Transient CFD investigation of a photocatalytic multi-tube reactor

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Is your building sick?

Most businesses don't know...
Introduction

- **Sick Building Syndrome (SBS)**
  - Accumulation of pollutants (VOCs, NOx, CO,...)
  - Stringent heat-insulation measures
  - Insufficient ventilation
  - People spend 90% of their time indoors

- **Possible solutions**
  - Source control
  - Ventilation
  - Air purification

- **Our goal**
  - Integration of photocatalytic reactor in ventilation systems
Photocatalysis: Applications

- Water purification/desinfection
- Air purification
- Self-cleaning materials
Photocatalysis: How does it work?

- **Photocatalysis in our application:**
  - Activation of a photocatalyst to degrade indoor air pollution (VOCs)
  - **Catalyst:** increases reaction rate without being consumed

- **Diagram:**
  - **Pollutant (VOC) + UV light → TiO₂**
  - **TiO₂**
  - **H₂O + CO₂**

- **Benefits:**
  - Cost-effective
  - No waste steams
  - Mild reaction conditions
Experimental setup
Experimental data (FTIR)
Comsol Multiphysics: Geometry

Photocatalytic reactor: Glass tubes

Inlet

Connecting tubes

FTIR

Outlet
Comsol Multiphysics: 
*Meshing*

*User-controlled mesh:*
- 54,000 prism elements
- 18,000 tetrahedral elements
Comsol Multiphysics: Laminar flow (spf)

- Stationary solver:

Photocatalytic reactor: Glass tubes
Comsol Multiphysics:
*Transport of diluted species (tds)*

- **Time-dependent solver:**
  - Pollutant concentration \((C_{Acal,bulk})\) coupled with the laminar flow
  - **Adsorption** defined as a flux from bulk to boundary \((N_{ads})\)
  - **Desorption** defined as a flux from boundary to bulk \((N_{des})\)

1. \(-\mathbf{n} \cdot \left( -D \nabla C_{Acal,bulk} + \mathbf{u} \cdot C_{Acal,bulk} \right) = -N_{ads} + N_{des}\)
2. \(N_{ads} = k_{ads} C_{Acal,bulk} (1 - \theta_{Acal})\)
3. \(N_{des} = k_{des} \theta_{Acal}\)
Comsol Multiphysics:
**Boundary ODE (bode)**

- **Time-dependent solver:**
  - Photocatalytic reaction rate \((R_{pc})\)
  - Acetaldehyde surface concentration \((C_{Acal,ads})\)

1. \( R_{pc} = k_{pc} C_{Acal,ads} \)
2. \( \frac{\partial C_{Acal,ads}}{\partial t} = N_{ads} - N_{des} - R_{pc} \)
Comsol Multiphysics: 
*Optimization module (opt)*

- Goal: fitting the experimental concentration profiles by adapting the kinetic parameters
  - Adsorption reaction rate constant \( (k_{ads}) \)
  - Desorption reaction rate constant \( (k_{des}) \)
  - Photocatalytic reaction rate constant \( (k_{pco}) \)
  - Maximum surface coverage \( (\Gamma_s) \)

- How?: Sparse Nonlinear OPTimizer (SNOPT) algorithm
  - To find the local minimum of a least-squares objective function
Comsol (lines) vs Experimental data (dots)

- Adsorption phase:
Comsol (lines) vs Experimental data (dots)

- Photocatalytic phase:
Comsol (lines) vs Experimental data (dots)

- Validation experiment:
Conclusion

- CFD/multiphysics is a versatile tool
  - To model the transient, dynamic behaviour of acetaldehyde through the reactor
  - To estimate the adsorption/desorption and photocatalytic rate constants
Thank you for your attention!