Sustainable Energy, Air & Water Technology
University of Antwerp

COMSOL CONFERENCE
2015 GRENOBLE

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

Siegfried Denys, Jeroen van Walsem

Siegfried.denys@uantwerpen.be

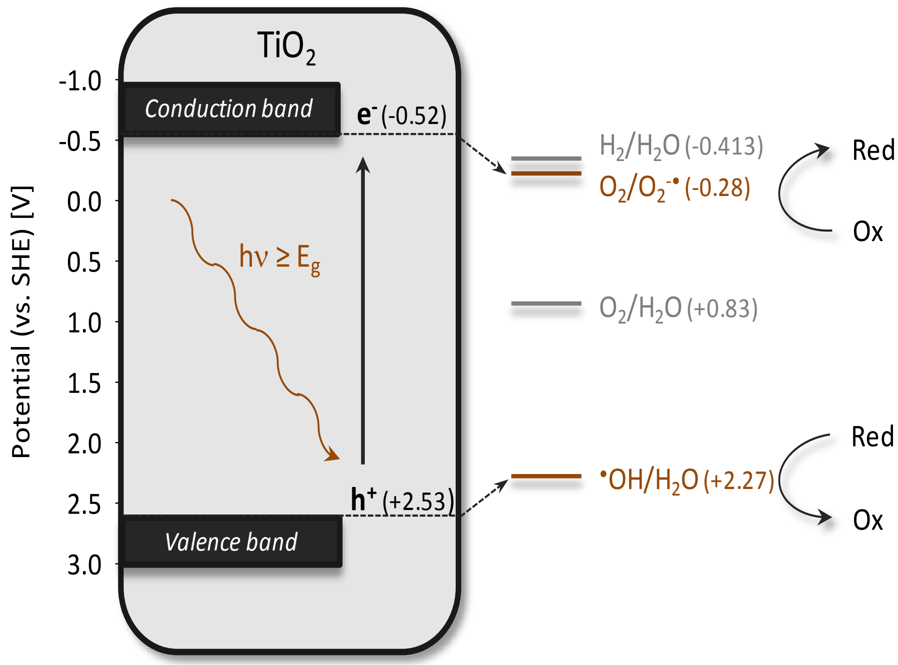
University of Antwerp

Photocatalysis: principle

Catalyst: increases reaction rate without being consumed

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

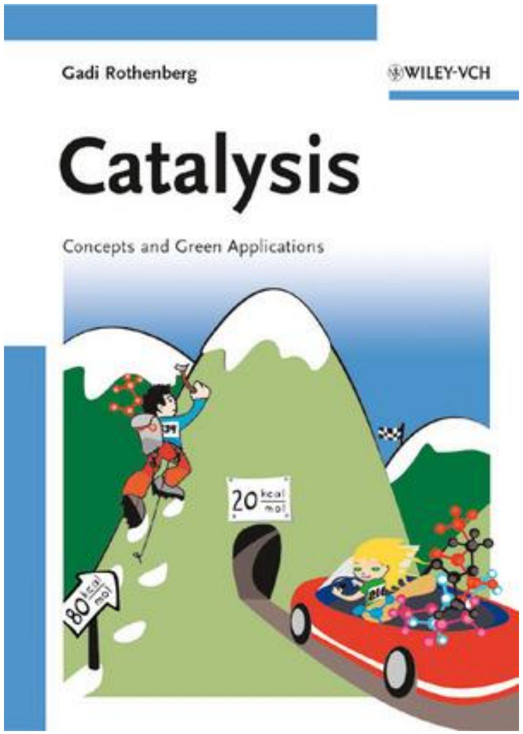
Most often titanium dioxide (TiO_2)



VOC's

↓

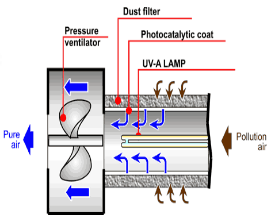
H_2O, CO_2



Photocatalysis: application fields

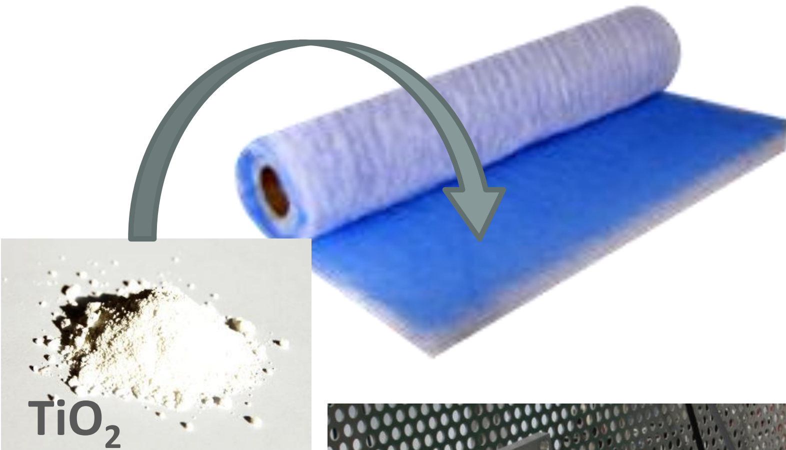
Water purification/desinfection

Air purification



Self-cleaning materials

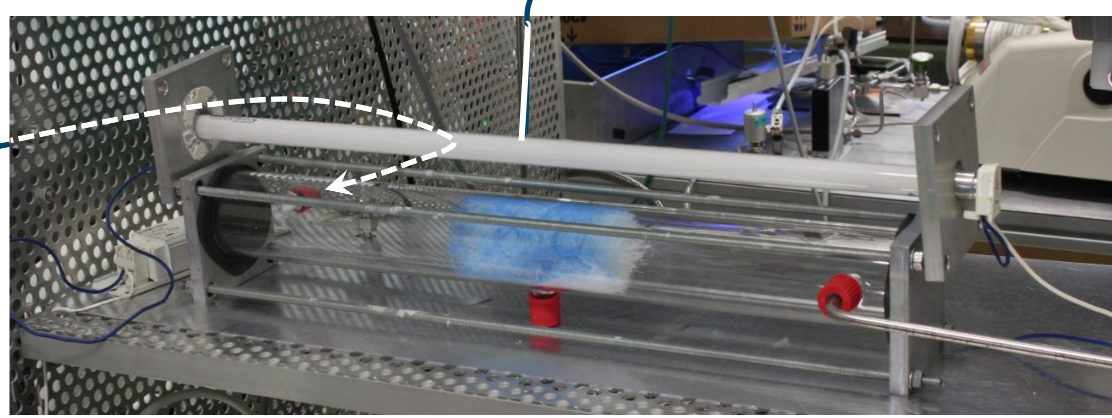
Gas phase photocatalytic fiber reactor



UV source

Inlet:

- air
- acetaldehyde
- controlled *C* and *Q*

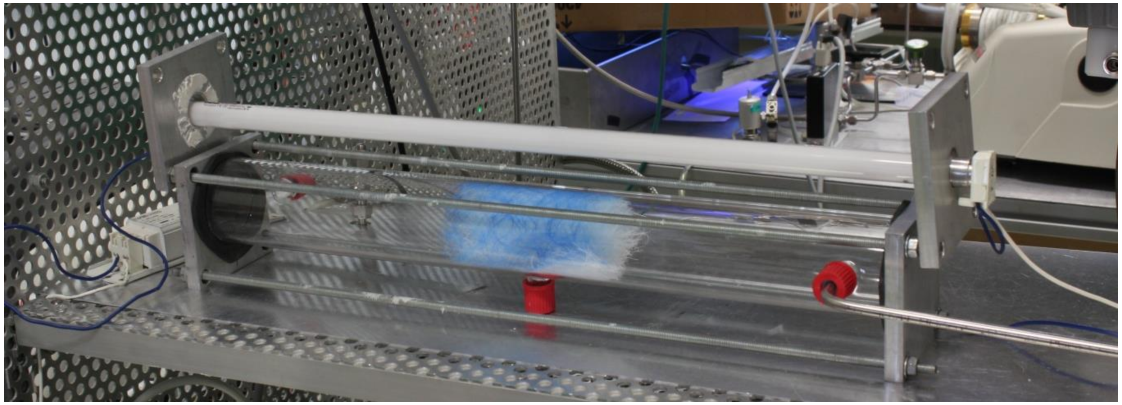


Tubular photoreactor

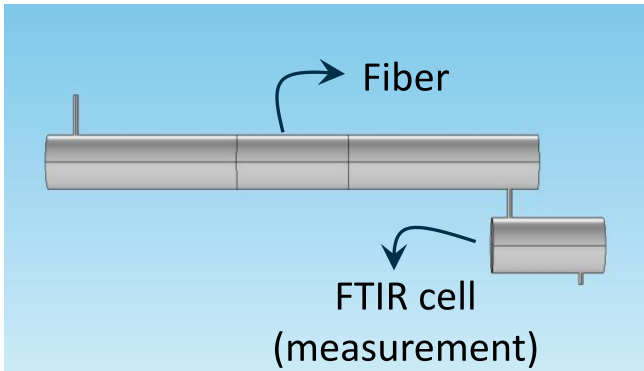
Outlet:
(to FTIR spectroscope)

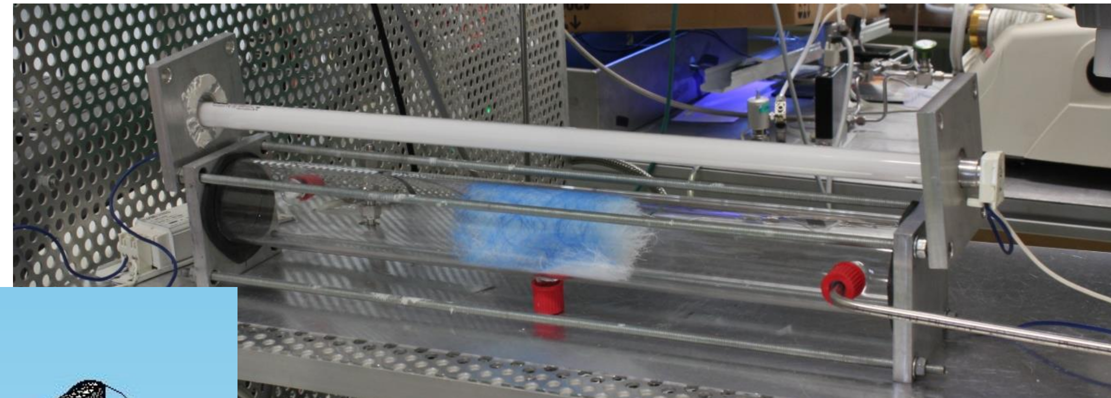
Comsol model: goals

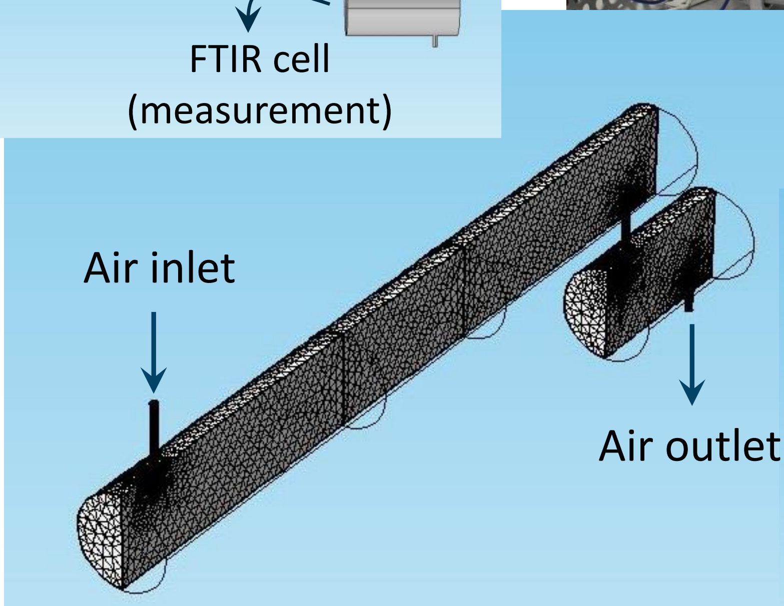
- To **model the transient, dynamic adsorption/desorption** of acetaldehyde as contaminated air flows through the reactor
- To **estimate** the adsorption/desorption **rate constants**

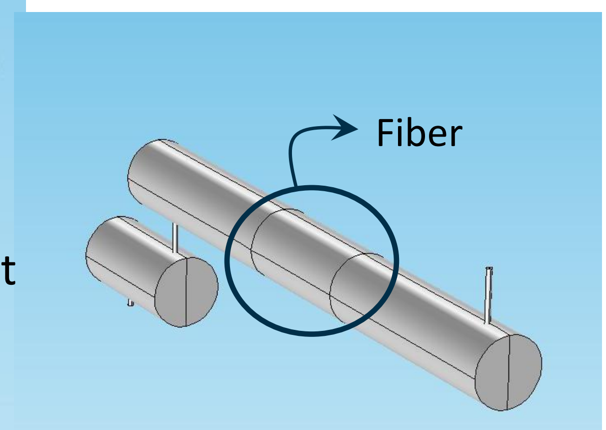


Comsol model: geometry









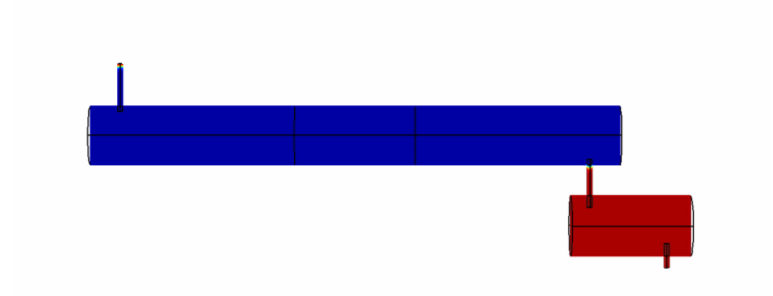
Approx . 80,000 tetrahedral cells + refinement

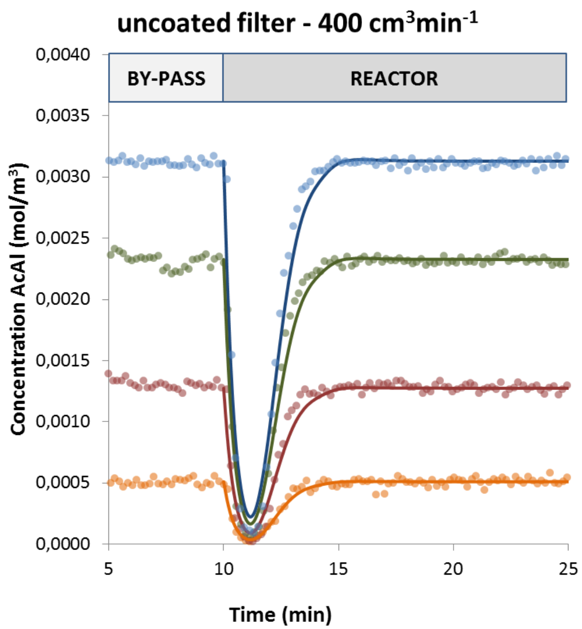
Comsol model: Physics

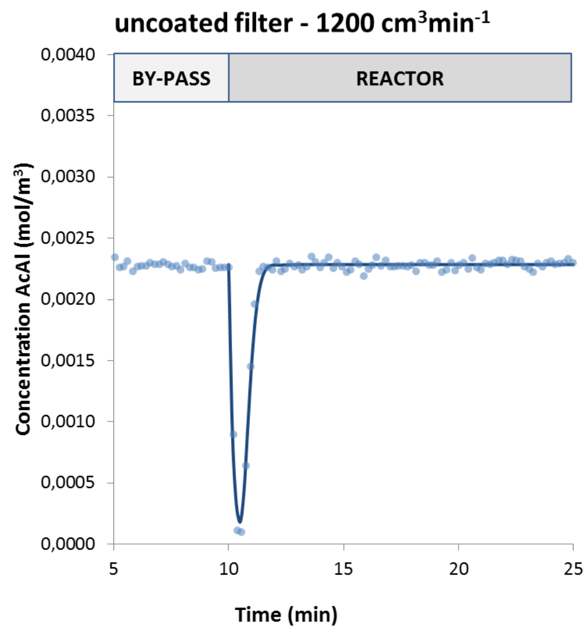
- Laminar flow (Re < 800)
- Darcy equation (single-phase gas flow in a porous medium)
  - ☞ **stationary solver**
- Species transport in porous media (incl. free flow)
  - ☞ **time dependent solver**

$$\frac{\partial C_{Acal,bulk}}{\partial t} = \nabla \cdot \left(D \nabla C_{Acal,bulk} \right) - \mathbf{u} \cdot \nabla C_{Acal,bulk}$$

Comsol results: no adsorption





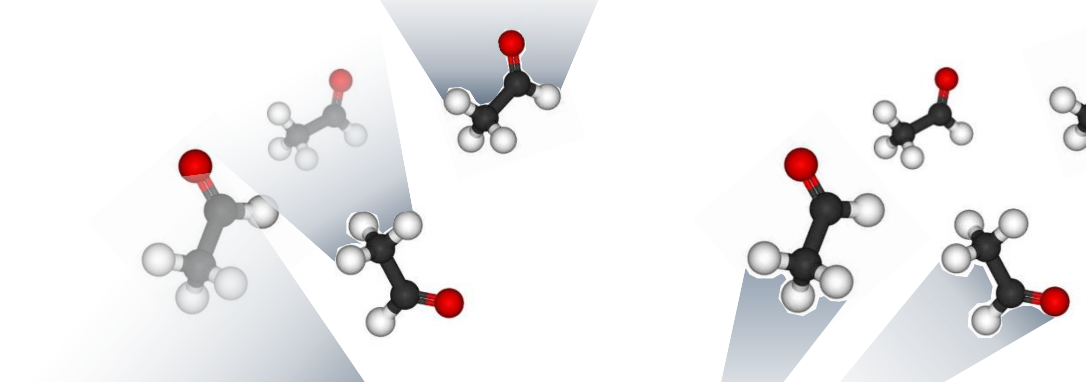


Langmuir adsorption/desorption

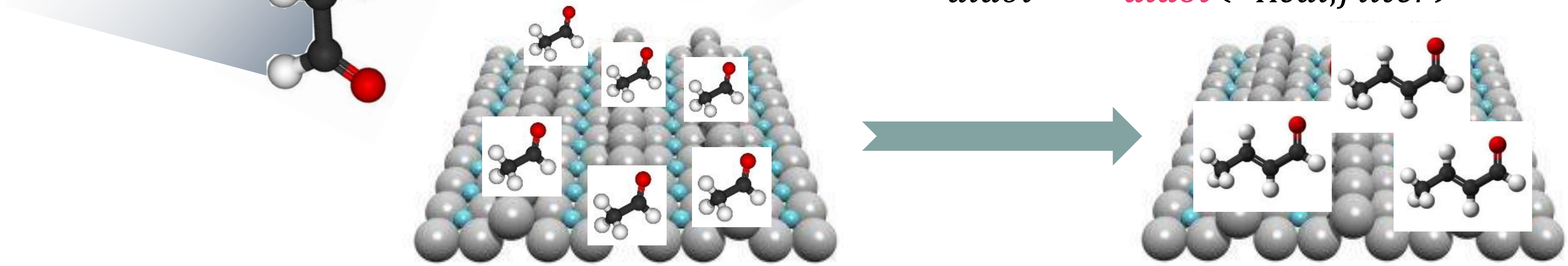
$$r_{ads} = \boldsymbol{k_{ads}} C_{Acal,bulk}(1 - \theta_{Acal})$$

$$r_{des} = \boldsymbol{k_{des}} \theta_{Acal}$$

$$\theta_{Acal} = \frac{C_{Acal,filter}}{\Gamma_{filter}}$$



$$r_{aldol} = \boldsymbol{k_{aldol}} (C_{Acal,filter})^2$$



Comsol physics incl. adsorption/desorption

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

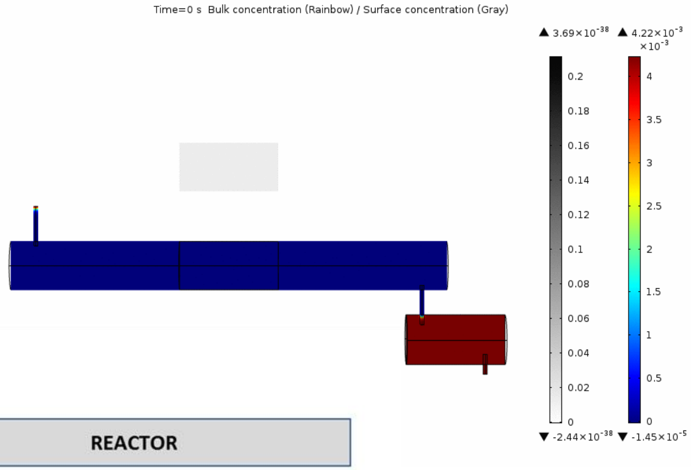
$$\frac{\partial C_{Acal,bulk}}{\partial t} = \nabla \cdot \left(D \nabla C_{Acal,bulk}\right) - \mathbf{u} \cdot \nabla C_{Acal,bulk} - r_{ads} + r_{des}$$

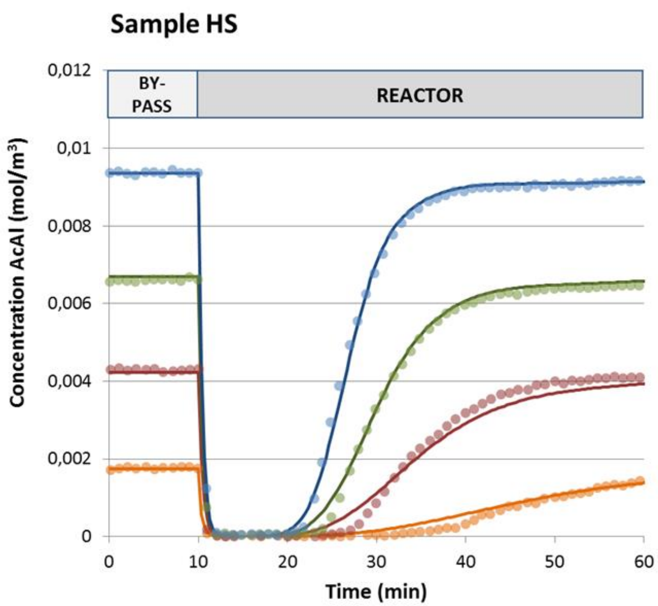
$$\frac{\partial C_{Acal,filter}}{\partial t} = r_{ads} - r_{des} - r_{aldol}$$

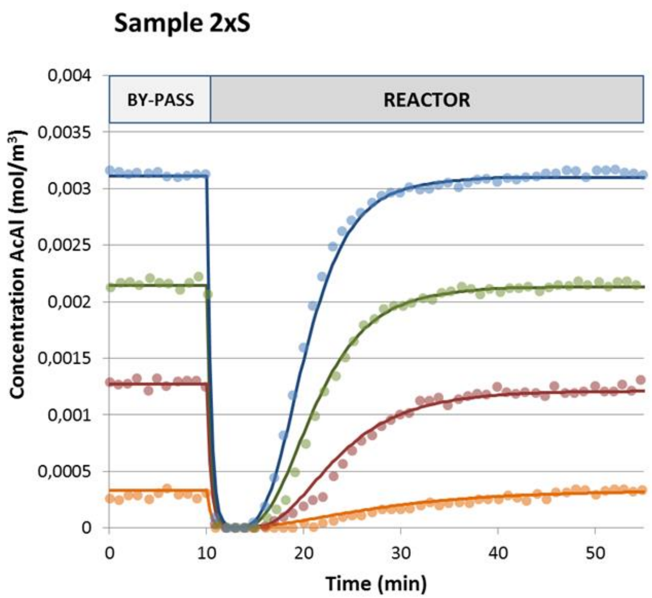
$$Obj = \sum_{t} \left(C_{Acal,out,exp,t} - C_{Acal,out,CFD,t}\right)^2$$

Comsol results incl. adsorption/desorption

	Parameters from analysis (exp)		Parameters from Comsol optimization	
	Γ_{filter} (mol kg^{-1})	K (m^3 mol^{-1})	Γ_{filter} (mol kg^{-1})	K (m^3 mol^{-1})
Sample A	0.0126	255	0.0119	220
Sample B	0.0425	222	0.0382	221







Conclusions

- CFD/multiphysics is a versatile tool for parameter estimation:
  - Time dependent solution
  - Spatial distribution

    1 vs several experiments
  - Implicit correction for air displacement
  - Extension of Langmuir model