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 (TiO₂) with UV-light to degrade indoor air pollution (VOCs)

\[ \text{Pollutant (VOC)} \rightarrow \text{TiO}_2 \rightarrow \text{UV} \rightarrow \text{H}_2\text{O} + \text{CO}_2 \]

Substrate
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 trajectories and irradiance graph](image_url)
Ray Optics

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

Optimization  Validation

[Graphs showing irradiance (W/m²) vs. position for different scenarios]
Ray Optics

- Prediction at low irradiance

![Graphs showing prediction at low irradiance](image-url)
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:

![FTIR measurements chart]

- Table:

<table>
<thead>
<tr>
<th>Bypass</th>
<th>Photocatalytic phase</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>FTIR measurements</td>
</tr>
</tbody>
</table>

- Graph:

- X-axis: time (s)
- Y-axis: Acetaldehyde outlet concentration (mol/m³)
Laminar flow

- CFD-simulation of velocity profile and pressure (inlet flow rate of 500 cm²/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. \( \frac{\partial C_{Acal,ads}}{\partial t} = R_{ads} - R_{des} - R_{pco} \)
3. \( k_{pco}(I) = \begin{cases} 
  k_0 I, & I < 10 \text{ W/m}^2 \\
  k_0 \sqrt{I_0 \cdot I}, & I > 10 \text{ W/m}^2 
\end{cases} \)
Optimization Module

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

![Graph showing concentration profiles over time for Bypass and Photocatalytic phase, comparing model predictions to FTIR measurements.](image-url)
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:

![Graph](attachment:image.png)
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?