Modeling Transient Adsorption/Desorption Behavior in a Gas Phase Photocatalytic Fiber Reactor

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Photocatalysis: principle

**Catalyst:** increases reaction rate without being consumed

**Photo-catalyst:** catalyst activated by (UV-)light

Most often titanium dioxide (TiO$_2$)
Photocatalysis: application fields

- Water purification/desinfection
- Self-cleaning materials
- Air purification
Gas phase photocatalytic fiber reactor

Inlet:
• air
• acetaldehyde
• controlled C and Q

Outlet:
(to FTIR spectroscope)

UV source

Tubular photoreactor

Introduction
Fiber reactor
Comsol model
Comsol model incl. adsorption/desorption
Conclusions
Comsol model: goals

- To model the transient, dynamic adsorption/desorption of acetaldehyde as contaminated air flows through the reactor
- To estimate the adsorption/desorption rate constants
Comsol model: geometry

Approx. 80,000 tetrahedral cells + refinement
Comsol model: Physics

- Laminar flow (Re < 800)
- Darcy equation (single-phase gas flow in a porous medium)
  - stationary solver
- Species transport in porous media (incl. free flow)
  - time dependent solver

\[ \frac{\partial C_{Acal,\text{bulk}}}{\partial t} = \nabla \cdot (D \nabla C_{Acal,\text{bulk}}) - \mathbf{u} \cdot \nabla C_{Acal,\text{bulk}} \]
Comsol results: no adsorption

- Uncoated filter - 400 cm³ min⁻¹
  - BY-PASS
  - REACTOR

- Uncoated filter - 1200 cm³ min⁻¹
  - BY-PASS
  - REACTOR
Langmuir adsorption/desorption

\[ r_{ads} = k_{ads} C_{Acal, bulk} (1 - \theta_{Acal}) \]

\[ r_{des} = k_{des} \theta_{Acal} \]

\[ \theta_{Acal} = \frac{C_{Acal, filter}}{\Gamma_{filter}} \]

\[ r_{aldol} = k_{aldol} (C_{Acal, filter})^2 \]
Comsol physics incl. adsorption/desorption

- Laminar flow (Re < 800)
- Darcy equation (single-phase gas flow in a porous medium)
  - \(\text{stationary solver}\)
- Species transport in porous media (incl. free flow)
- Domain ODE
  - \(\text{time dependent solver + optimization solver (SNOPT)}\)

\[
\frac{\partial C_{Acal,\text{bulk}}}{\partial t} = \nabla \cdot (D \nabla C_{Acal,\text{bulk}}) - \mathbf{u} \cdot \nabla C_{Acal,\text{bulk}} - r_{ads} + r_{des}
\]

\[
\frac{\partial C_{Acal,\text{filter}}}{\partial t} = r_{ads} - r_{des} - r_{aldol}
\]

\[
\text{Obj} = \sum_{t} \left( C_{Acal,\text{out,exp},t} - C_{Acal,\text{out,CFD},t} \right)^{2}
\]
Comsol results incl. adsorption/desorption

<table>
<thead>
<tr>
<th>Sample</th>
<th>Parameters from analysis (exp)</th>
<th>Parameters from Comsol optimization</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \Gamma_{\text{filter}} ) (mol kg(^{-1}))</td>
<td>( \Gamma_{\text{filter}} ) (mol kg(^{-1}))</td>
</tr>
<tr>
<td>Sample A</td>
<td>0.0126</td>
<td>0.0119</td>
</tr>
<tr>
<td>Sample B</td>
<td>0.0425</td>
<td>0.0382</td>
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</tbody>
</table>
Conclusions

• CFD/multiphysics is a versatile tool for parameter estimation:
  • Time dependent solution
  • Spatial distribution
  • Implicit correction for air displacement
  • Extension of Langmuir model

1 vs several experiments