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

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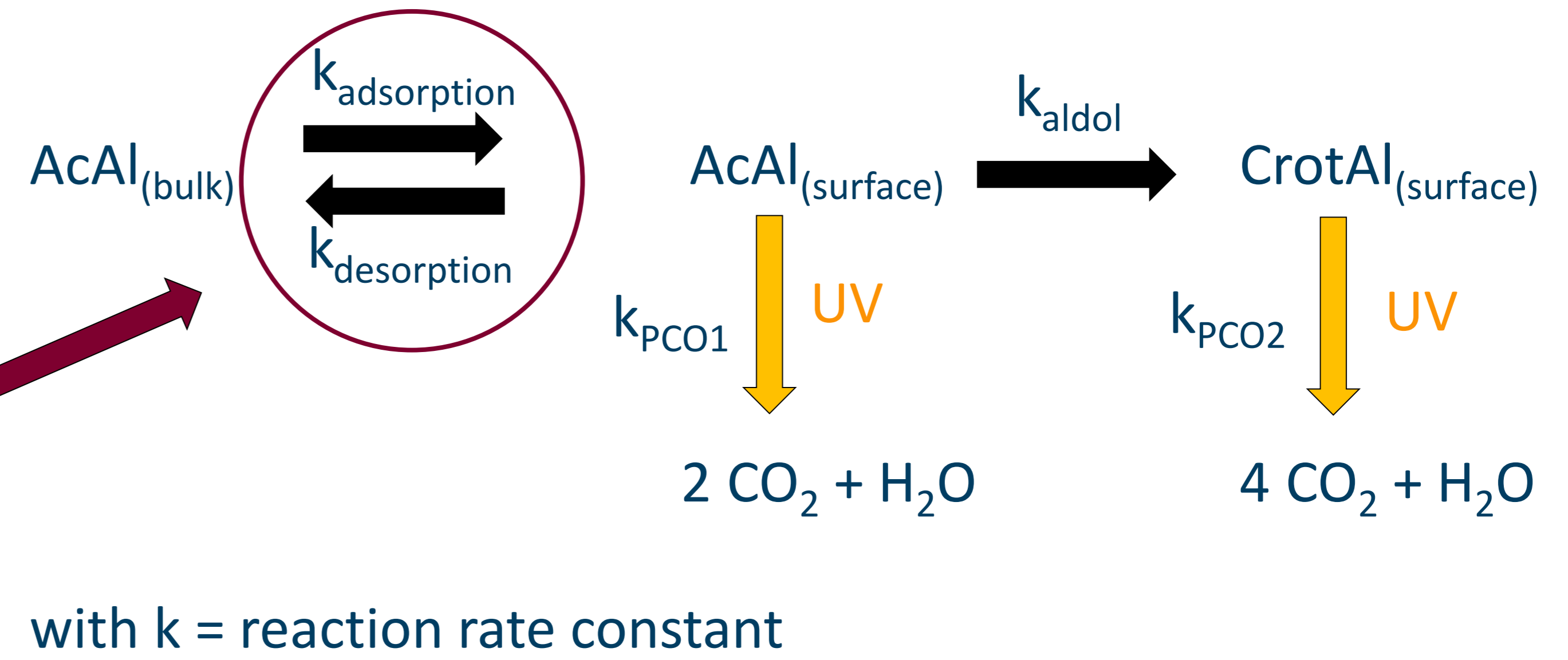
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Introduction

Goal : Abatement of indoor air pollution by the integration of a photocatalytic (PCO) TiO_2 coated reactor in HVAC systems

$$Pollutant\ (VOC) \xrightarrow{\ UV\ } H_2O + CO_2$$

How? : Estimating the adsorption/desorption parameters as vital information for the design and development of the reactor

## Reaction kinetics of PCO acetaldehyde mineralization

$$AcAl_{(bulk)} \underset{k_{desorption}}{\overset{k_{adsorption}}{\rightleftharpoons}} AcAl_{(surface)} \xrightarrow{k_{aldol}} CrotAl_{(surface)}$$

$AcAl_{(surface)}$ with k_{PCO1} UV → $2\ CO_2 + H_2O$

$CrotAl_{(surface)}$ with k_{PCO2} UV → $4\ CO_2 + H_2O$

with k = reaction rate constant

3D plot of the acetaldehyde concentration in a gas phase PCO fiber reactor

Acetaldehyde bulk concentration (**AcAl_bulk**) at time 17 minutes

FTIR cel (measurement)
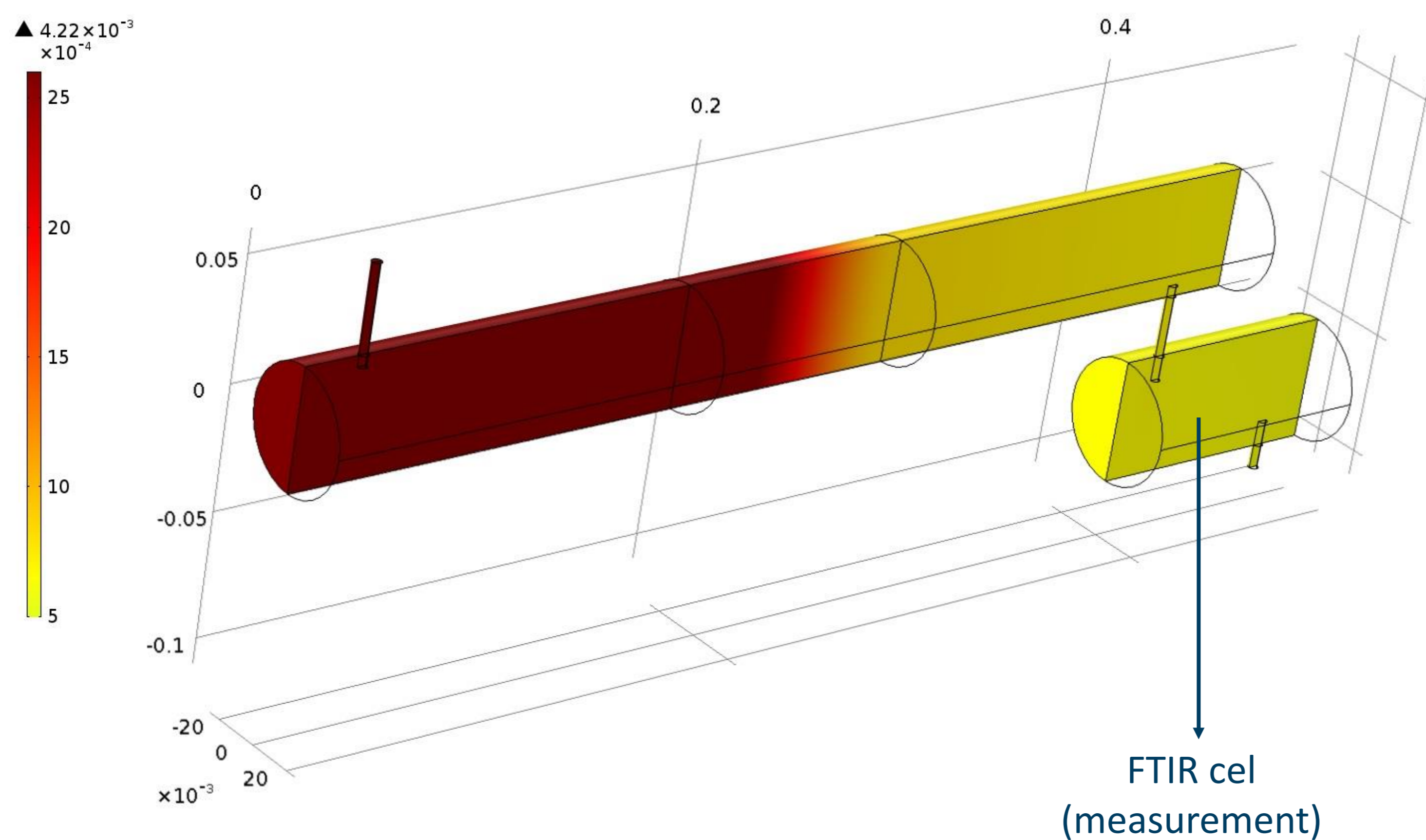
Acetaldehyde surface concentration (**AcAl_surface**) at time 17 minutes

Inlet   Fiber reactor   Outlet
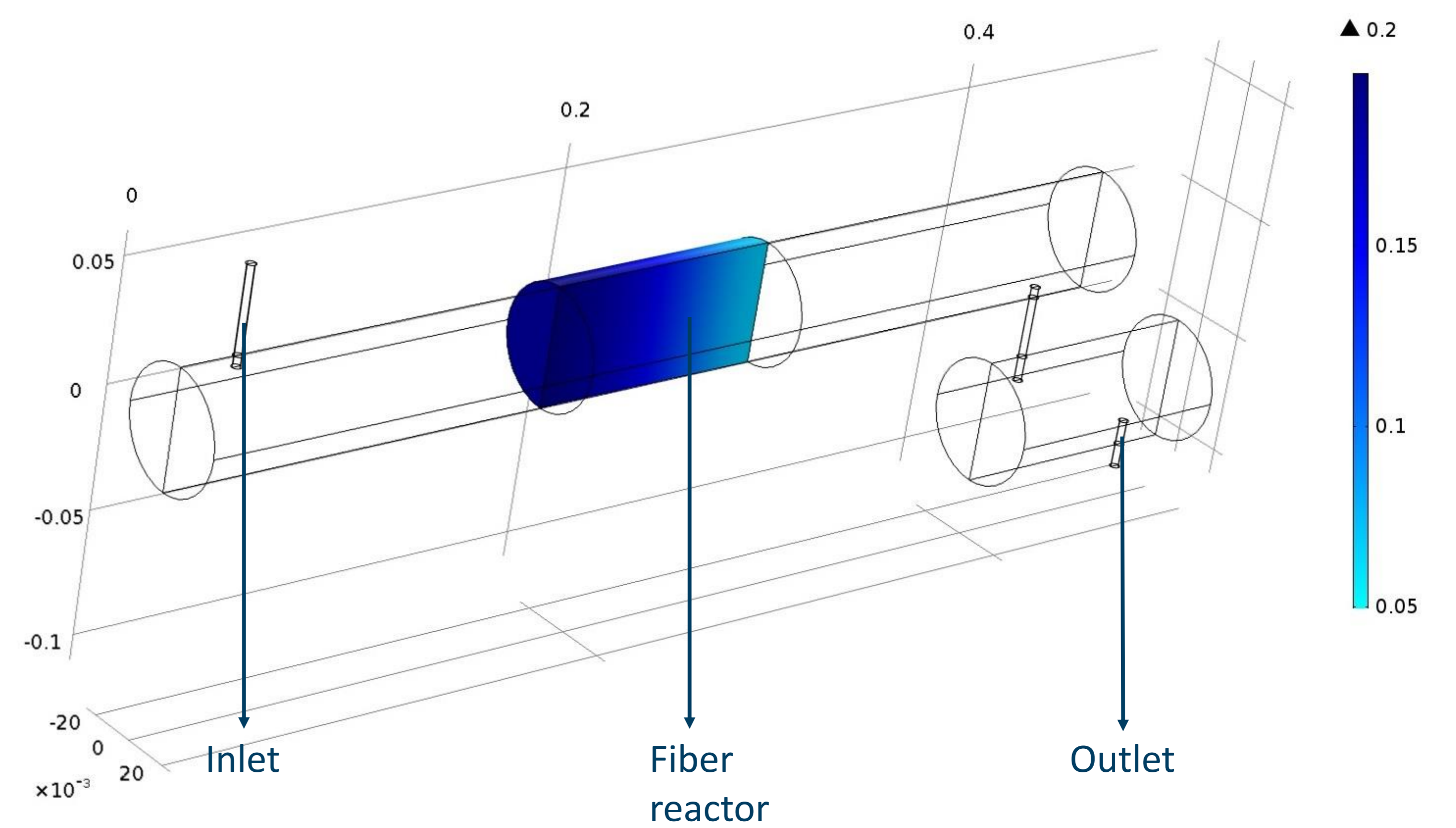
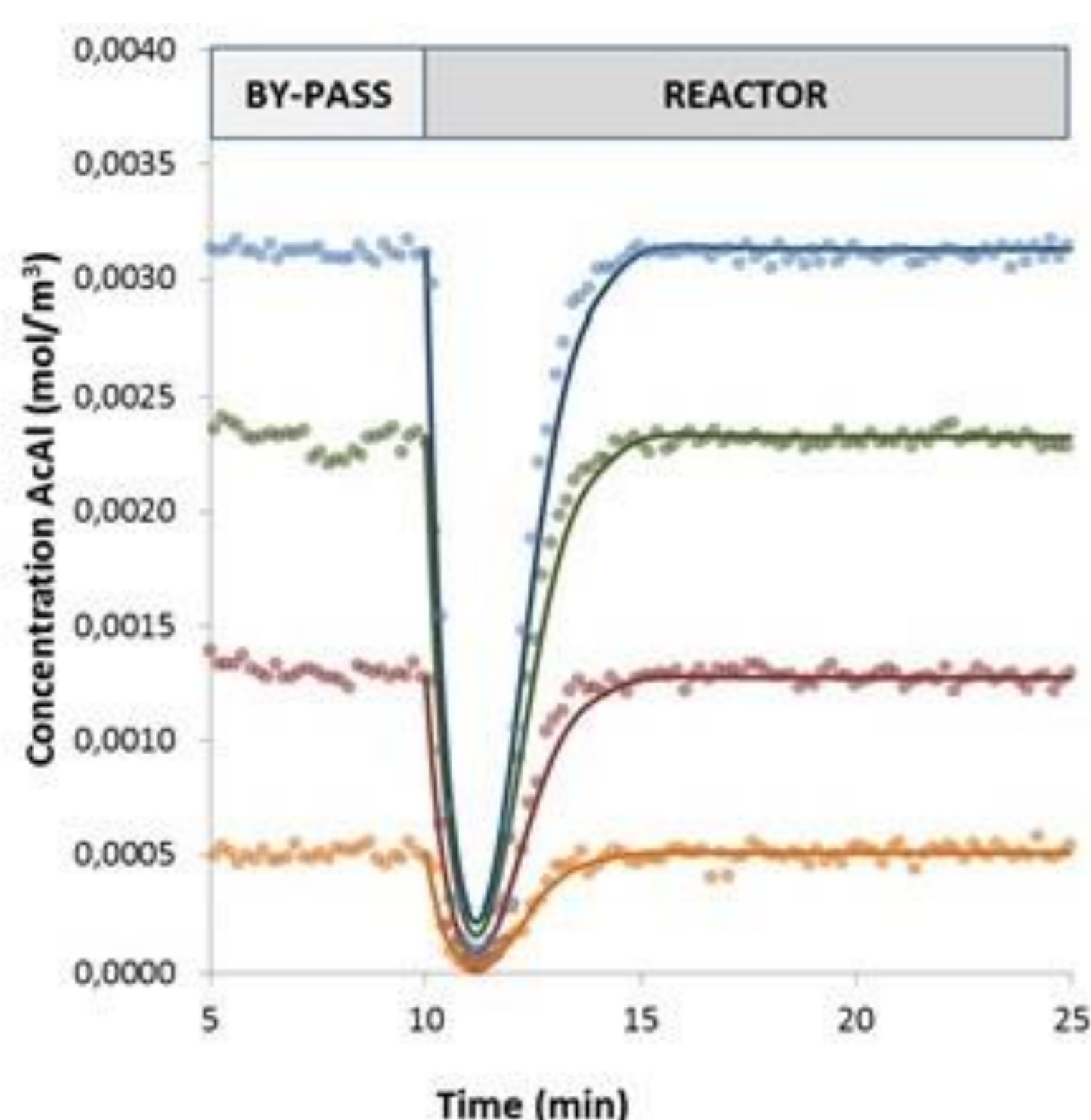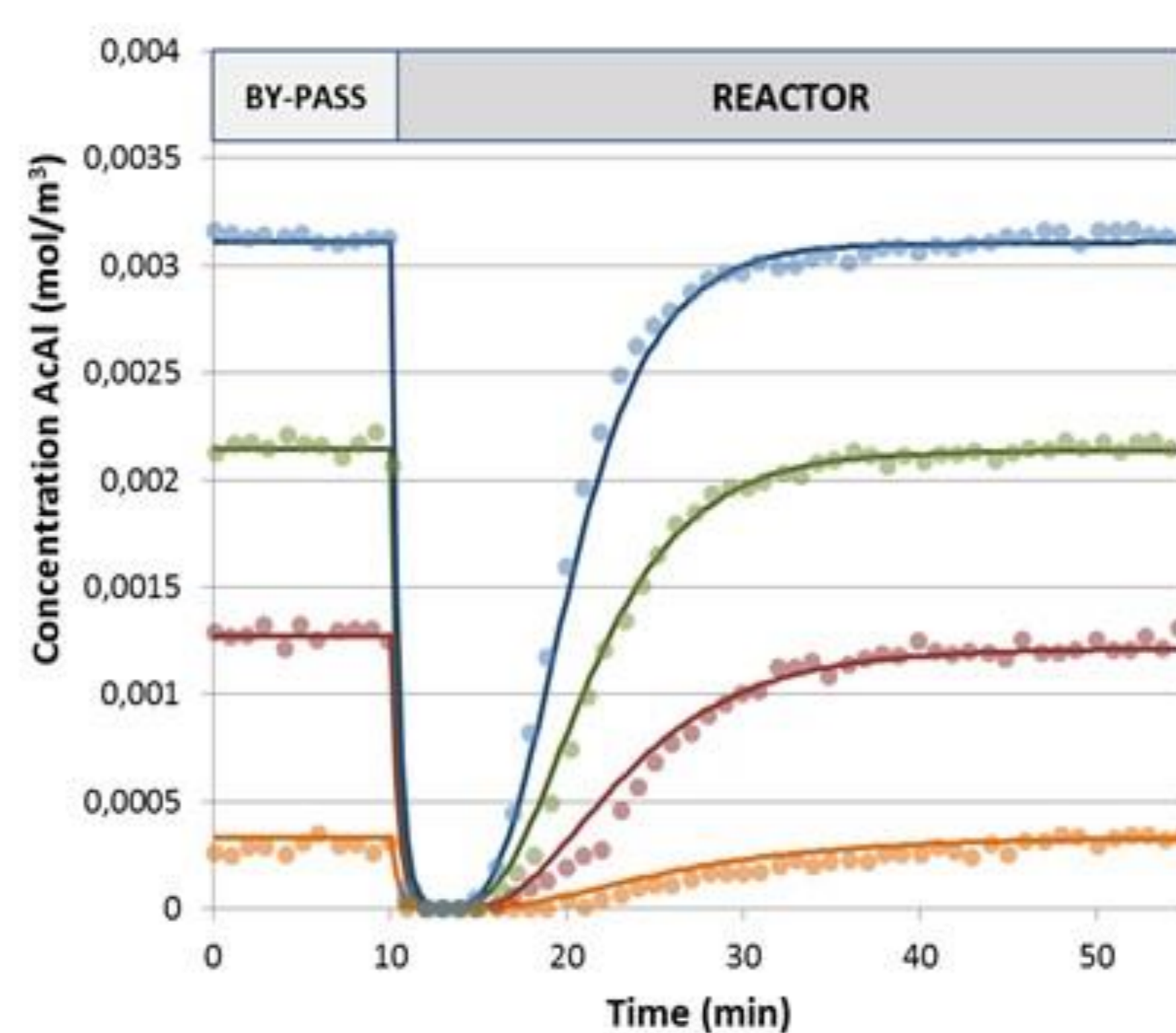## Using experimental data for parameter estimation

Goal : Determing the kinetic parameters $k_{adsorption}$, $k_{desorption}$, Γ_{filter} using Comsol optimization module in junction with the CFD calculations

Adsorption of acetaldehyde on uncoated fibers

VERSUS

Adsorption of acetaldehyde on TiO_2 coated fibers

Optimized $k_{adsorption}$ $k_{desorption}$ Γ_{filter}

CFD is useful to unravel adsorption/desorption behavior and to study the photocatalytic reaction mechanism