COMSOL CONFERENCE
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Predictive Model for UV Light Irradiation and Reaction Kinetics in a Photocatalytic Reactor

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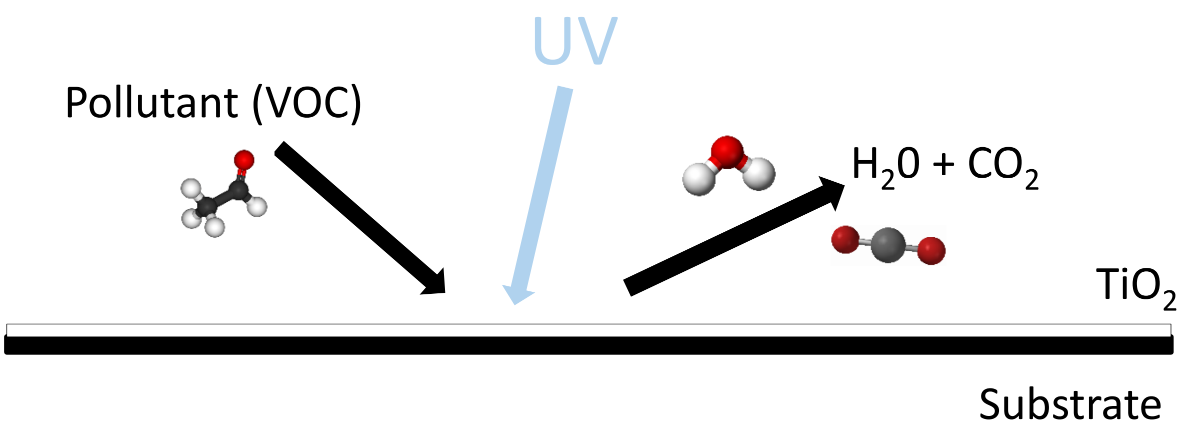
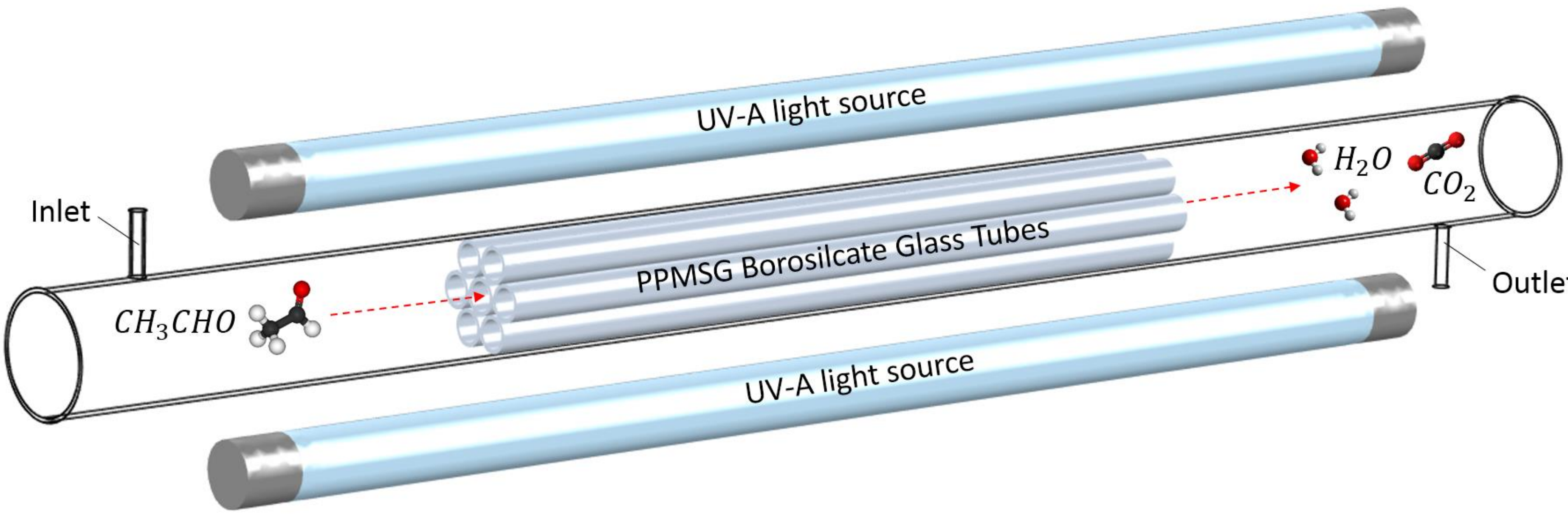
Photocatalysis: How does it work?

- Photocatalysis in our application:
  - Activation of a photocatalyst (TiO_2) with UV-light to degrade indoor air pollution (VOCs)

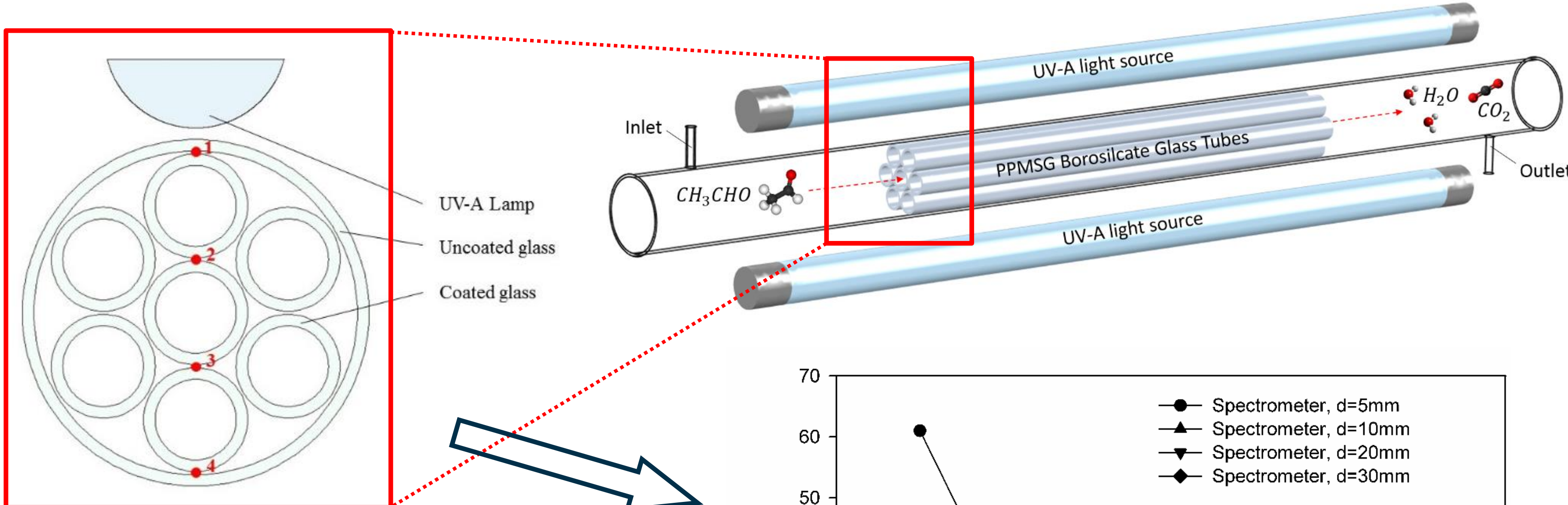


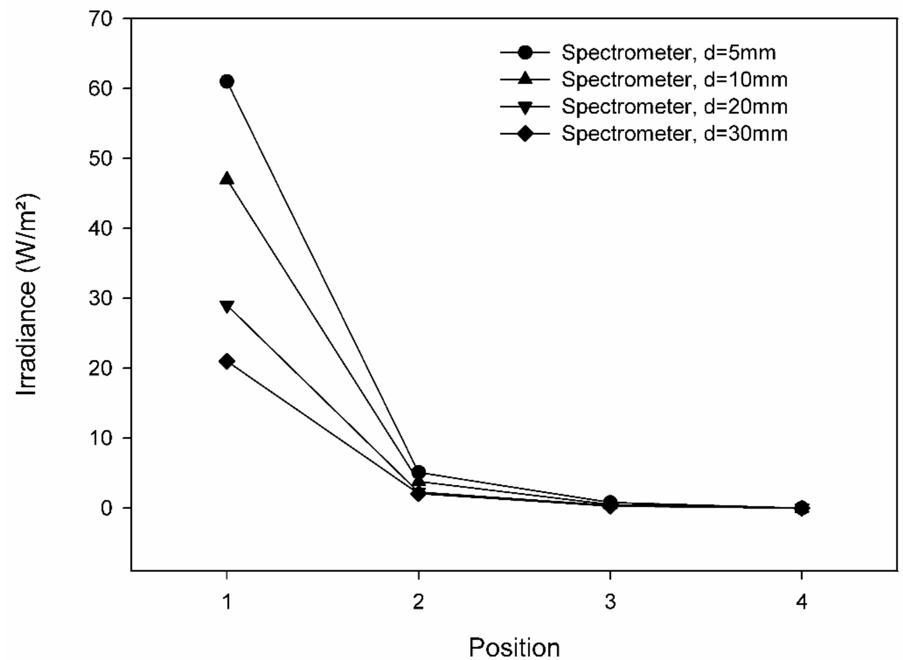
Photocatalytic multi-tube reactor



- Goal: Development of a model to predict distribution of UV-light intensity and pollutant concentration

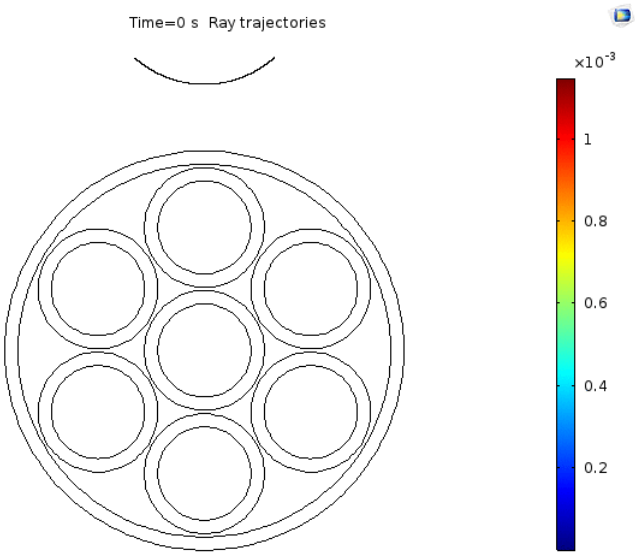
UV-irradiance measurements



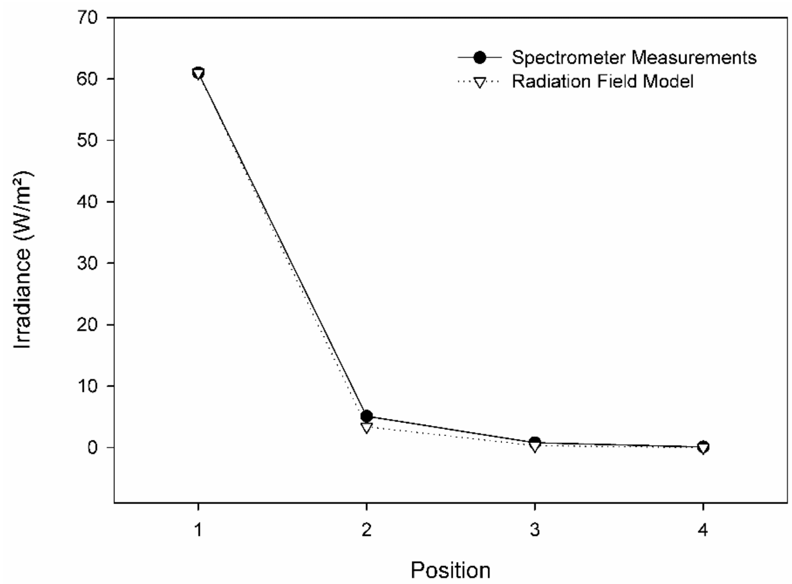


Ray Optics

- Light is simulated as rays with a certain amount of power (W) and intensity (W/m²)
- Initial guess for optical parameters such as refractive index and layer thickness of the coating (based on literature values):

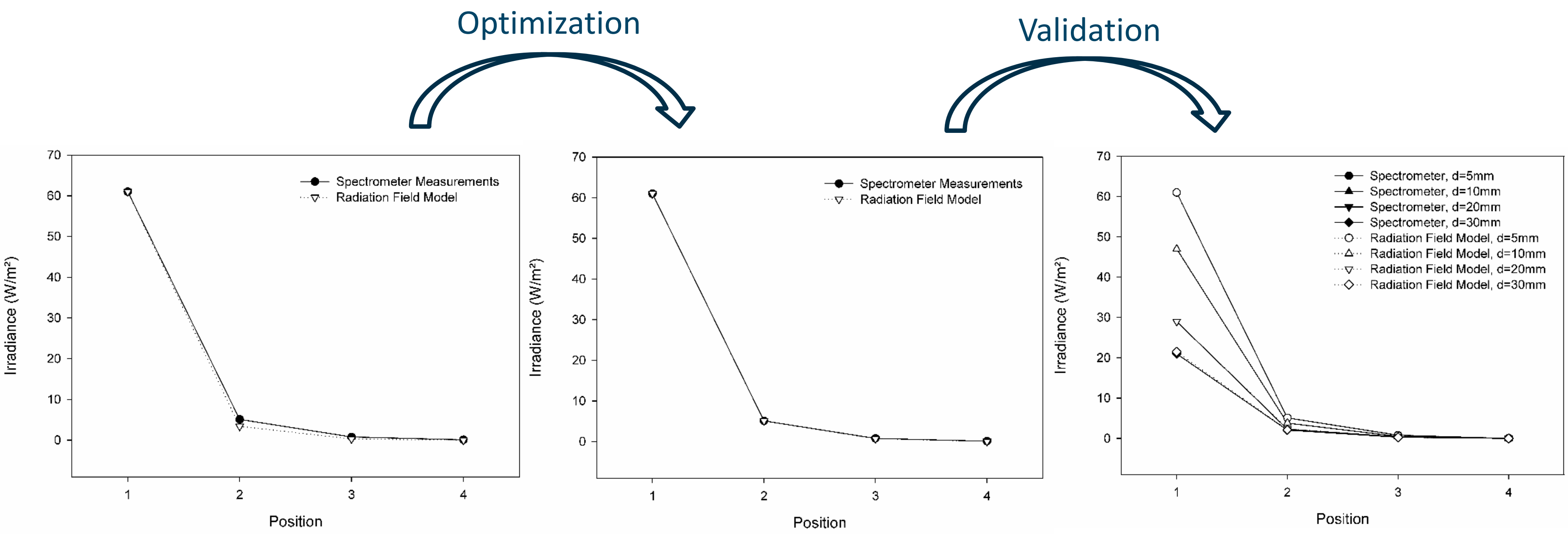


Ray Power (W)



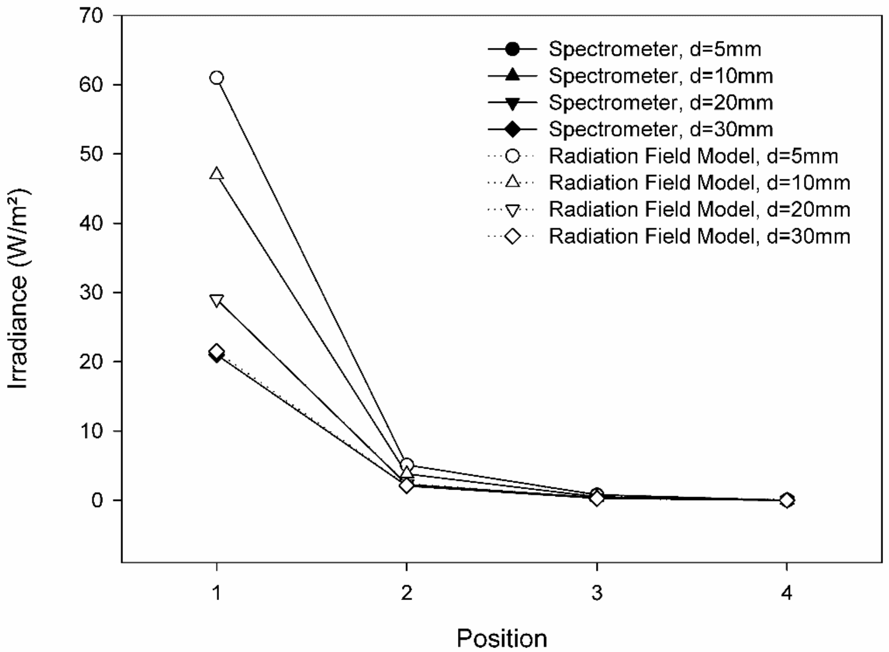
Ray Optics

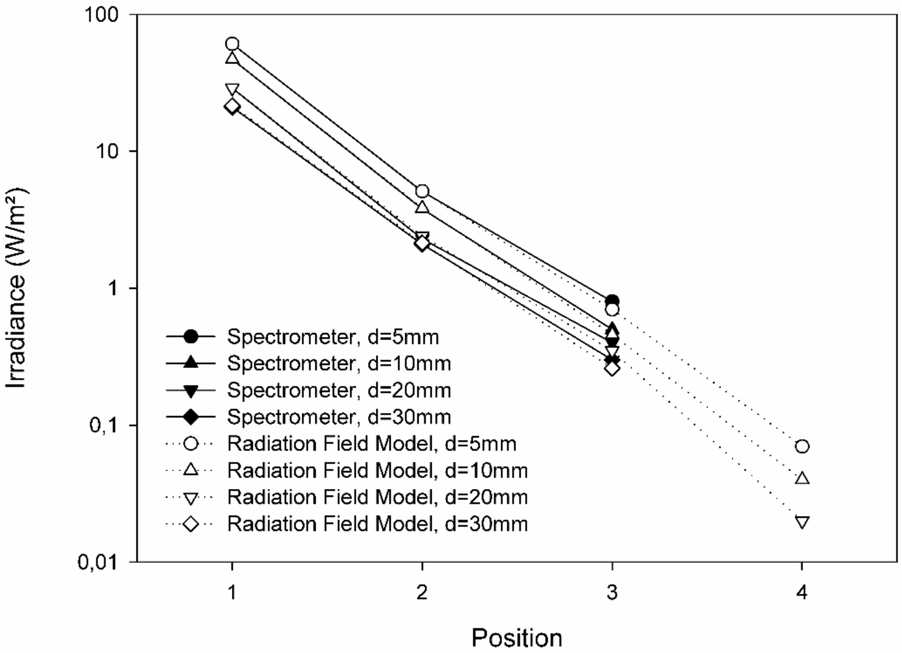
- Light is simulated as rays with a certain amount of power (W) and intensity (W/m²)
- Optimization of optical parameters:



Ray Optics

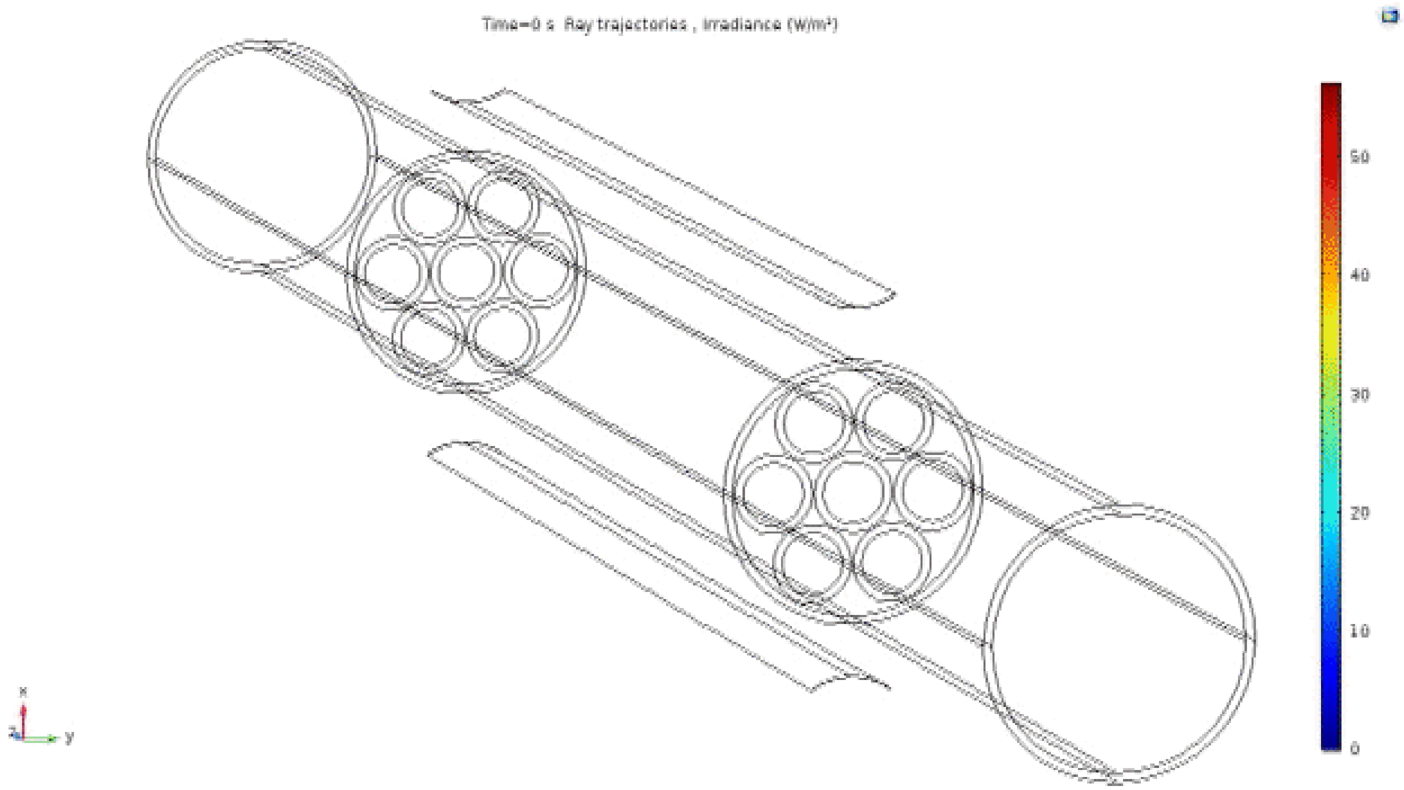
- Prediction at low irradiance





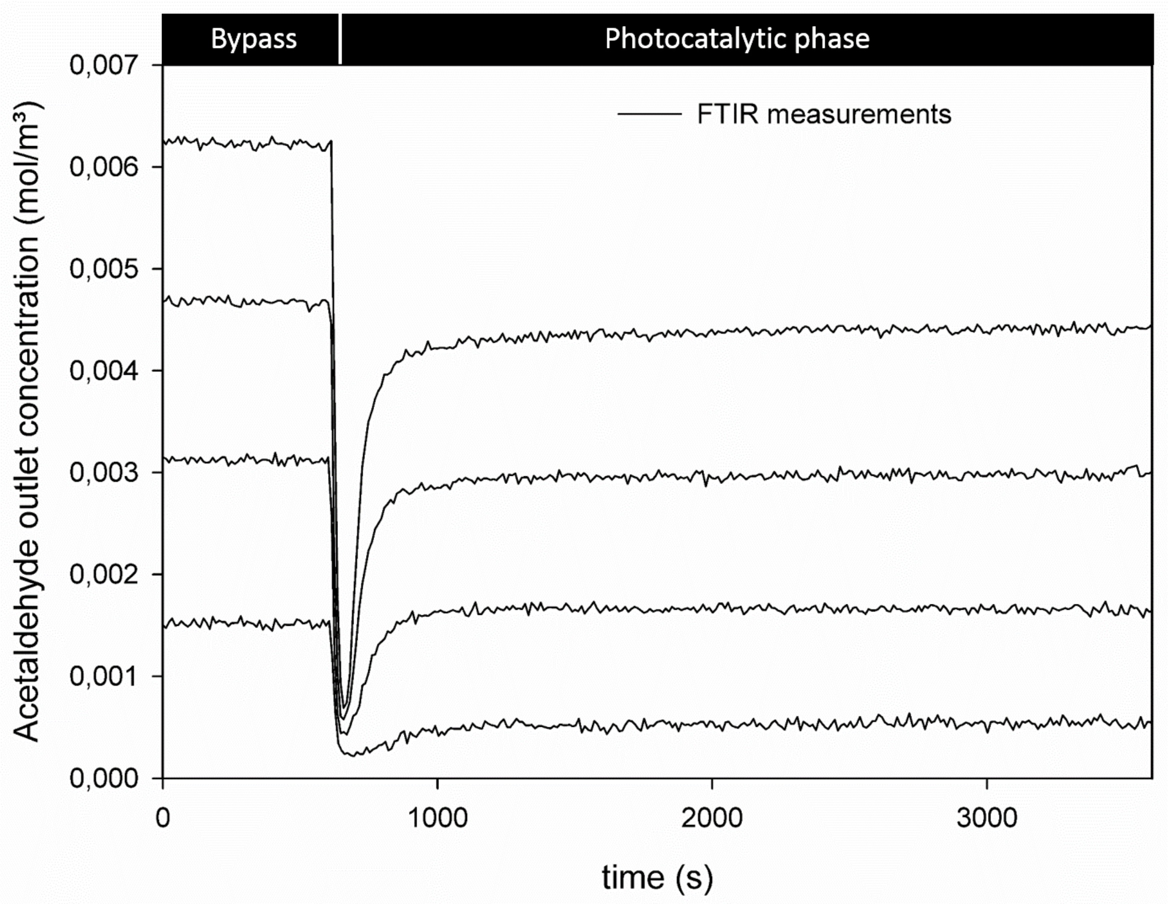
Ray Optics

- The optimized parameters are used to simulate the irradiance distribution on the catalytic surface in a 3D-model:



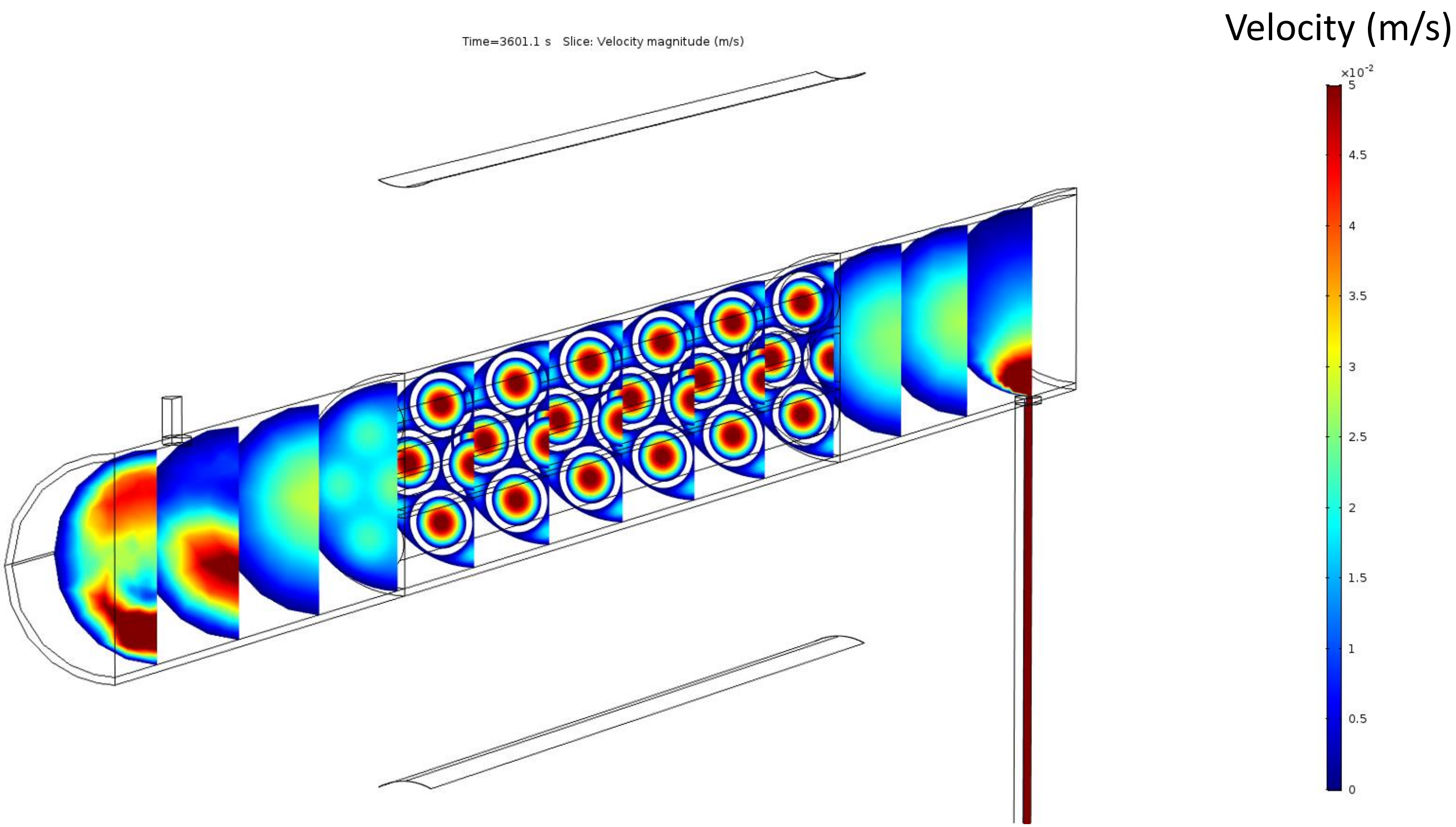
FTIR measurements

- Assembling experimental data for model calibration:



Laminar flow

- CFD-simulation of velocity profile and pressure (inlet flow rate of 500 cm³/min)



Transport of Diluted Species

- Pollutant concentration ($C_{Acal,bulk}$) coupled with the laminar flow
- Adsorption defined as a flux from bulk to boundary (R_{ads})
- Desorption defined as a flux from boundary to bulk (R_{des})

1. $-\mathbf{n} \cdot \left(-D\nabla C_{Acal,bulk} + \mathbf{u} \cdot C_{Acal,bulk}\right) = -R_{ads} + R_{des}$
2. $R_{ads} = k_{ads} C_{Acal,bulk} (1 - \theta_{Acal})$
3. $R_{des} = k_{des} \theta_{Acal}$

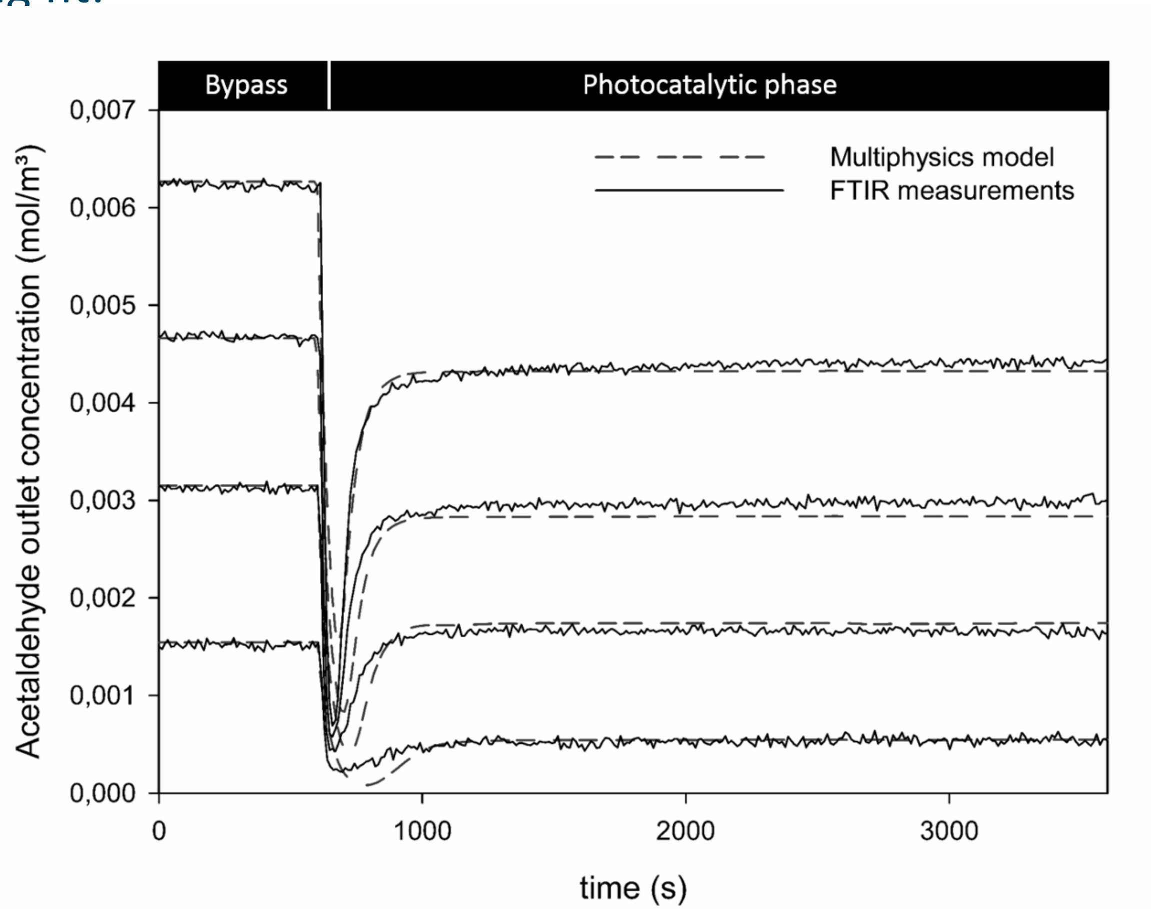
Boundary ODE

- Photocatalytic reaction rate (R_{pco})
- Acetaldehyde surface concentration ($C_{Acal,ads}$)

1. $R_{pco} = k_{pco} C_{Acal,ads}$
2. $\dfrac{\partial C_{Acal,ads}}{\partial t} = R_{ads} - R_{des} - R_{pco}$
3. $k_{pco}(I) = \begin{cases} k_0 I & , I < 10\ W/m^2 \\ k_0\sqrt{I_0 \cdot I} & , I > 10\ W/m^2 \end{cases}$

Optimization Module

- Fitting the experimental concentration profiles by adapting the kinetic parameters (k_{ads}, k_{des} & k_0)
- Resulting fit:



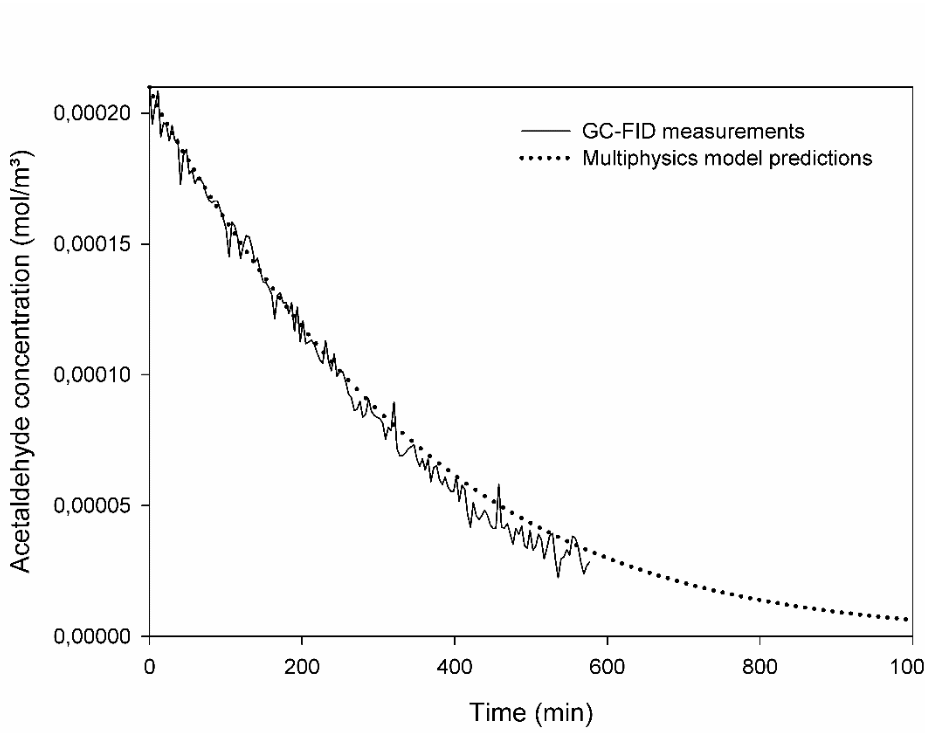
Model Validation

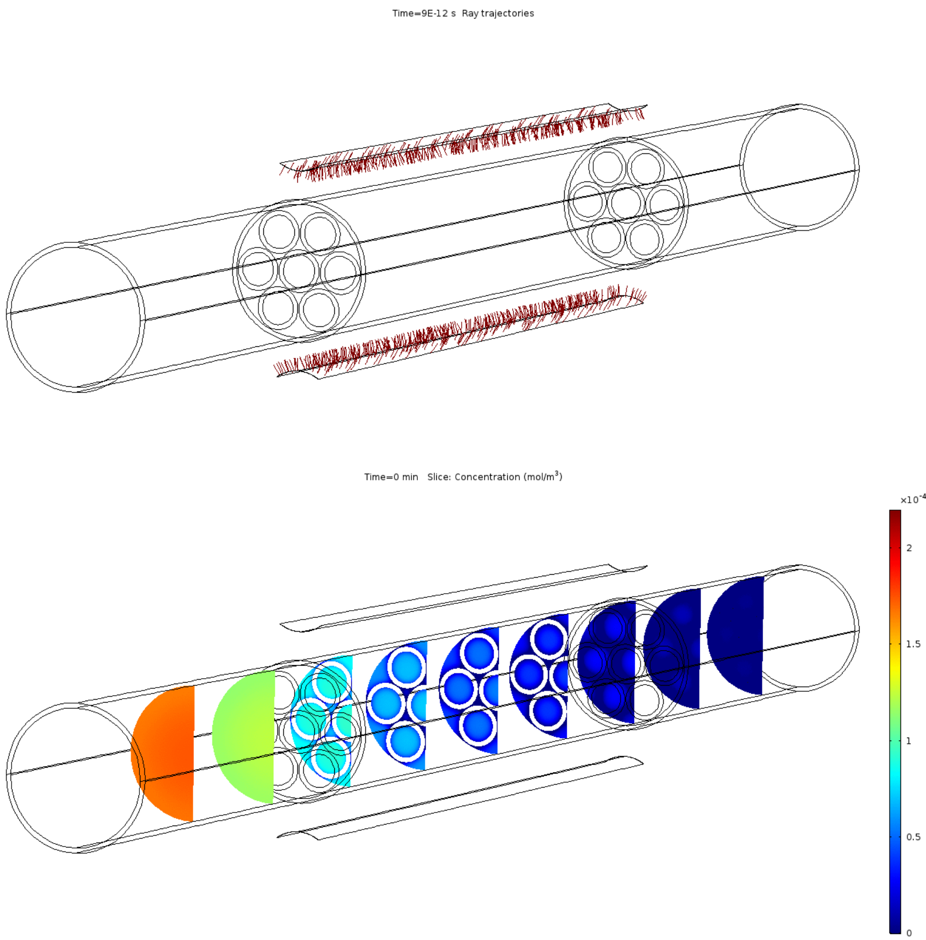
- Air-tight climate chamber:

a) Air homogenization fans
b) Septum
c) Air-tight hatch
d) Compact GC-FID
e) Multi-tube reactor

Model Validation

➢ Air-tight climate chamber:





Conclusion

- Multiphysics model is a versatile tool:
  - Accurate prediction of transient pollutant concentrations under different conditions
  - Optimization of reactor design and light source configuration to improve photocatalytic performance

Thank you for your attention!
Questions?

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