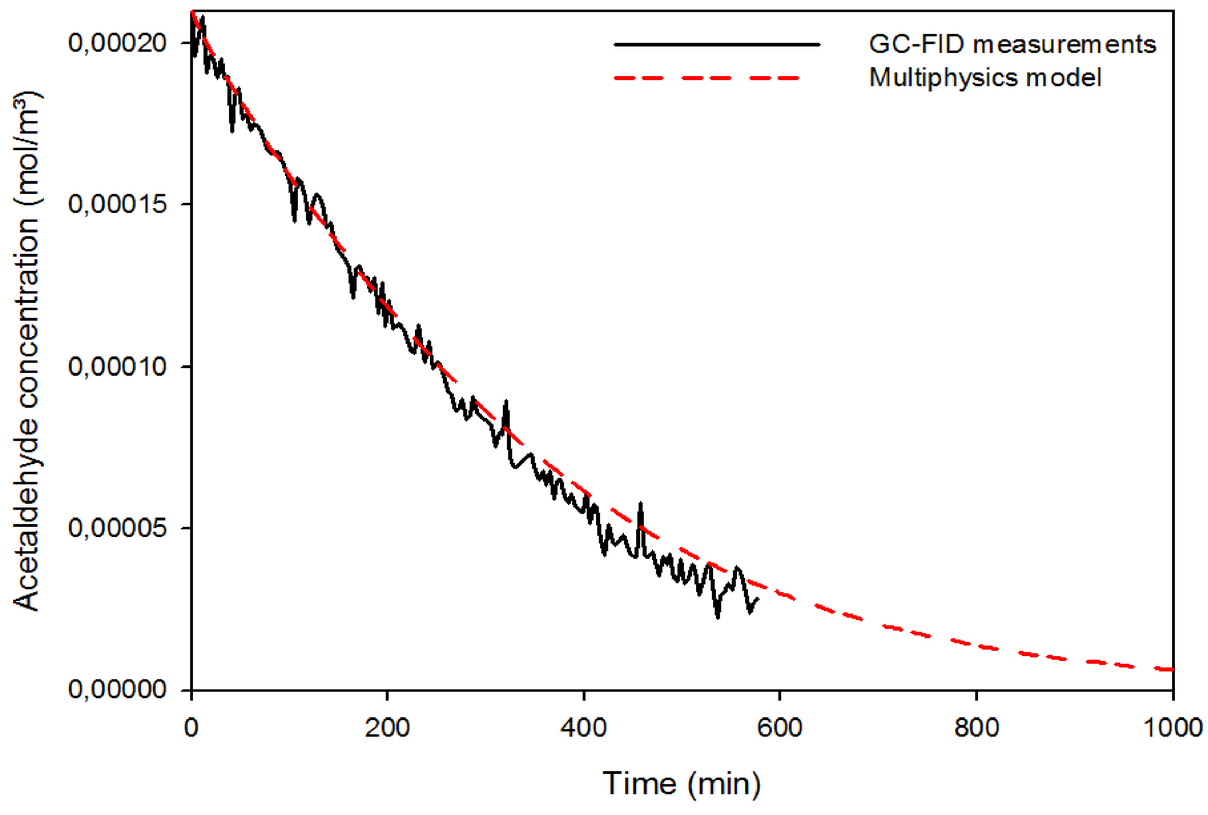


Figure 2: GC-FID measurements (solid line) of acetaldehyde concentration at challenging operating conditions and the resulting fit of the Multiphysics model simulation (dotted line)

Conclusion: Multiphysics modeling is a useful and convenient tool for designing and upscaling photocatalytic devices.