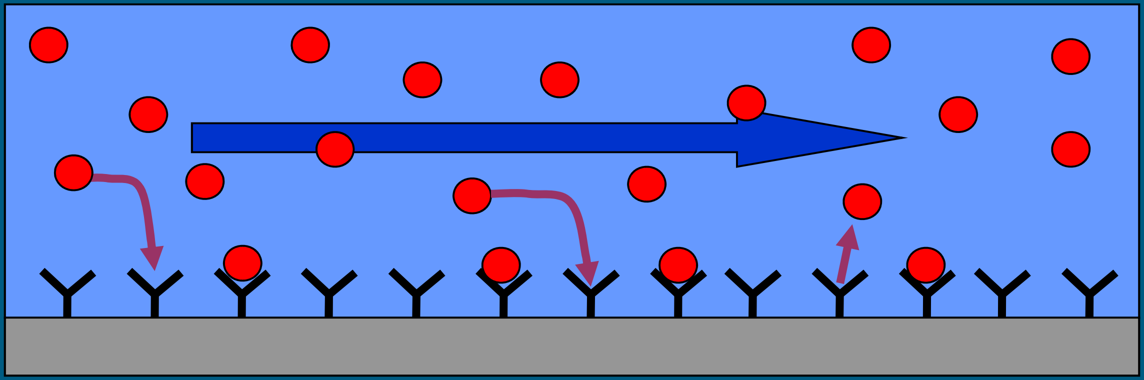
Presented at the COMSOL Conference 2009 Milan

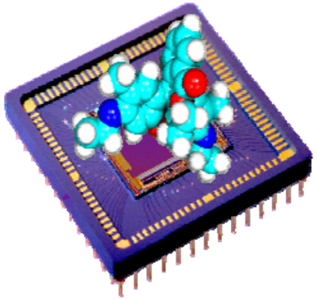
Mitglied der Helmholtz-Gemeinschaft

Chemical Reactions in a µ-fluidic T-Sensor: Numerical Comparison of 2D and 3D Models

15 October 2009 | Remo Winz



The Cµ Research Group



Why Cµ was formed:

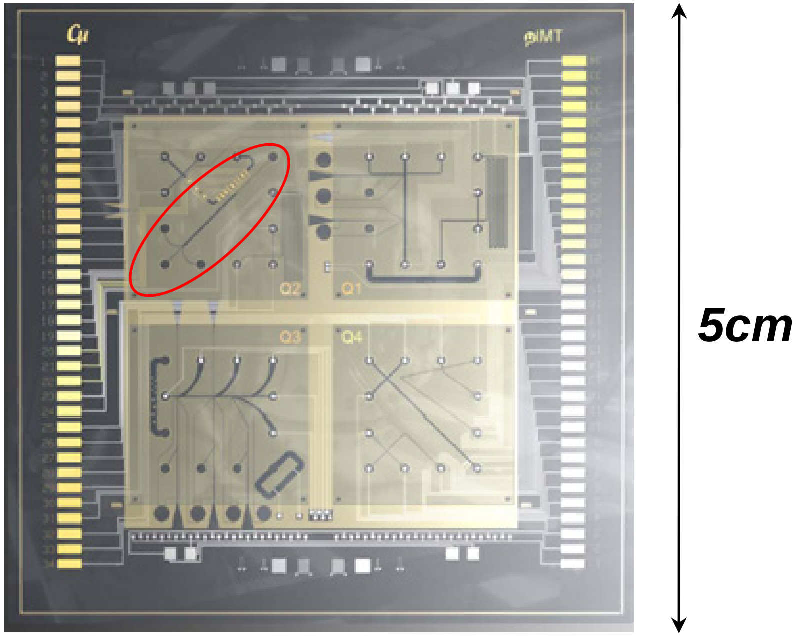
- focus & merge expertise (chemistry, microsystems)

Cµ mission:

- explore chemical processes under develop of intelligent microsystem devices e.g. for lab-on-chip technology.

Lab-on-Chip Systems:

Combining fluidic parts with (electro-) analytical ones

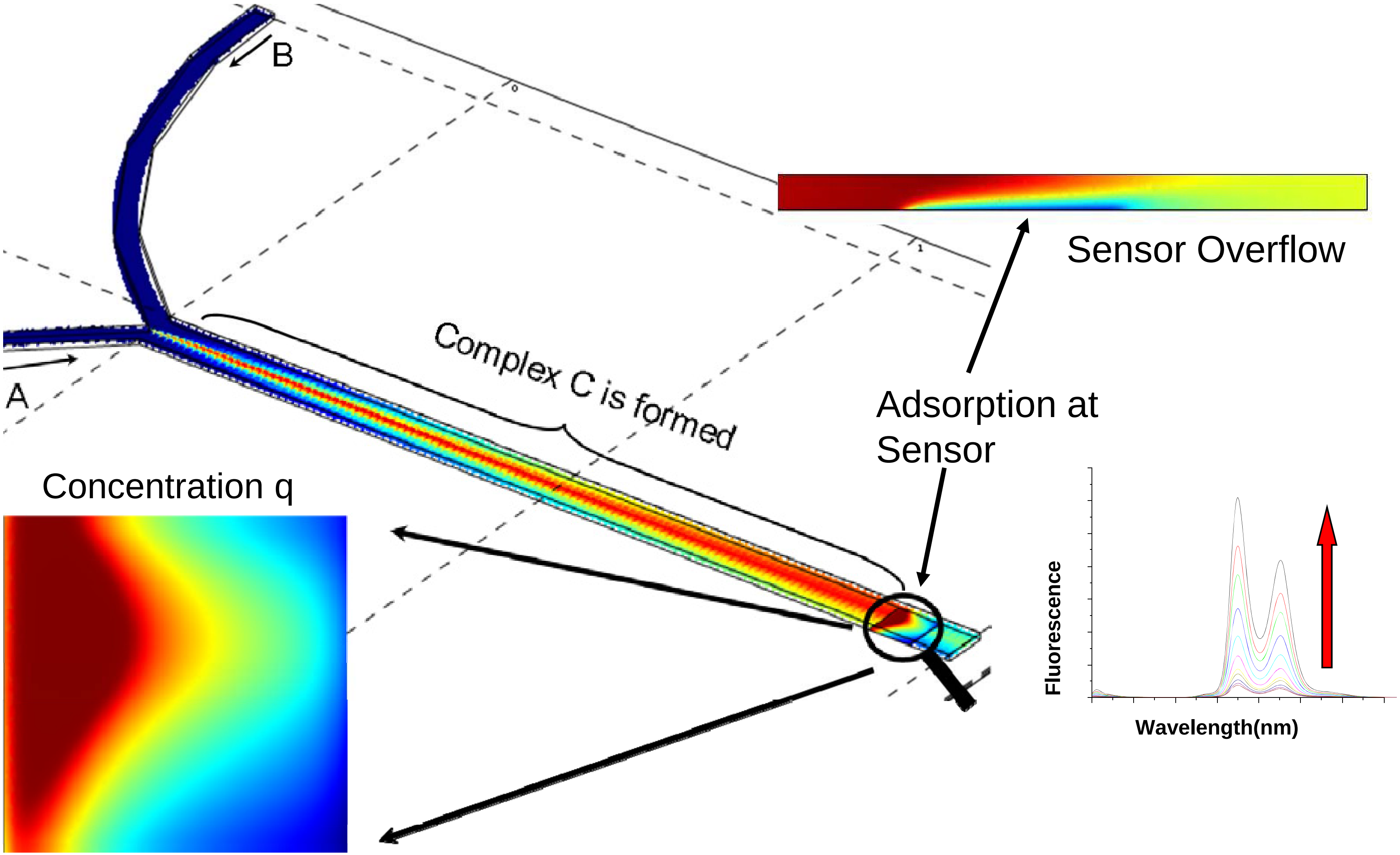


Fluidic Microchip, by Cµ-team Prof. Dr. M. Böhm, Nov. 2005

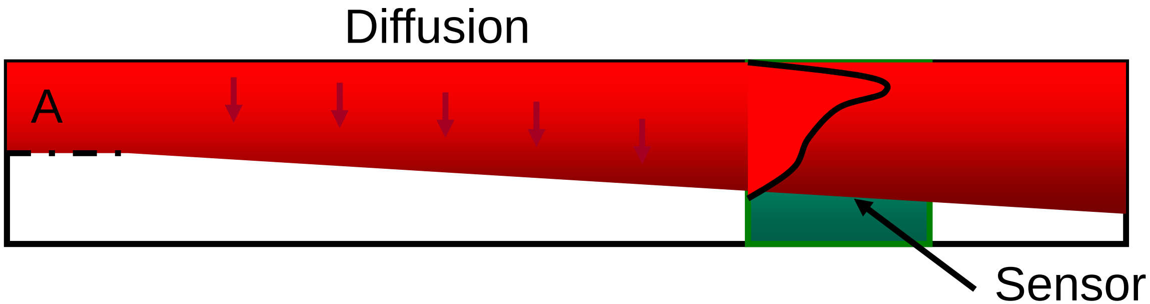
5cm

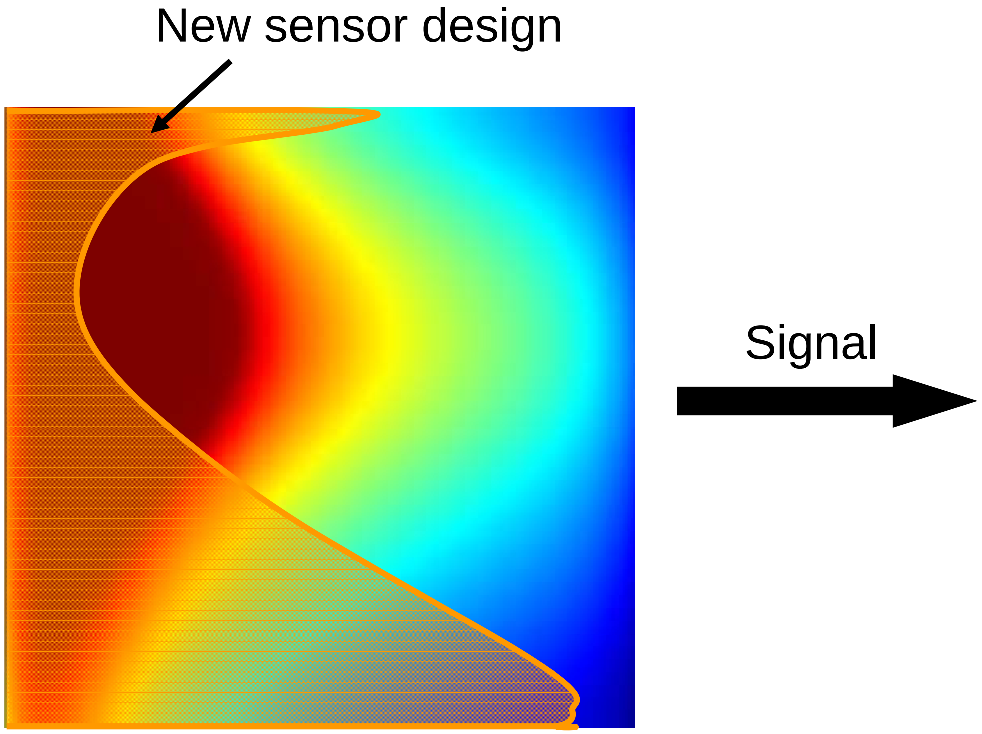
Content

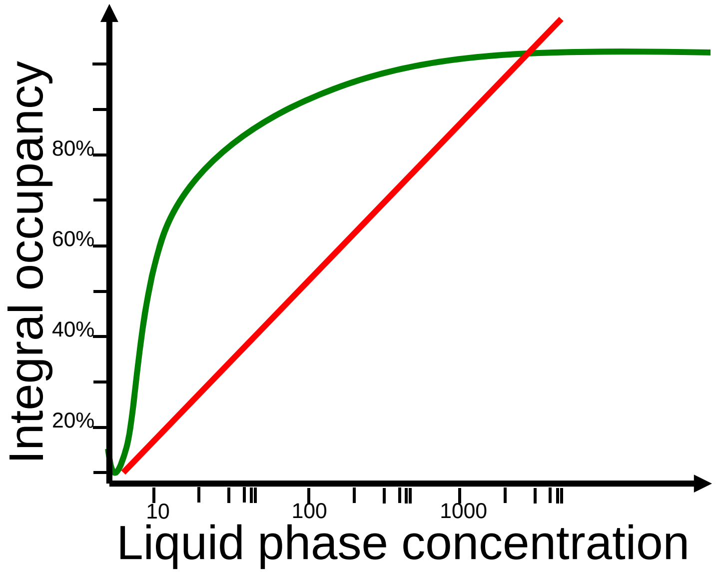
3D T-Sensor with Reaction



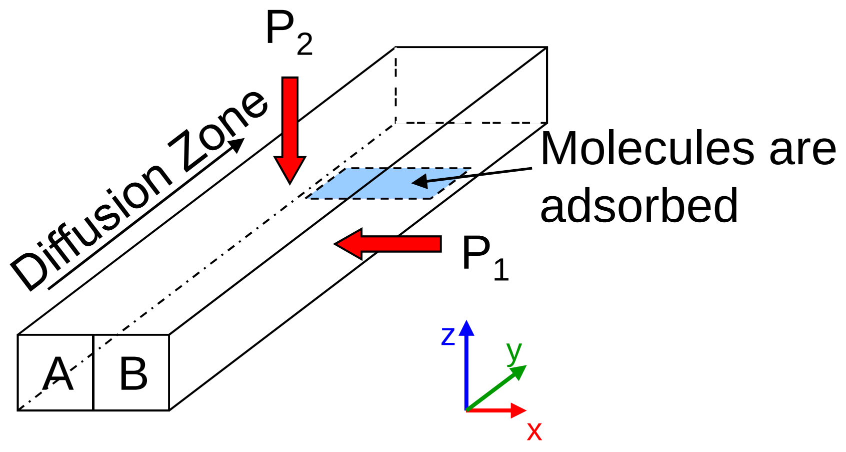
Sensor Design

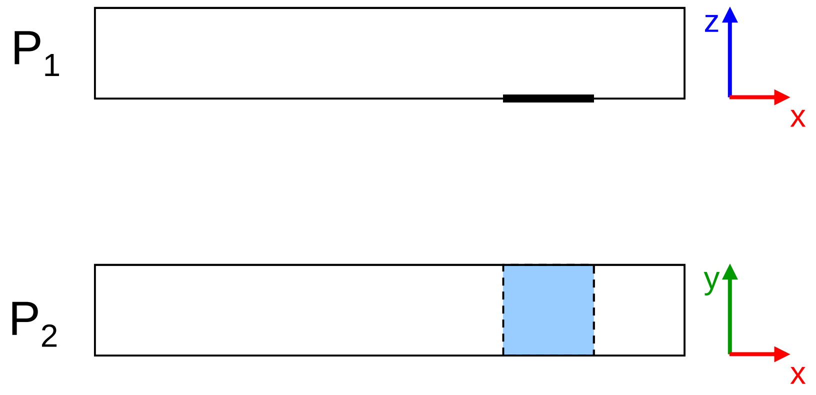




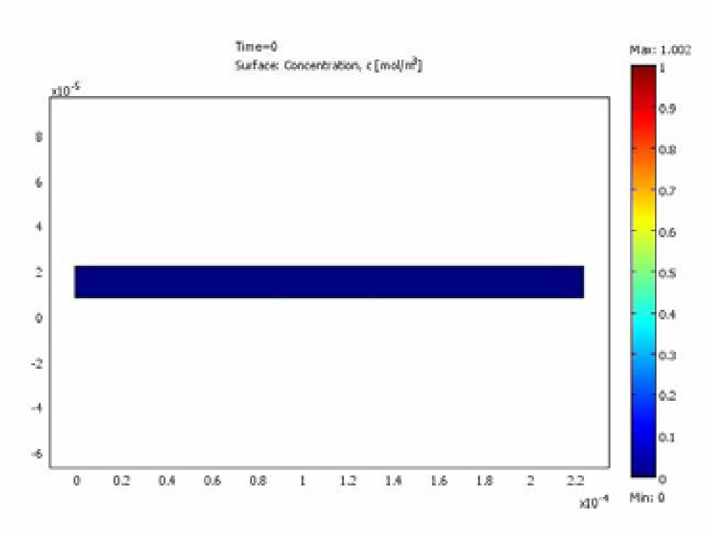


Projections from 3D to 2D

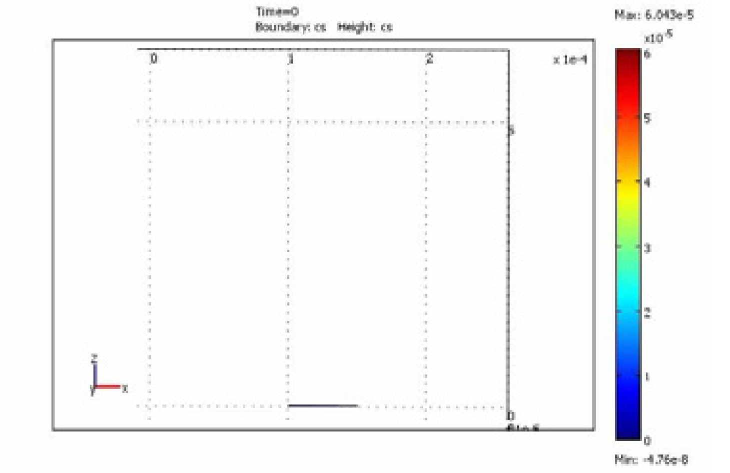




Projection P_1:

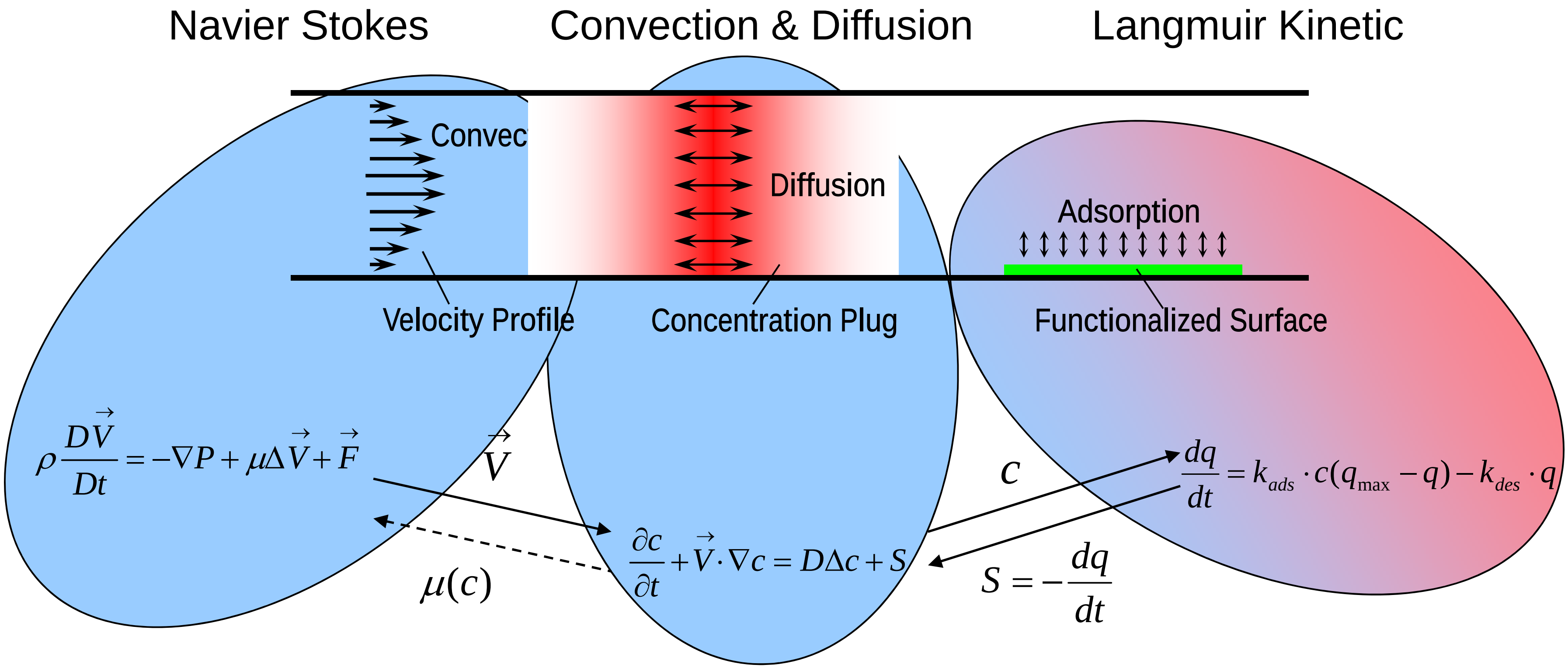


Sensor Load:



Winz et. al. [2007]

The Mathematical Model



$$\rho \frac{D\vec{V}}{Dt} = -\nabla P + \mu \Delta \vec{V} + \vec{F}$$

$$\frac{\partial c}{\partial t} + \vec{V} \cdot \nabla c = D \Delta c + S$$

$$\frac{dq}{dt} = k_{ads} \cdot c(q_{\max} - q) - k_{des} \cdot q$$

$$S = -\frac{dq}{dt}$$

Diffusion:	0.45e-9 m²/s	Inlet Concentration:	1e-3 mol/m³
Velocity:	6.6e-4 m/s	Receptors density:	3.32e-6 mol/m²
Adsorption:	4.4e4 m³/mol/s		≈ 2 rec./nm²
Desorption:	1e-1 1/s	Degrees of Freedom:	~ 650.000 (P_2)

Reaction, Film Diffusion and Adsorption

Reaction Equation

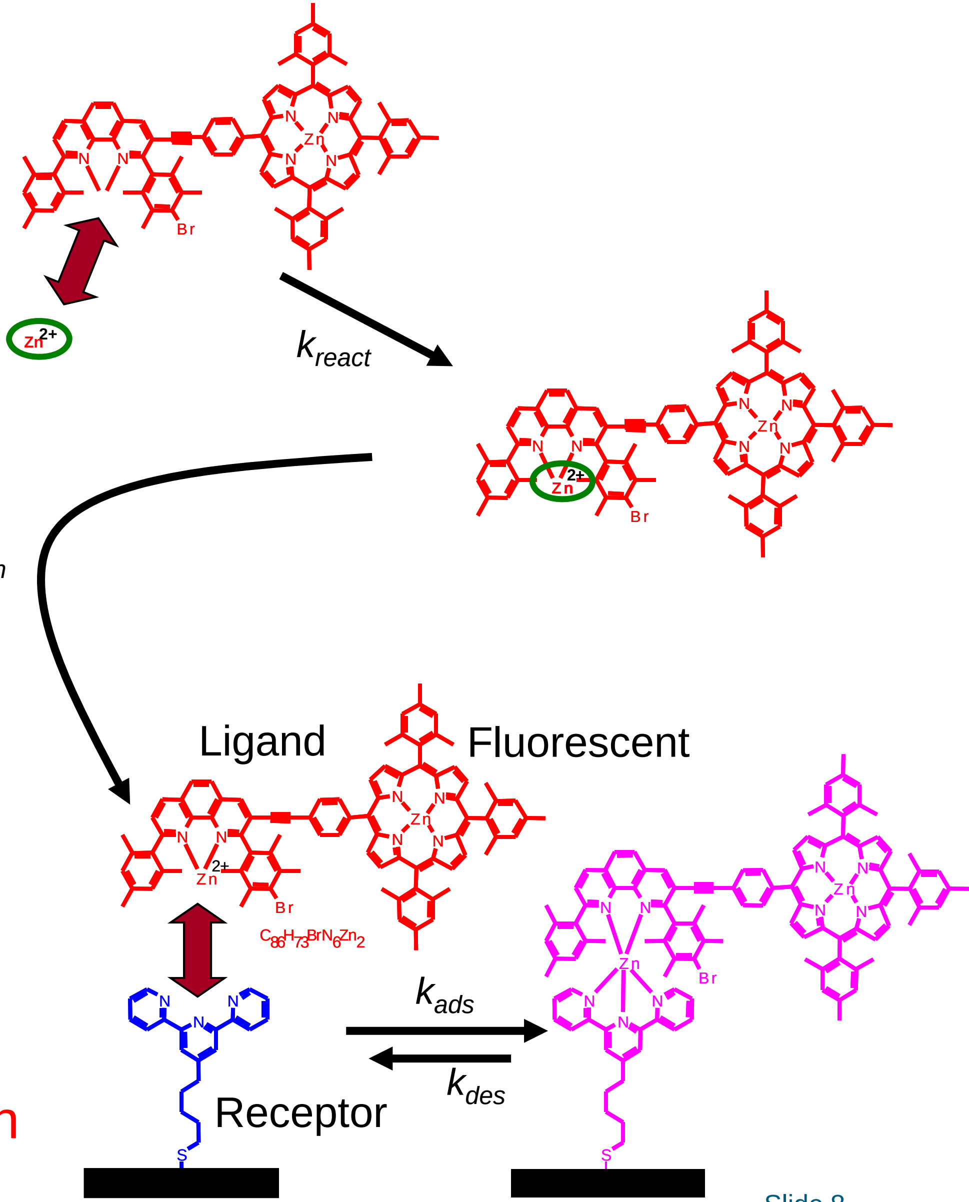
$$\frac{\partial c_C}{\partial t} = k_{react} \cdot c_A \cdot c_B$$

Film Diffusion

$$\frac{\partial c_f}{\partial t} = k_{film} \cdot (c_C - c_f)$$

Sorption Kinetic

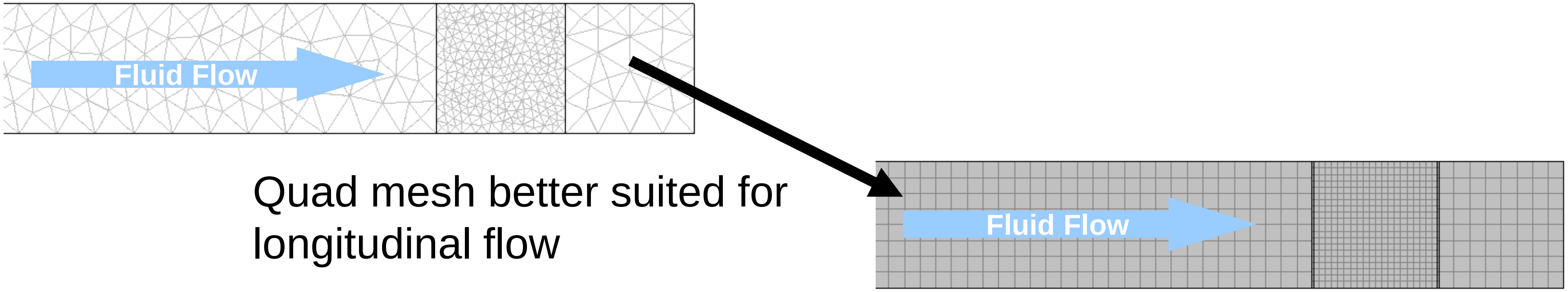
$$\frac{dq}{dt} = \underbrace{k_{ads} \cdot c_f (q_{\max} - q)}_{\text{Adsorption}} - \underbrace{k_{des} \cdot q}_{\text{Desorption}}$$



Numerics & Implementation

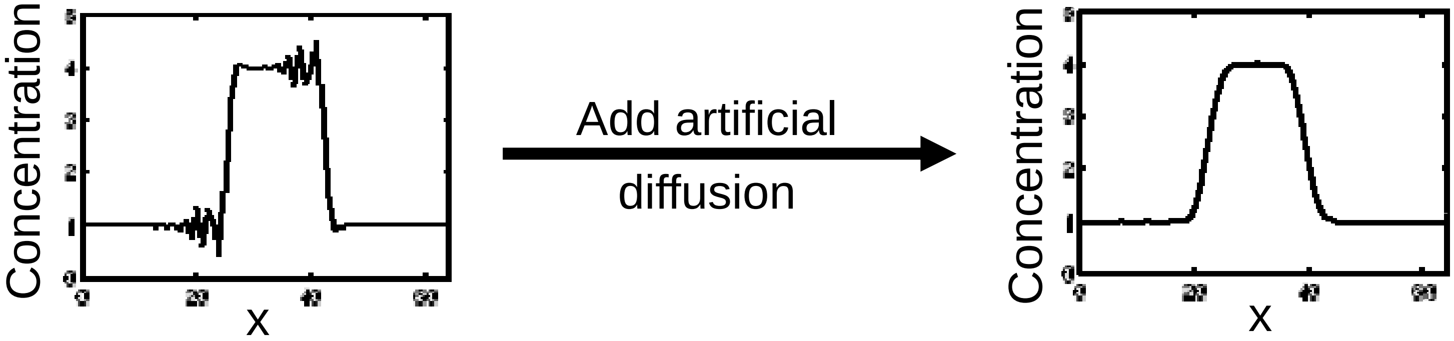
Aim: Receive a stable and precise solution

- Refined mesh in the region of strong kinetics



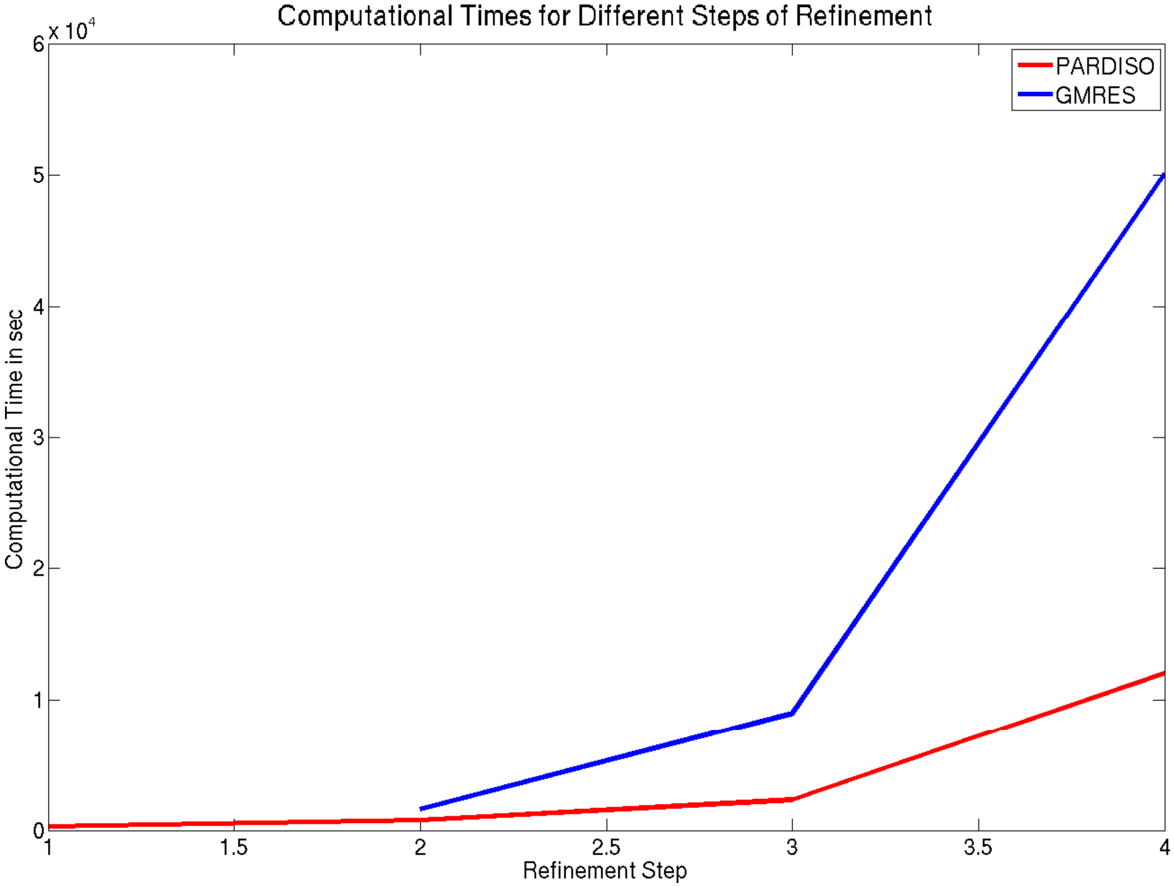
Quad mesh better suited for longitudinal flow

- Numerical stabilization techniques



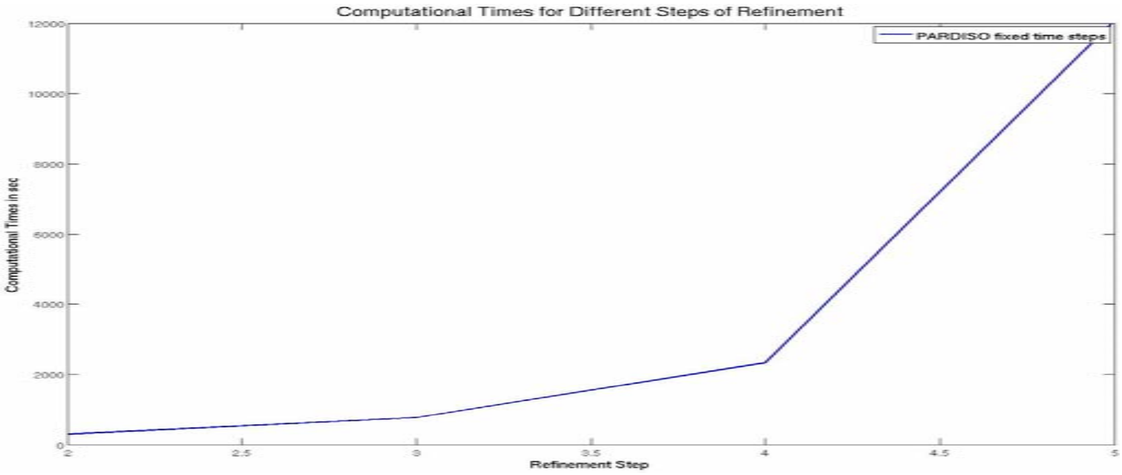
Direct vs. iterative Solvers

- Solvers: PARDISO and GMRES (with ILU precond.)
  - Computational Times: GMRES increasingly slow
  - Accuracy: negligible influence

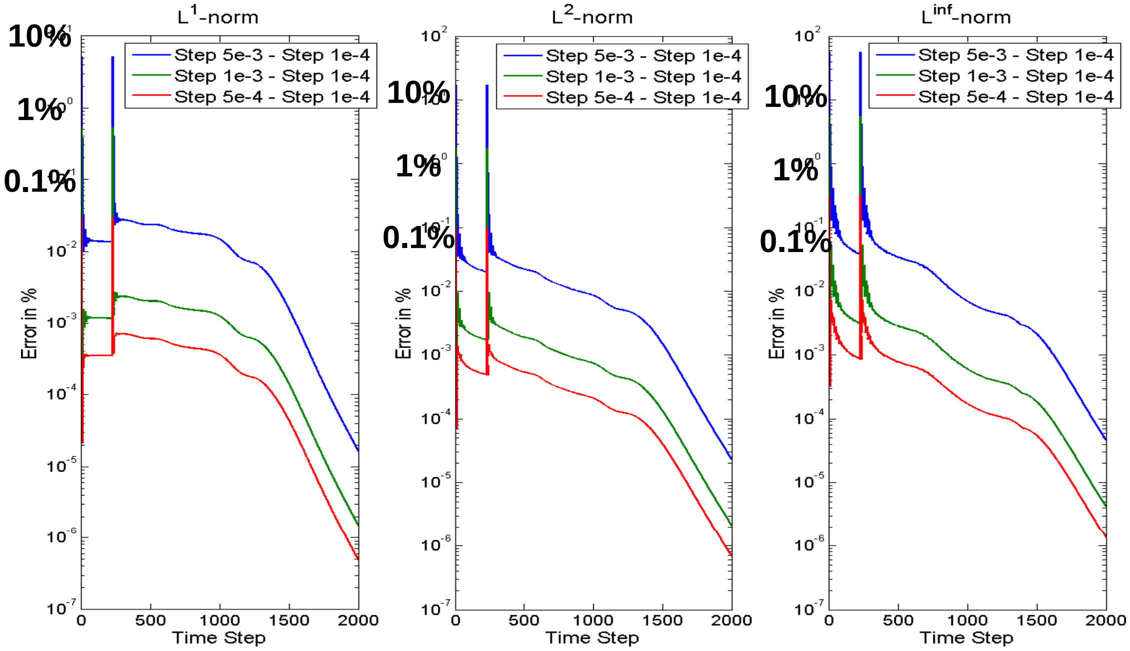


Numerical Considerations: Time Discretization

- Computation Times
    - fixed time steps
    - increasing effort

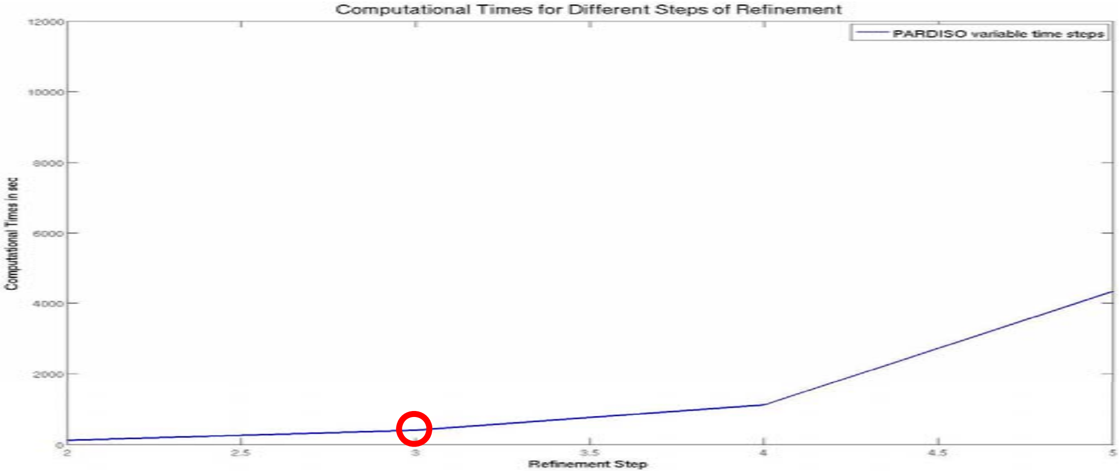


- Accuracy
    - compared with ‘best’ solution
    - no significant improvement
    - major error at plug

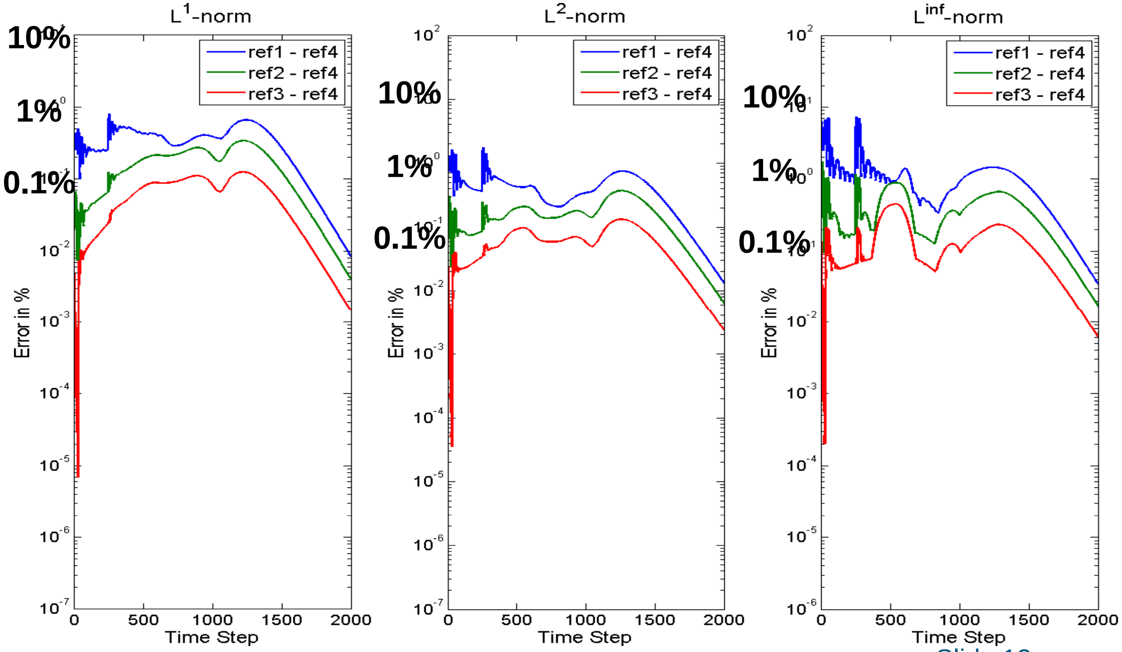


Numerical Considerations: Space Discretization

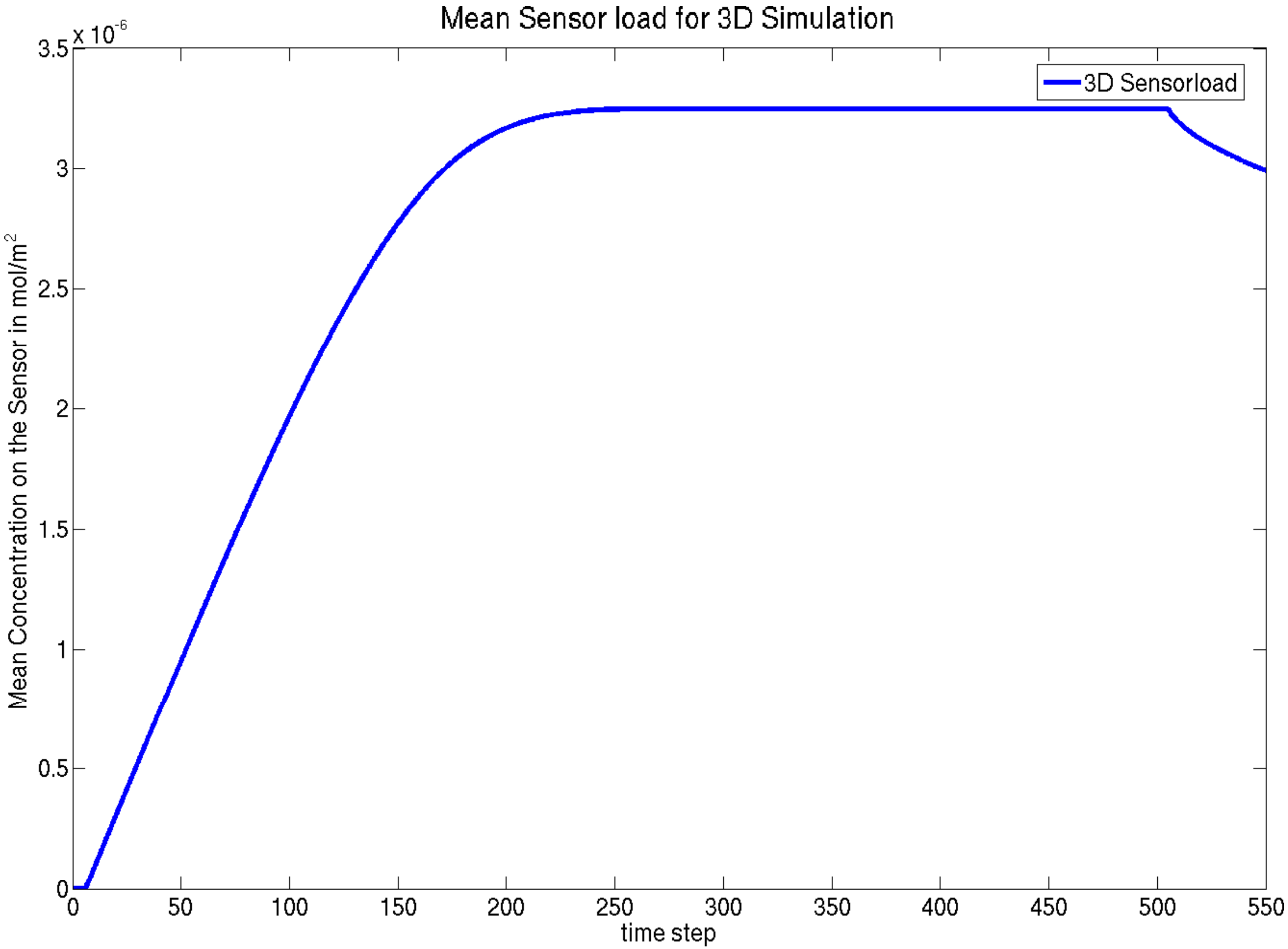
- Computation Times
  - variable time steps



- Accuracy
  - compared to next refined solution
  - better at plugs
  - improvement on refinement steps

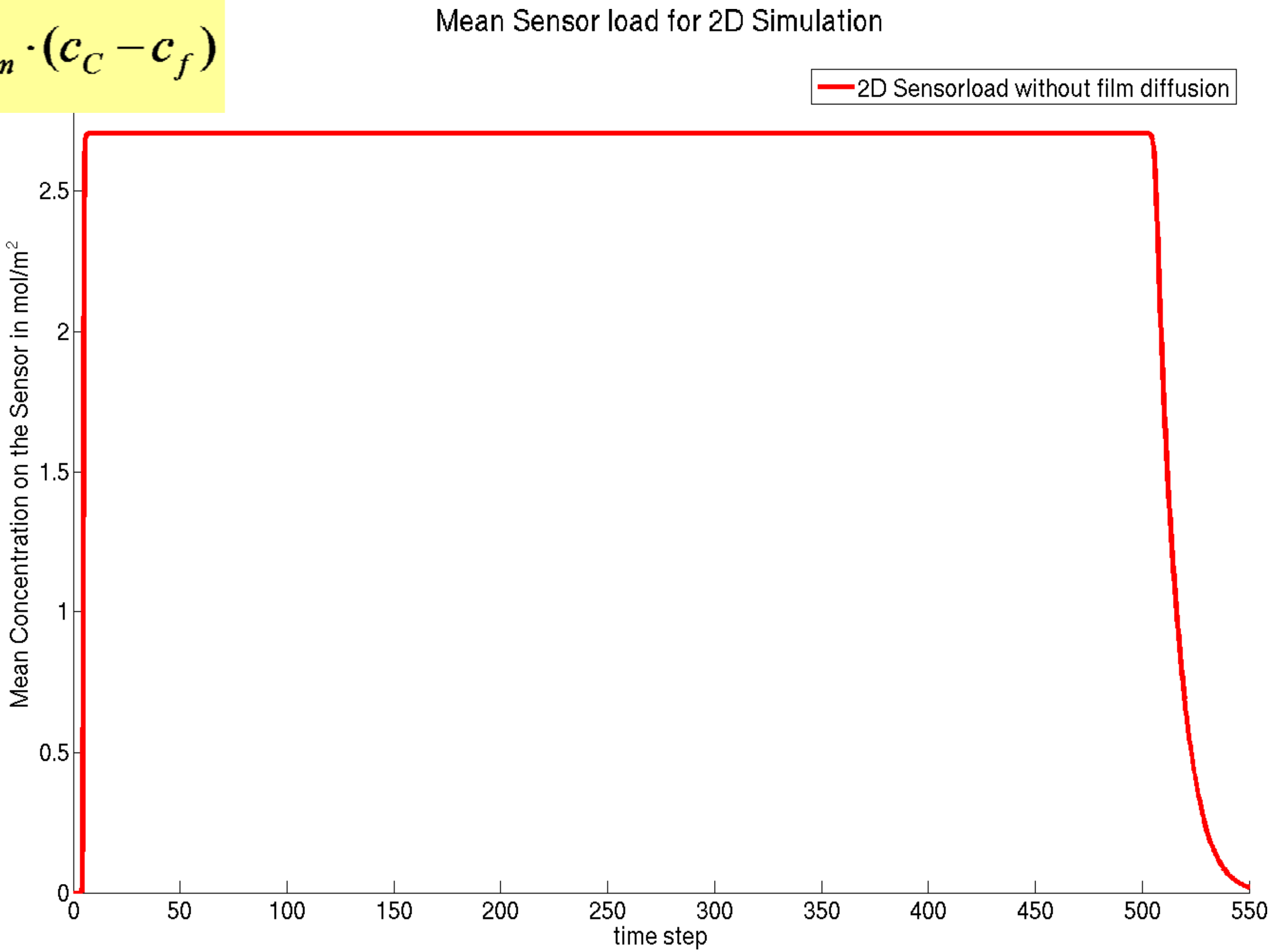


Mean Sensor Load 3D Simulation



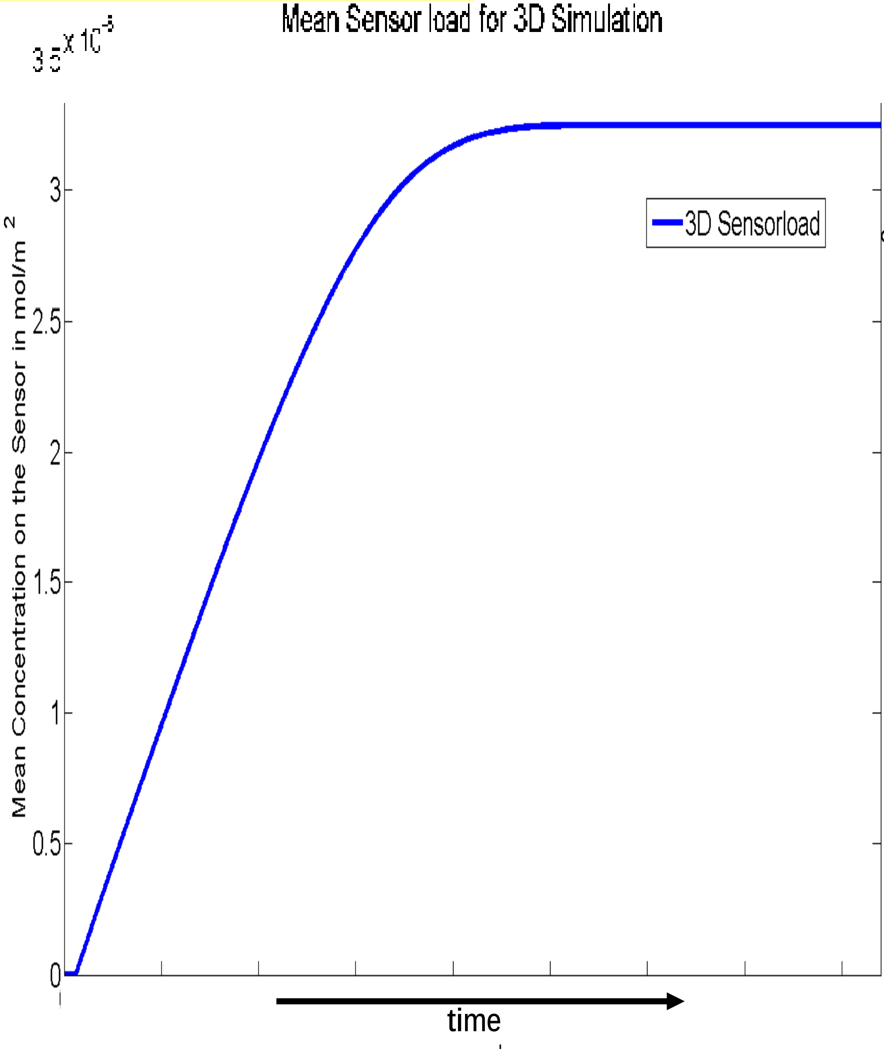
Mean Sensor Load 2D Simulation

$$\frac{\partial c_f}{\partial t} = k_{film} \cdot (c_C - c_f)$$

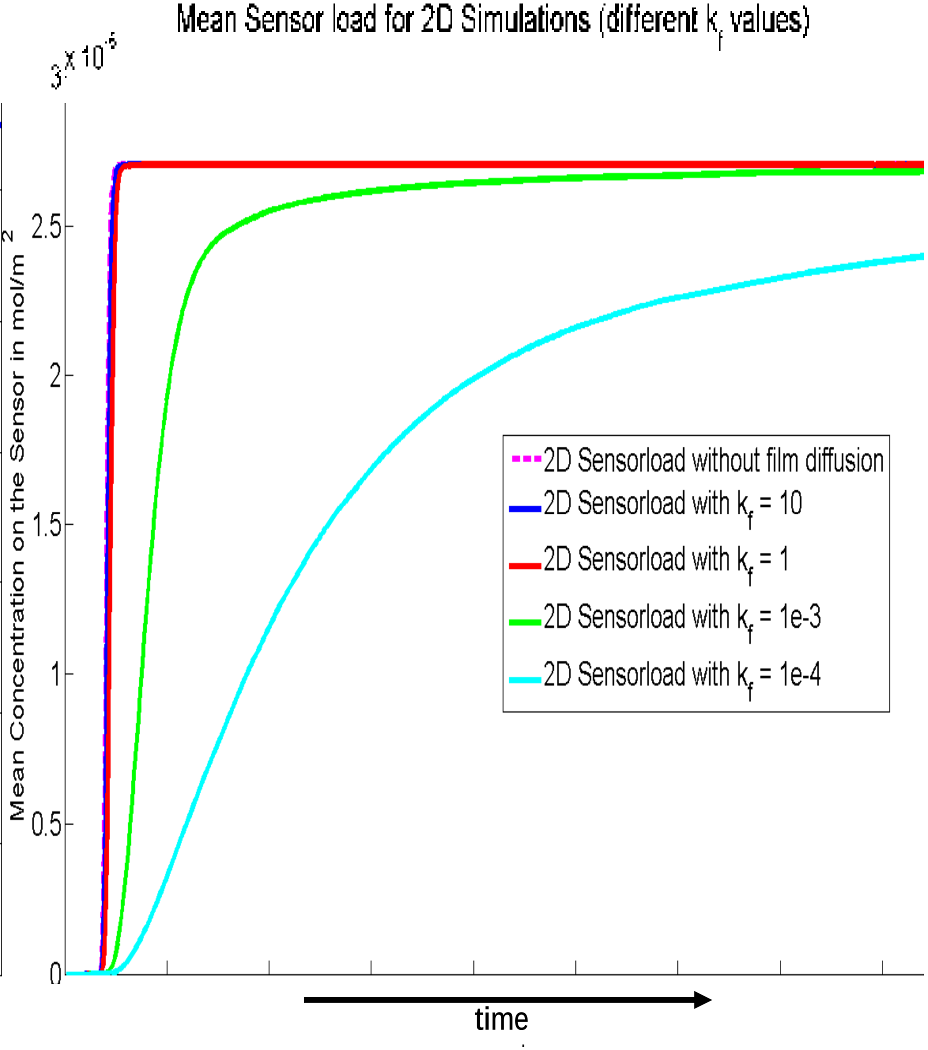


Adjusting k_f

$$\frac{\partial c_f}{\partial t} = k_{film}\cdot(c_C - c_f)$$

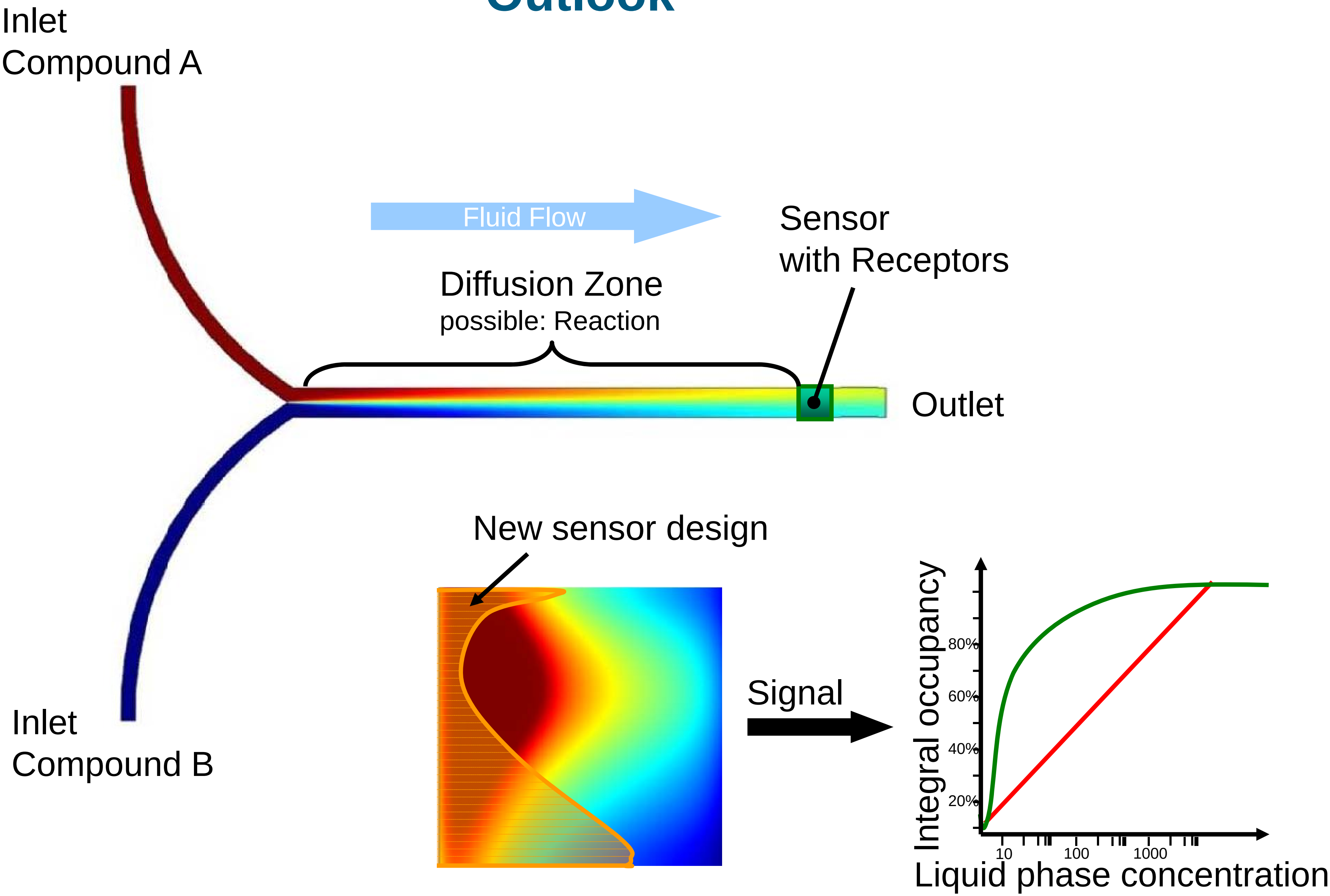


Mean Sensor load for 3D Simulation



Mean Sensor load for 2D Simulations (different k_f values)

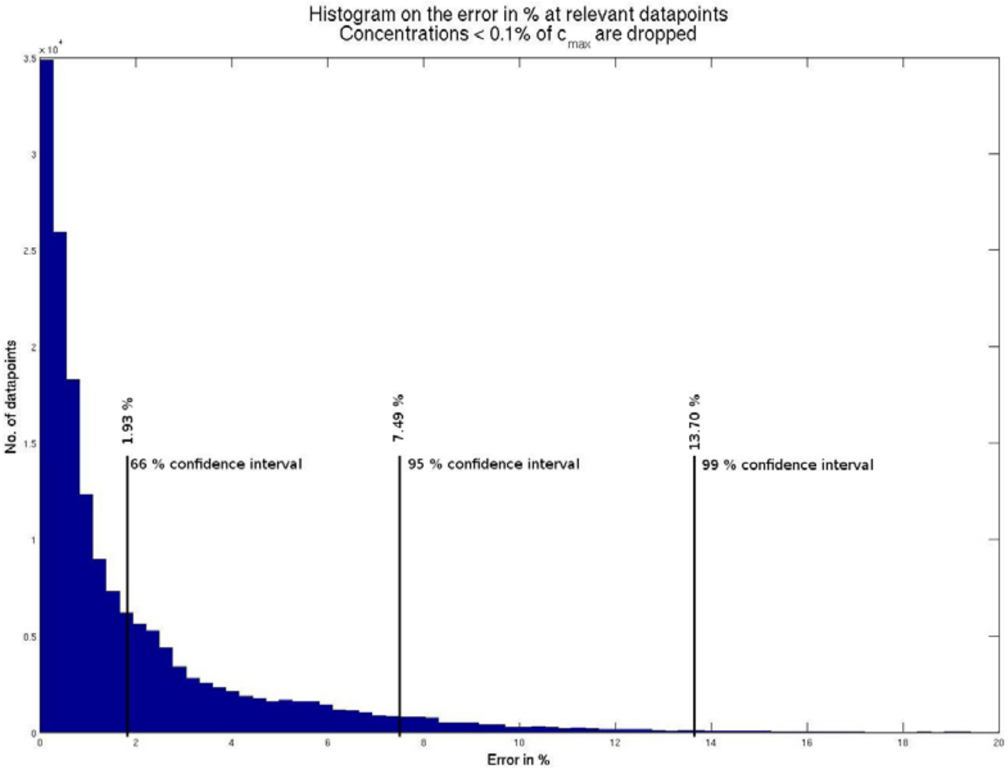
Outlook


Inlet
Compound A
Fluid Flow
Sensor
with Receptors
Diffusion Zone
possible: Reaction
Outlet
Inlet
Compound B
New sensor design
Signal
Integral occupancy
80%
60%
40%
20%
10
100
1000
Liquid phase concentration

Comparison of Comsol and deal.II

- Comsol Model
  - Streamline diffusion used

- deal.II Model
  - uses Upwind scheme
  - fixed time stepping



- Concentrations < 0.1 % of c_{max} dropped
- Comparison of concentrations