COMSOL 2009 Conferences

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Modeling of a DBD Reactor for the Treatment of VOC "

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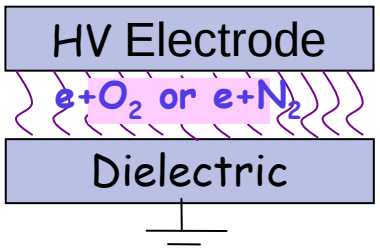
The process

Air
(N_2, O_2)

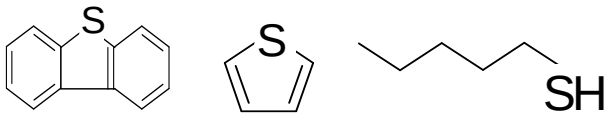
Dielectric Barrier Discharge



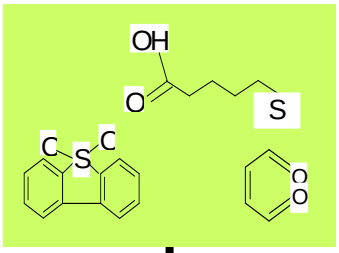
Active species
$O(1D)$, O_3, $O_2(1\Delta g)$, ...

+

Pollutant(VOC)



Partial oxidation
(low energy)



Complete oxidation
(high energy)

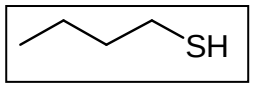
SO_2, CO_2

Trapping on fluidised or fixed bed

Bioremediation

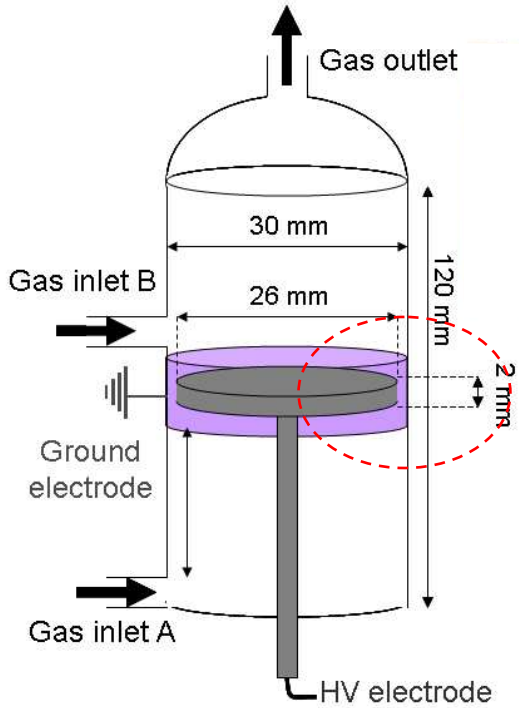
Clean air

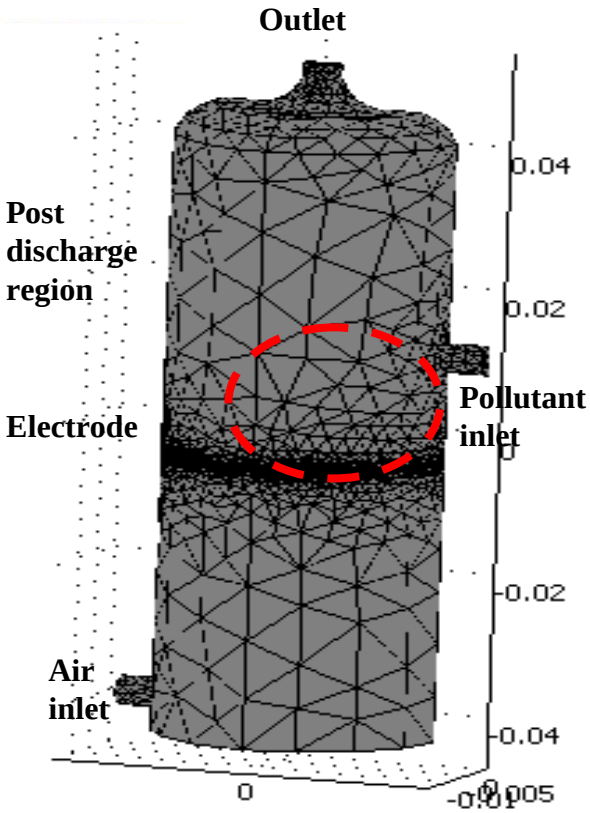
Molecule model:
Butane-thiol-1



The reactor and simulation domain

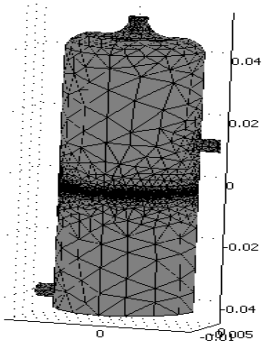
whole domaine





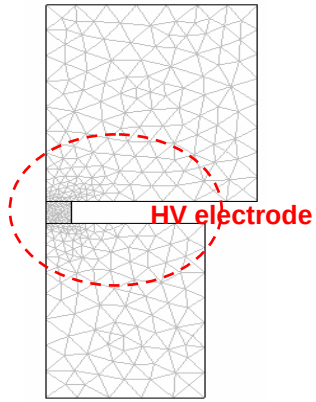
Flow simulation 3D

Diffusion of pollutant



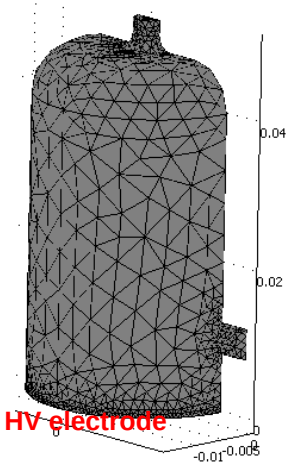
Discharge region simulation 2D

Production of active species (O, O3, …)

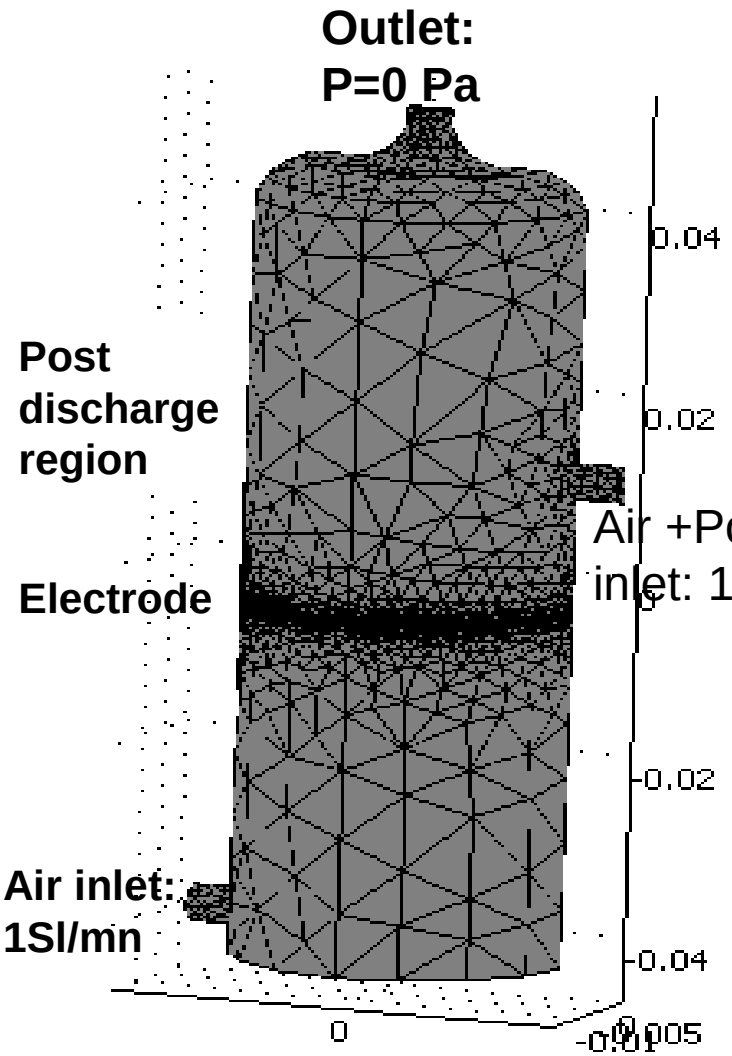


Post discharge simulation 3D

Reaction of active species with the pollutant

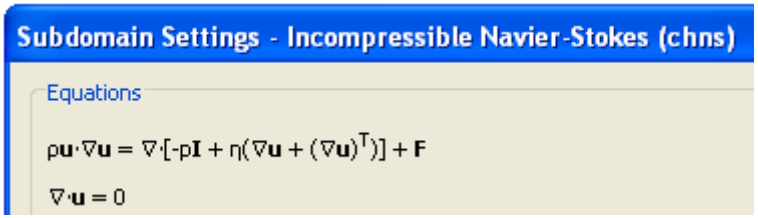


Flow simulation



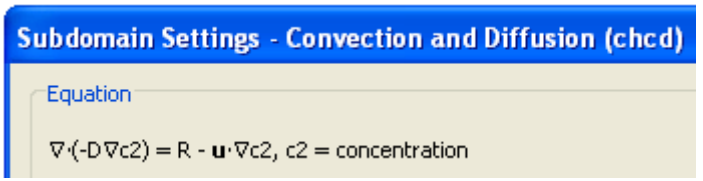
Models used:

1/ Navier-Stokes incompressible (chns)



Velocity and Pressure fields

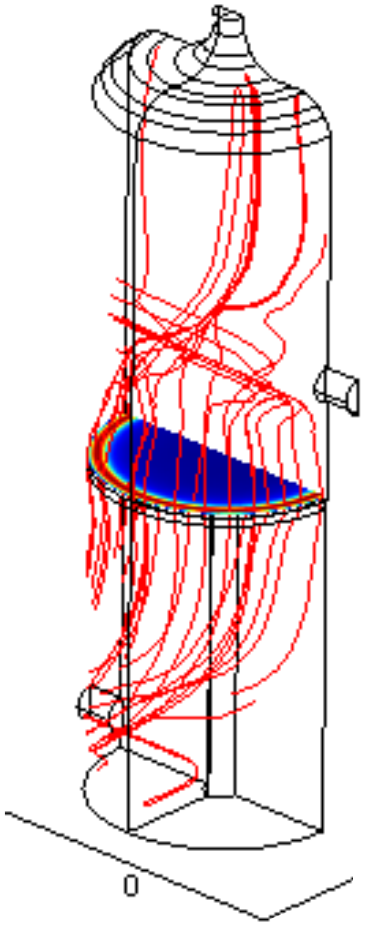
2/ Convection and Diffusion (chcd)

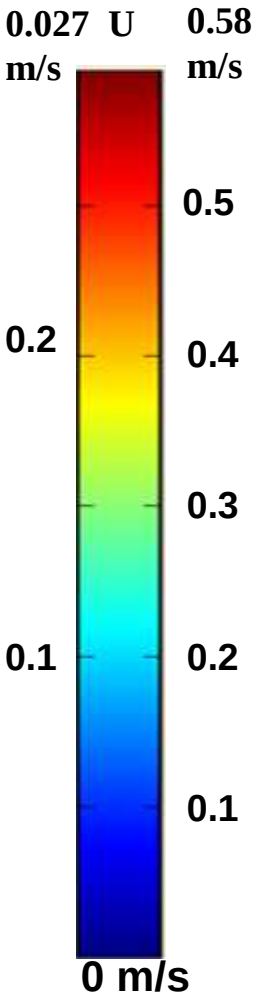


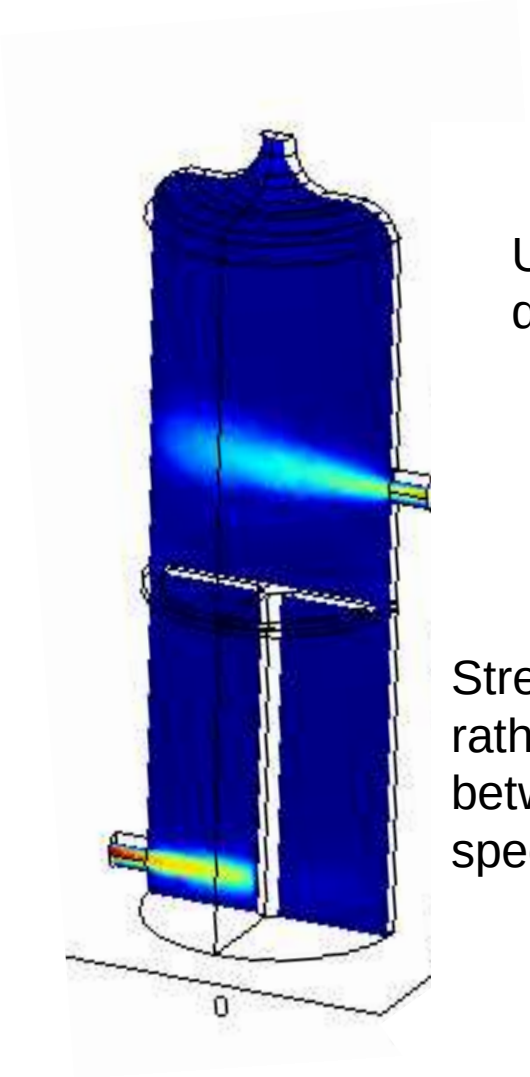
Concentration of pollutant in the reactor

Flow simulation

1/ Navier-Stokes incompressible (chns)





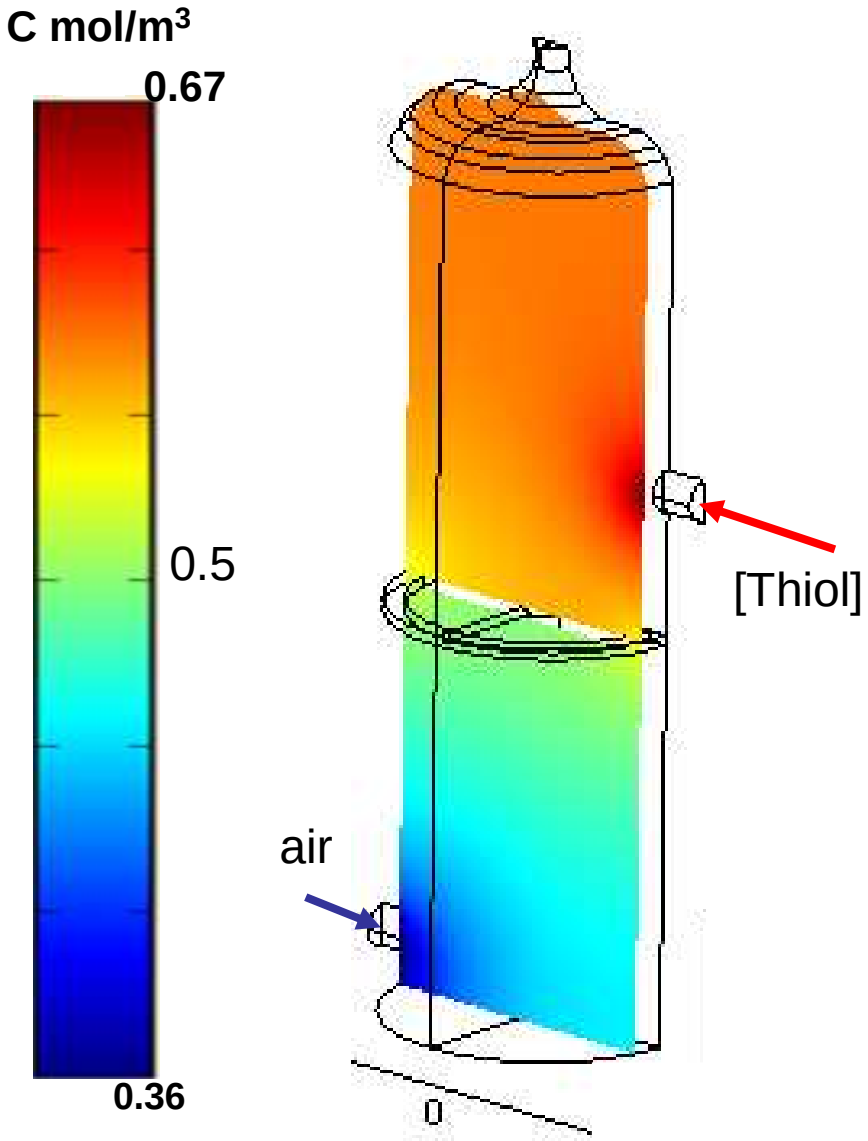


U_{max}=0.25 m/s in the discharge region

Streamlines show a rather good mixing between of active species and the pollutant

Flow simulation

2/ Convection and Diffusion (chcd)



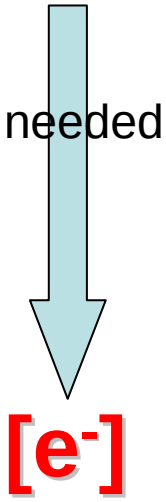
Diffusion of thiol in the discharge region.

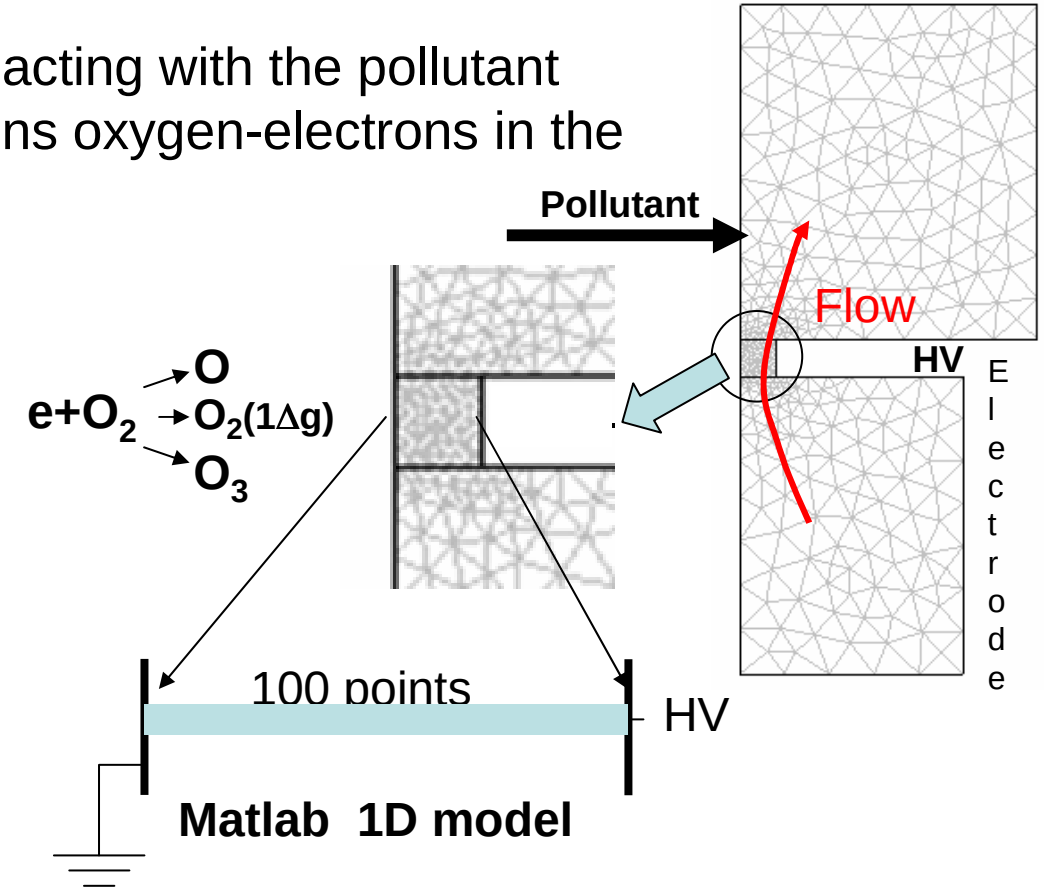
Experimental results show a film formation in the discharge region.

Change of the design of the reactor is necessary

Electron density determination

The active species reacting with the pollutant are created by colisions oxygen-electrons in the discharge region





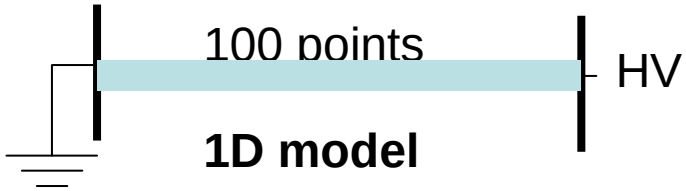
Calculation by resolution of a system of 4 equations:

Equation of Poisson **and three continuity equations, for electrons, positive ions and negative ions**

Discharge region simulation 2D

Electron density determination

Resolution of 4 coupled equations:



Equation of Poisson $\nabla^2\varphi = -\frac{e}{\varepsilon}(n_p - n_e - n_n)$ **relating V with distribution of local densities of charges.**

three continuity equations: for electrons, positive ions and negative ions:

$$\frac{\partial n_j}{\partial t} + \nabla.\Gamma_j = S_j \qquad \text{with} \qquad \Gamma_j = -D_j \nabla n_j + sign(q_j) n_j \mu_j E$$

Flux of particles — **Source term for particles j** — **Diffusion flux** — **Flux due to the drift of charged particles**

***J**: **e** for electrons , **p** for positive ions and **n** for negative ions*

The species are created by the reactions

$e + A \xrightarrow{\alpha} A^+ + 2e$ **Ionization**

$e + A^+ \xrightarrow{\beta} A$ $\quad A^- + A^+ \xrightarrow{\beta} A$ **Recombination**

$e + A \xrightarrow{\eta} A^-$ **Attachement**

$$S_e = (\alpha - \eta) n_e v_e - \beta n_e n_p \qquad S_p = \alpha n_e v_e - \beta n_e n_p - \beta n_n n_p \qquad S_n = \eta n_e v_e - \beta n_n n_p$$

Discretization Cranck Nicholson and linearization Raphson Newton

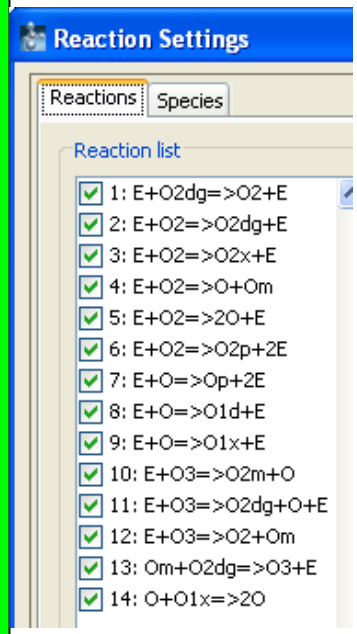
$\Rightarrow$ $[e^-] \cong 10^{14}\ cm^{-3}$

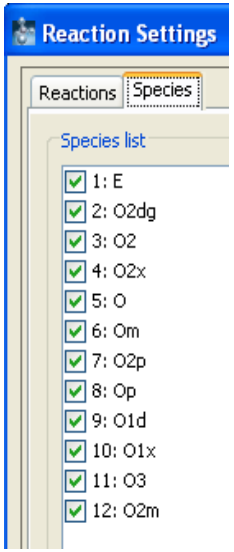
Discharge region simulation 2D

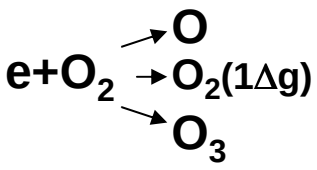
Reaction Engineering Lab

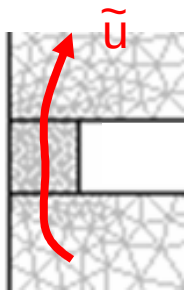
0D kinetic model of Willy Morscheidt: (LGPPTS)

14 reactions, 12 species



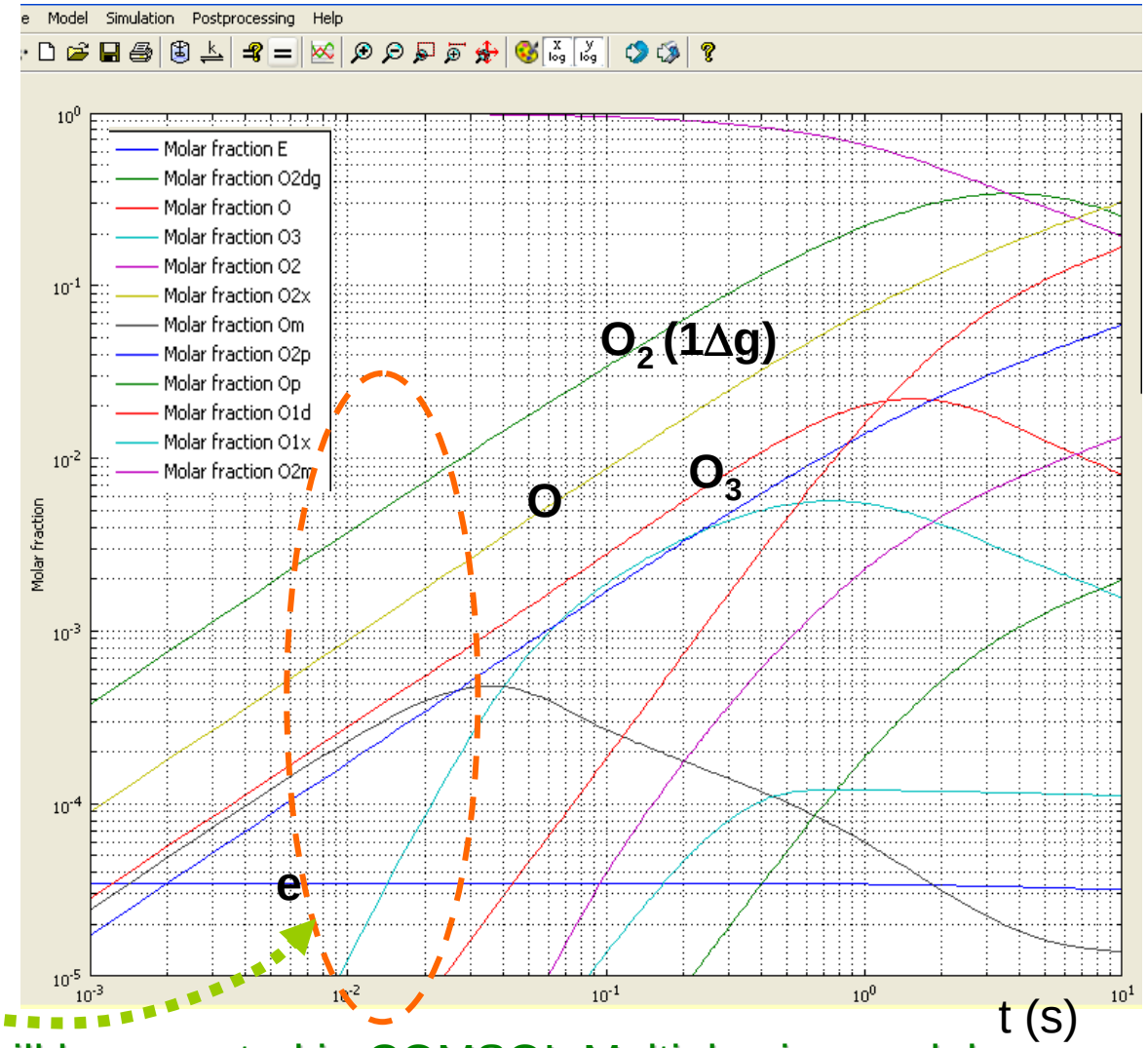






Average velocity: 0.15m/s

Residence time:~10ms

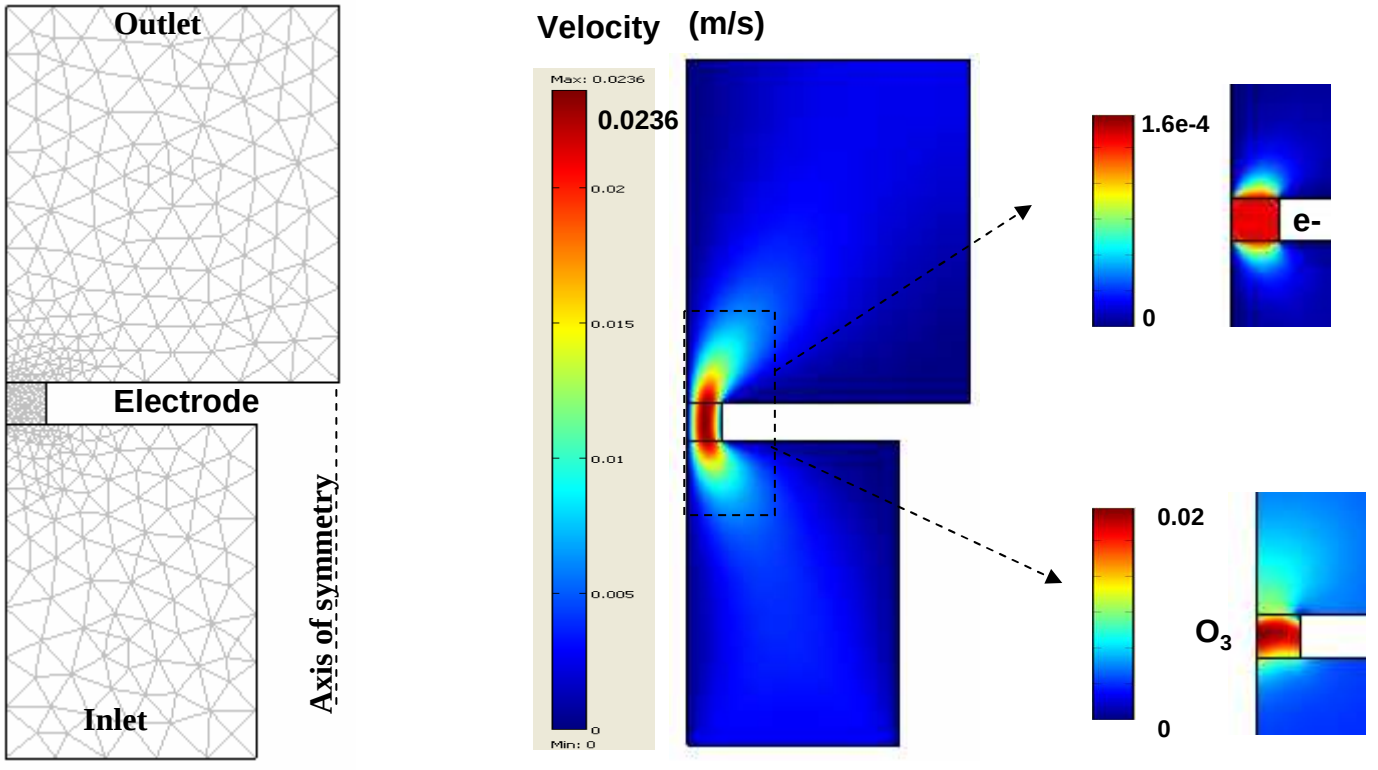


The model will be exported in COMSOL Multiphysics module

Discharge region simulation 2D

Flow and concentration fields

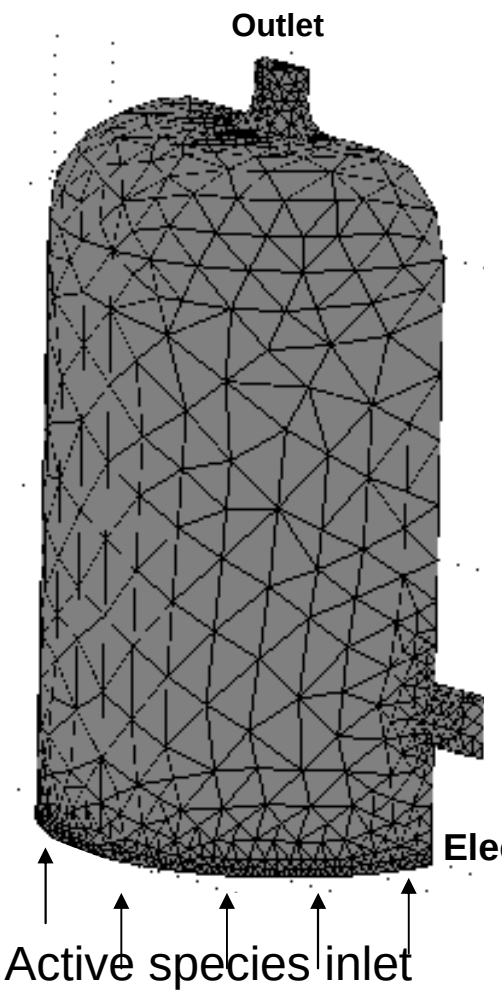
chns and ***chcd*** models



These concentrations and velocity will be used as Inlet BL in ***chcd*** and ***chns*** models respectively, in the post discharge reactor

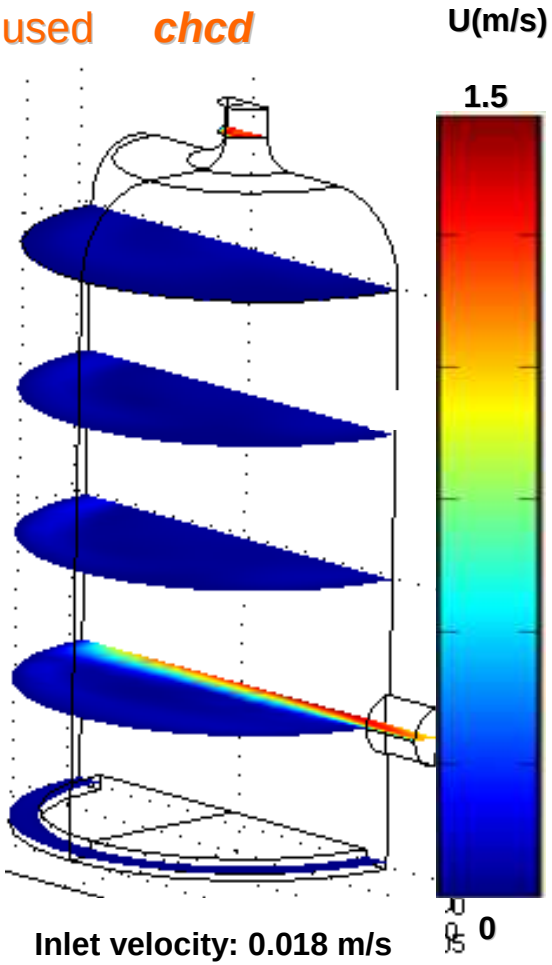
Post discharge region 3D simulation

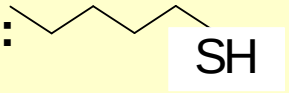
Set-up of 3D reactor and velocity field



model used ***chcd***

Residence time:
1 to 2 seconds



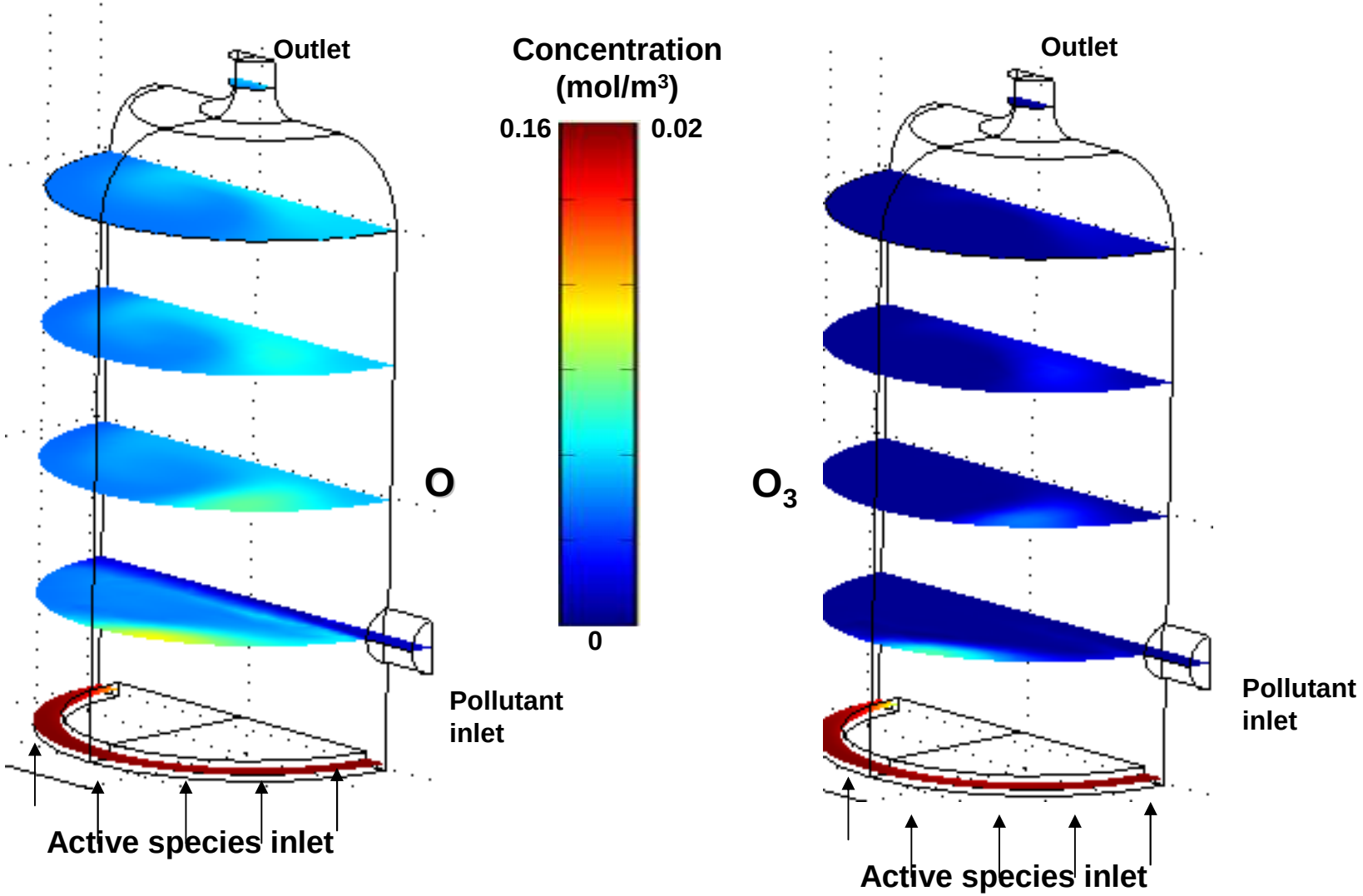
Reactions:  + O / O_3 → **Products**

Rate Constants (cm3/s)
K1=1.2e-12
K2=9.6e-12

Post discharge region 3D simulation

Concentration fields of reactants

model used ***chcd***

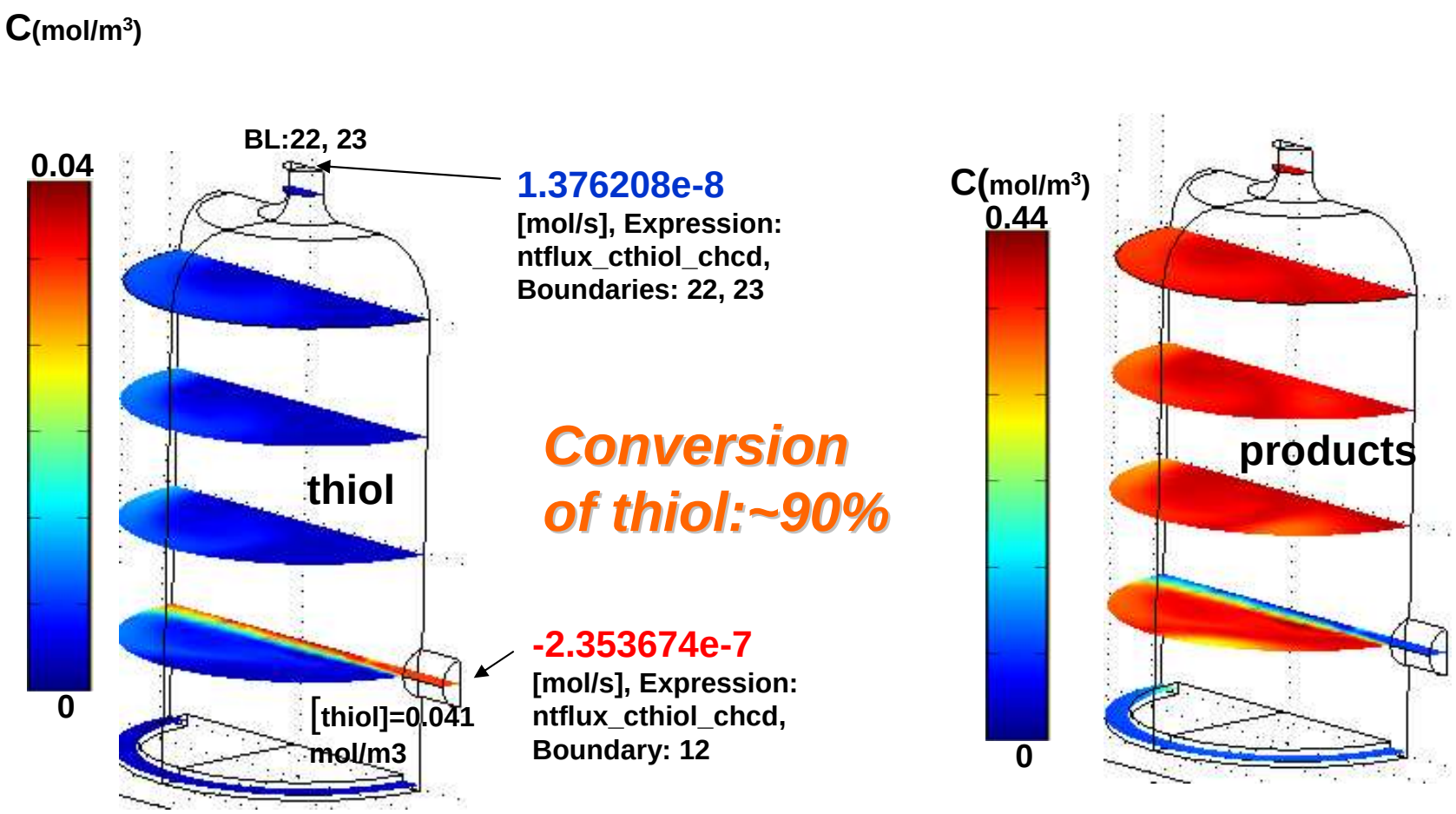


Concentrations of active species in the inlet BL from 2D model

Post discharge region 3D simulation

Concentration fields of pollutant and products

model used ***chcd***



Experimental results show a depletion from 40% to 100% depending on the induced specific energy

Conclusion

- It is possible to simulate a convection- diffusion process in 3D chemical reactor for the treatment of VOC. However due to the lack of CPU memory the reactor must be divided in 3 parts and the whole process must be treated sequentially. So the diffusion of the pollutant in the discharge region is not taken into account.

-Calculations show a qualitative agreement with experimental results. The prediction can be sensibly improved for kinetic models with more reactions.

Current and future work

-Use of more powerfull PC with larger memory for the treatment the whole process in one step.

--Implementation of the discharge model directly in COMSOL

Thank your for your attention

Questions?

Suggestions?

Any idea for the implementation of DBD model in COMSOL is welcome