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Vento

AGENTSCHAP INNOVEREN & ONDERNEMEN

Vlaanderen is ondernemen

Transient CFD investigation of a photocatalytic multi-tube reactor

J. van Walsem, J. Roegiers, S. Lenaerts & S. Denys

Sustainable Energy, Air & Water Technology
University of Antwerp

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

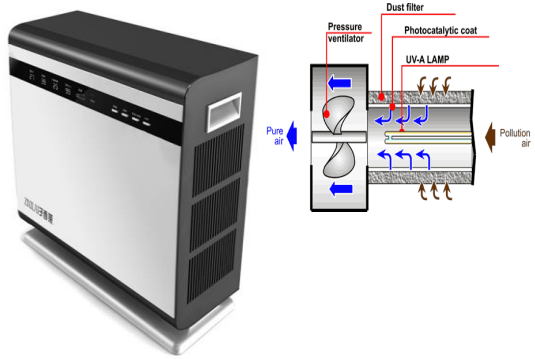
- Possible solutions
  - Source control
  - Ventilation
  - Air purification

- Our goal
  - Integration of photocatalytic reactor in ventilation systems

Photocatalysis: Applications

Water purification/desinfection

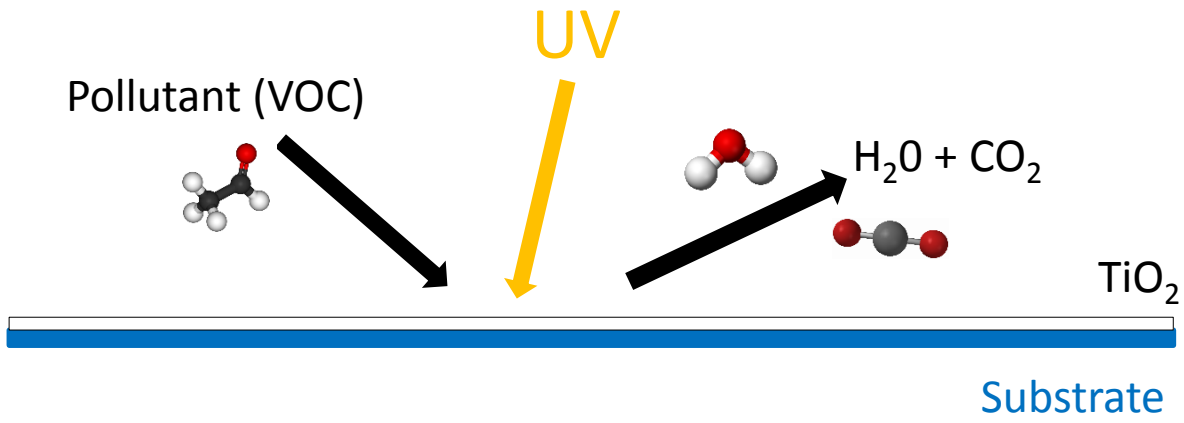
Air purification



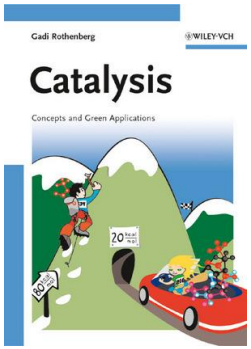
Self-cleaning materials

Photocatalysis: How does it work?

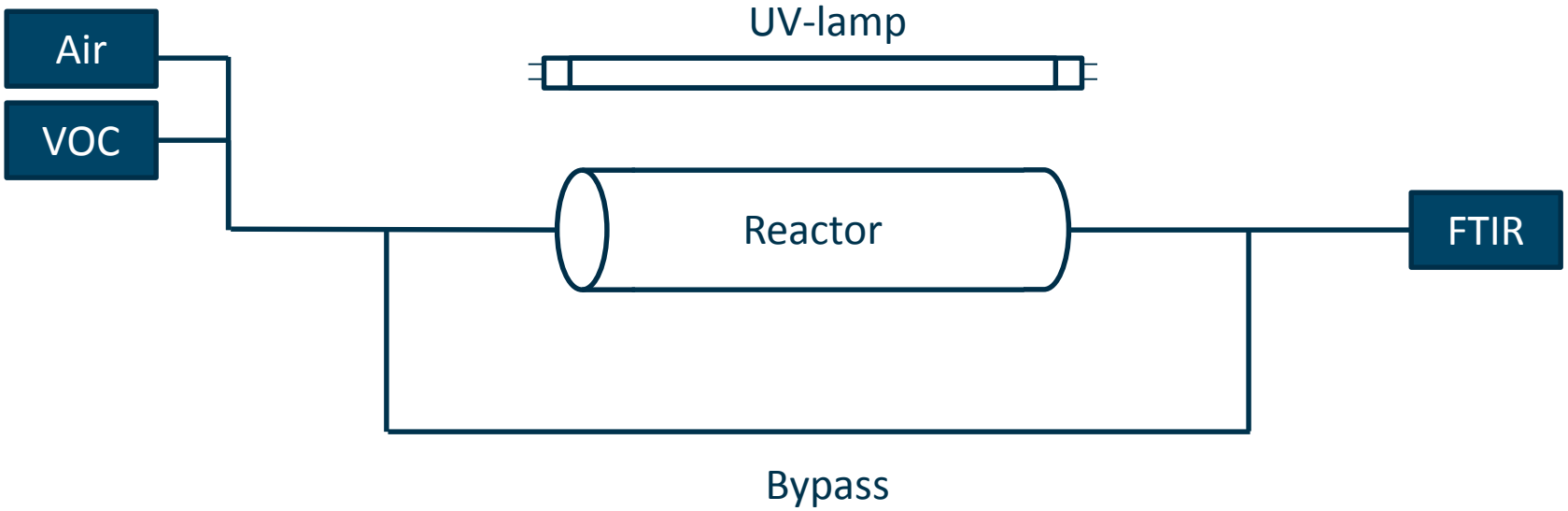
- Photocatalysis in our application:
  - Activation of a photocatalyst to degrade indoor air pollution (VOCs)
  - ***Catalyst***: increases reaction rate without being consumed



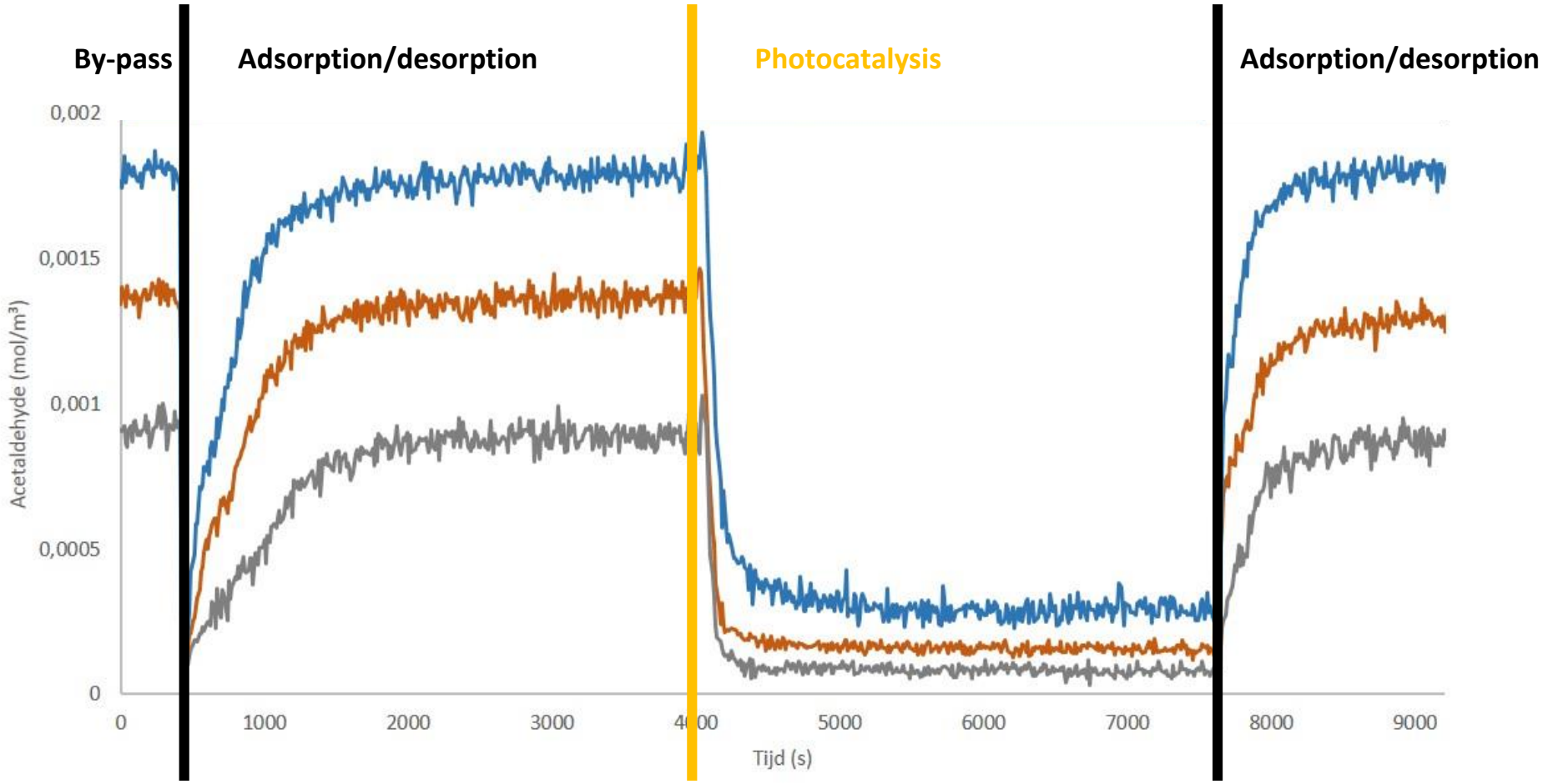
- ✓ Cost-effective
- ✓ No waste steams
- ✓ Mild reaction conditions



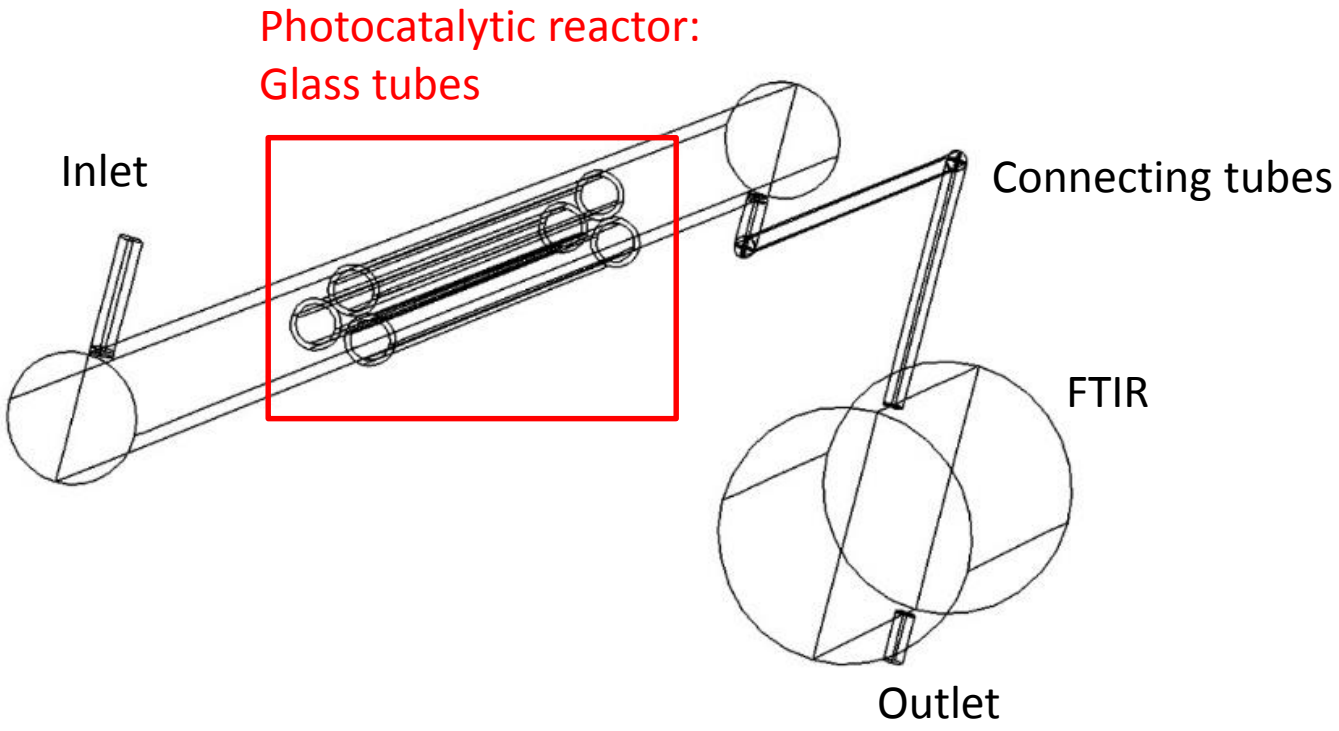
Experimental setup



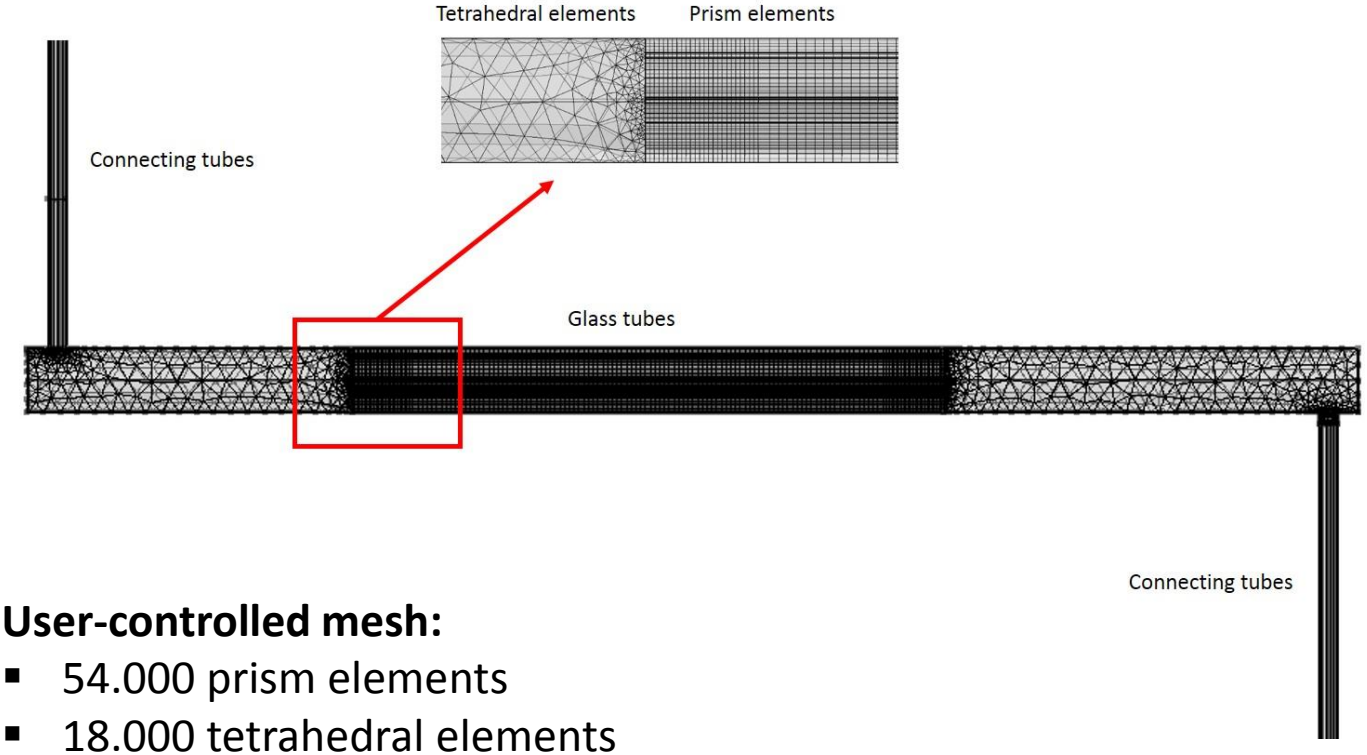
Experimental data (FTIR)



Comsol Multiphysics:
Geometry



Comsol Multiphysics:
Meshing

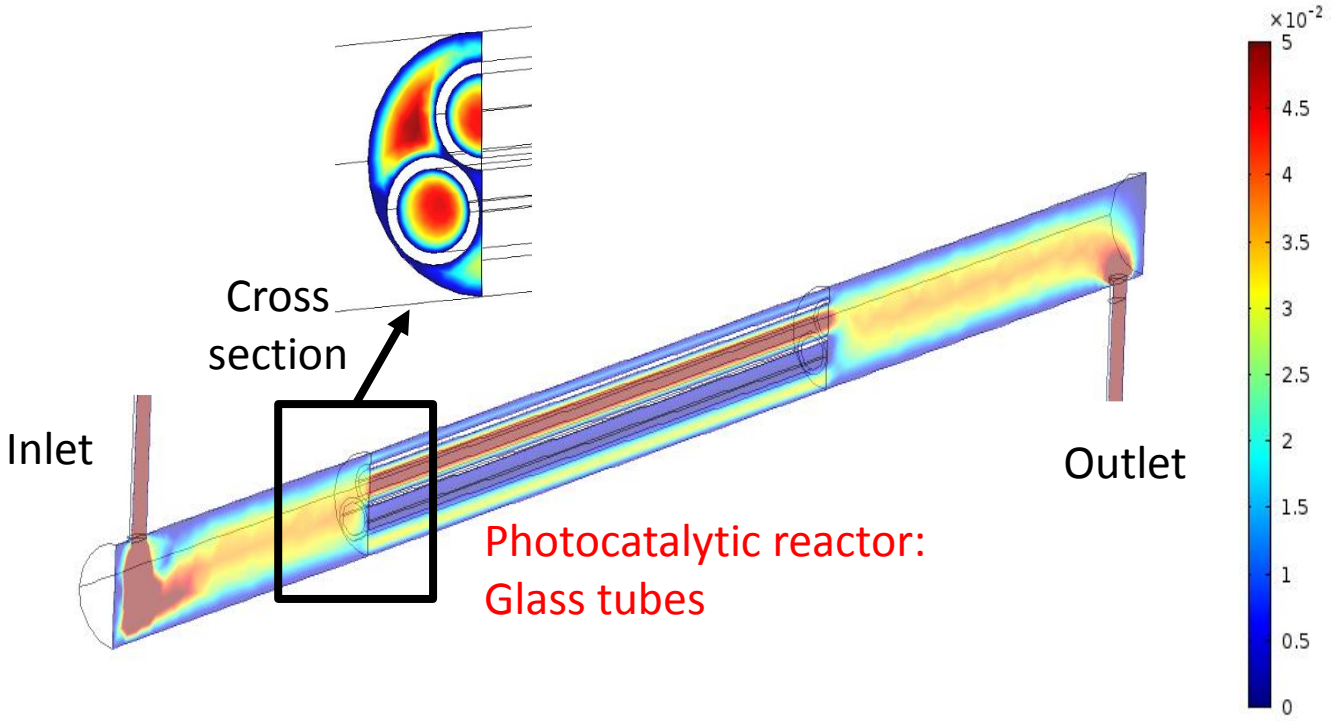


User-controlled mesh:

- 54.000 prism elements
- 18.000 tetrahedral elements

Comsol Multiphysics:
Laminar flow (spf)

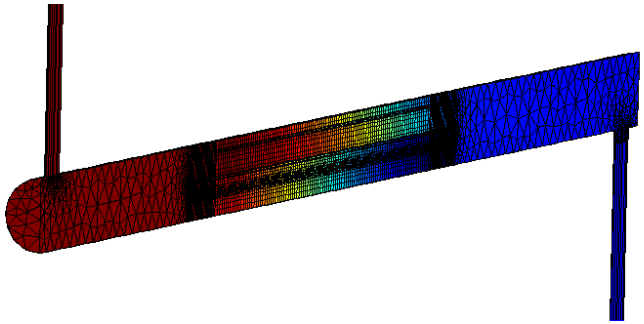
- Stationary solver:



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_{pco})
  - **Acetaldehyde surface concentration** ($C_{Acal,ads}$)

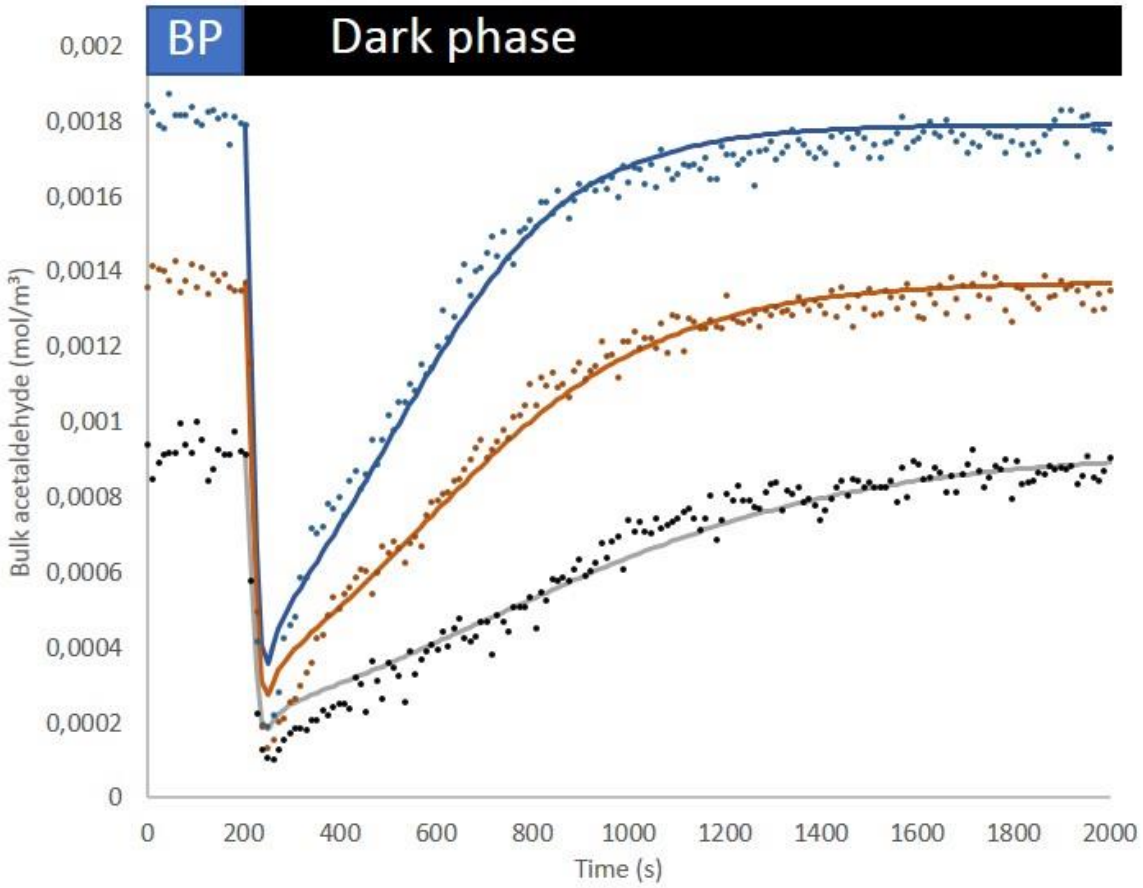
1. $R_{pco} = k_{pco} C_{Acal,ads}$
2. $\frac{\partial C_{Acal,ads}}{\partial t} = N_{ads} - N_{des} - R_{pco}$

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 *(Γ_s)*
- How?: Sparse Nonlinear OPTimizer (SNOPT) algorithm
  - To find the local minimum of a least-squares objective function

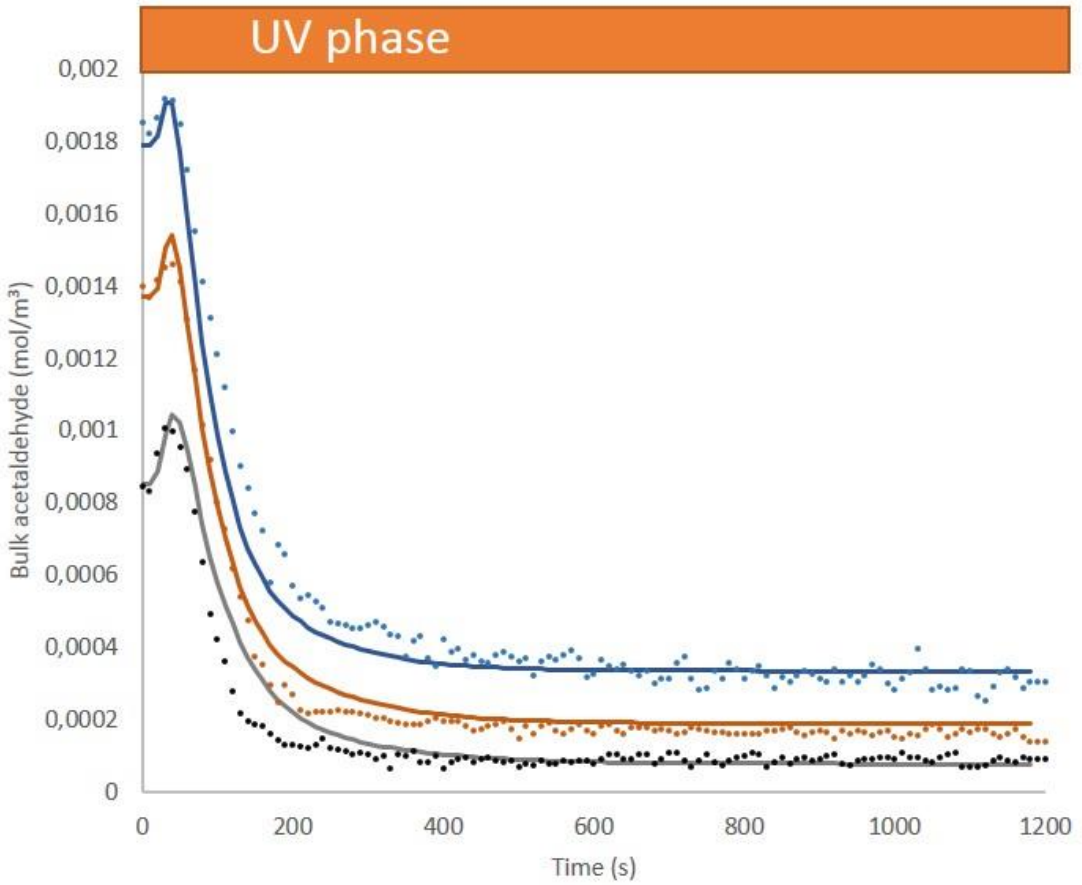
Comsol (lines) vs Experimental data (dots)

- Adsorption phase:



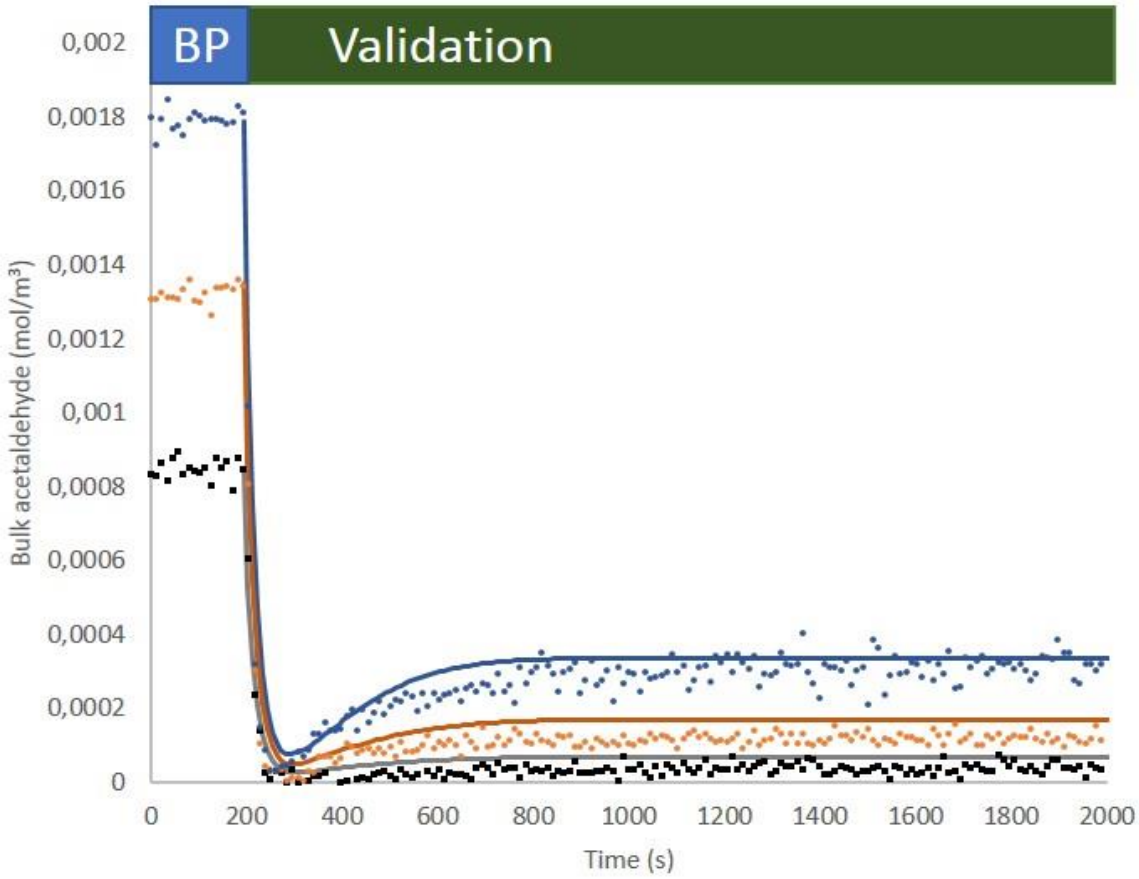
Comsol (lines) vs Experimental data (dots)

- 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

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Thank you for your attention!

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