COMSOL 2011 Conference

26 -28 october 2011, Stuttgart, Germany

Simulation of the degradation of methyl red by gliding arc plasma

Beyram Trifi [1, 2], Stephanie Ognier[2], Nizar Bellakhal[1, 3], Siméon Cavadias [2]

1 Laboratoire de Chimie Analytique et Electrochimie, Département de Chimie, Faculté des Sciences de Tunis, Université Tunis El Manar, Tunisie.

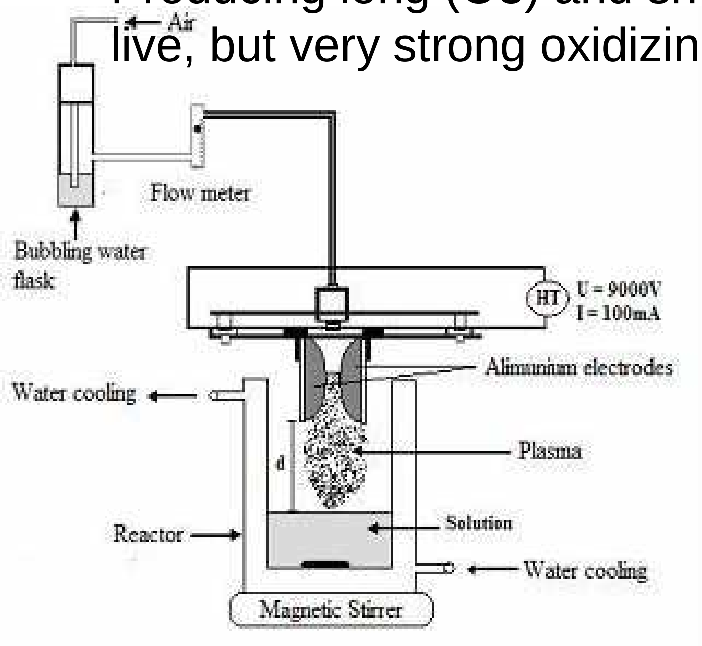
2 Laboratoire de Génie des Procédés Plasma et Traitement de Surface, Ecole Nationale Supérieure de Chimie de Paris, Université Pierre et Marie Curie, France.

3 Département de Chimie et de Biologie Appliquées, Institut National des Sciences Appliquées et de Technologie, B.P. N°676, 1080 Tunis Cedex, Tunisie.

The process

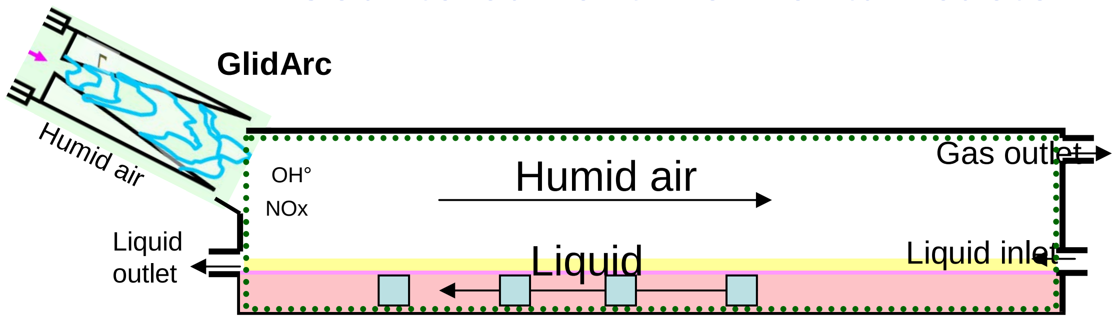
Treatment of water charged with organic pollutants by GlidArc reactor

Producing long (O3) and short (O, OH) live, but very strong oxidizing species



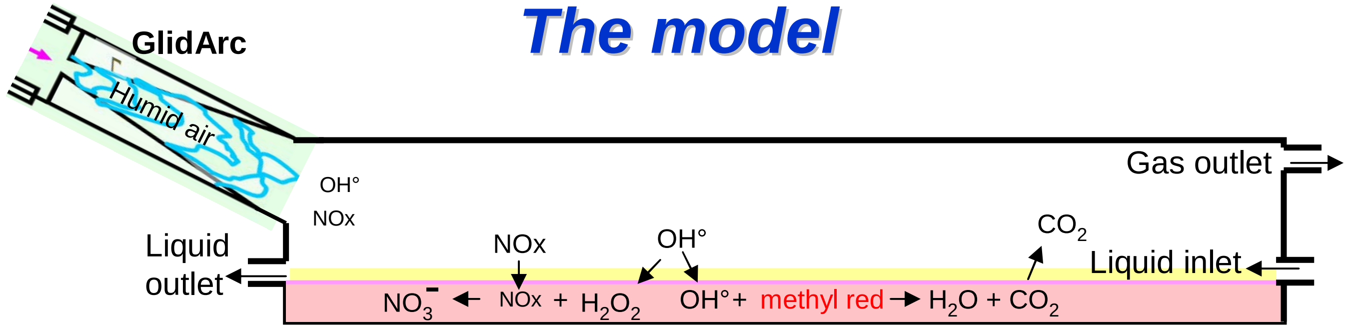
Good efficiency, but batch proces with very low contact area between gaz and water

Countercurrent horizontal reactor



- Continuous treatment
- Contact area increased
- Possibility of mixing

The model



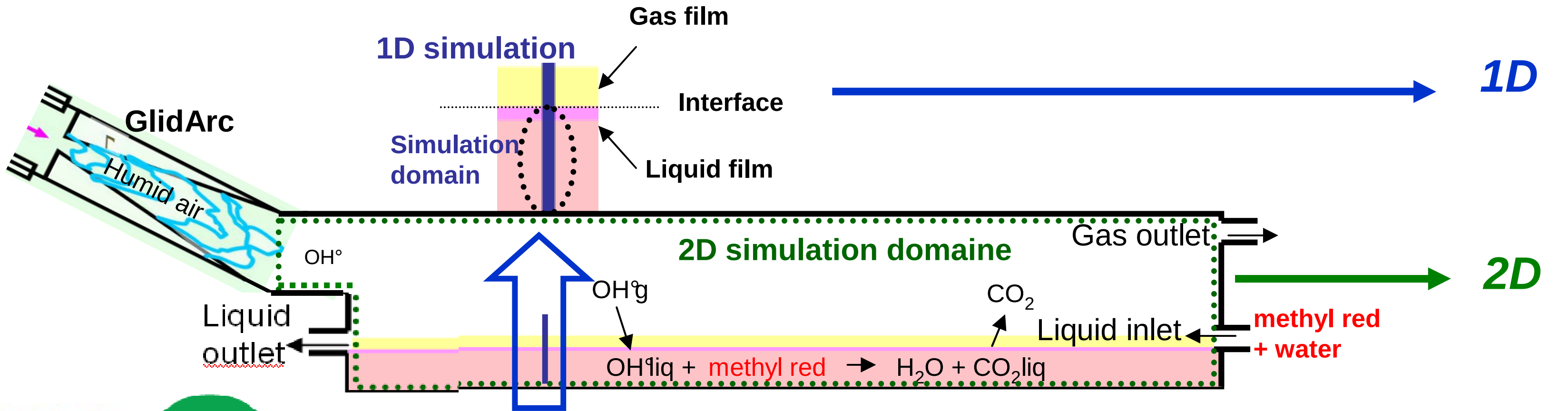
Kinetic model with 6 species and 5 reactions:

OH° + H_2O_2	**<----->**	**H_2O + HO_2°**	**(1)**
HO_2° + HO_2°	**<----->**	**H_2O_2 + O_2**	**(2)**
OH° + OH°	**<----->**	**H_2O_2**	**(3)**
HO_2° + OH°	**----->**	**H_2O + O_2**	**(4)**
OH° + mred	**----->**	**H_2O + CO_2**	**(5)**

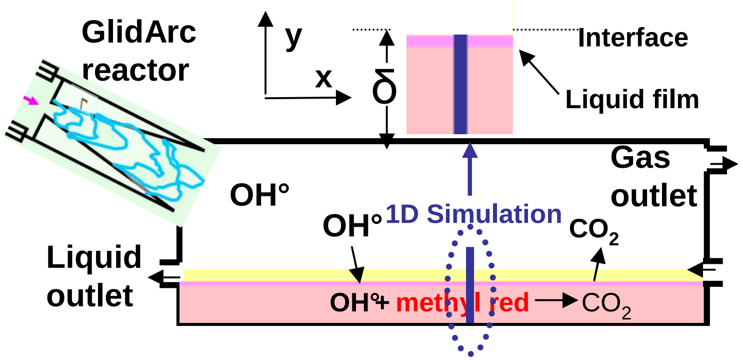
6 species
5 reactions → ***1D***

3 species
1 reaction → ***2D***

~~NO_x~~



1D diffusion model (setup)



Species: $OH°_l$, $HO_2°_l$, H_2O_2, O_2, mred, CO_2

$OH°_g$ is formed by by e^- - M_2 collisions in the GlidArc interelectrode region.

$OH°_g \rightarrow OH°_l \rightarrow$ diffusion, reaction liquid phase

$OH° + H_2O_2$	<----->	$H_2O + HO_2°$	(1)
$HO_2° + HO_2°$	<----->	$H_2O_2 + O_2$	(2)
$OH° + OH°$	<----->	H_2O_2	(3)
$HO_2° + OH°$	----->	$H_2O + O_2$	(4)
$OH°$ + mred	----->	$H_2O + CO_2$	(5)

$CO_{2g} \leftarrow CO_{2l}$

Diffusion in the liquid phase

Interface 1 gas liquid

2 bottom of the reactor

Model used ***chcdp*** **(see tutorial of Absorption in a Falling film)**

Equations solved in the domain:

$$-D_i \frac{\partial^2 c_i}{\partial y^2} + v_x \frac{\partial c_i}{\partial x} - \sum R_j = 0 \quad \text{in } \Omega$$

Diffusion flux **Convective flux** **Reaction rate of the reactions**

Velocity gradient dv_x/dy

$$v_x = 1.5 v_{av}\left(1 - \left(\frac{y}{\delta}\right)^2\right)$$

1D diffusion model (setup)

Boundary limit settings

$$OH_l^\circ : \ -D_i \frac{\partial c_i}{\partial x}(0,t) = k_{g,OH}\left(p_{OH} - c_{OH} H_{OH}\right)$$

$$-D_i \frac{\partial c_i}{\partial x}(0,t) = 0$$

for $HO_2{}^\circ{}_{,}$, H_2O_2, O_2 and mred

$$CO_{2l} : \ -D_i \frac{\partial c_i}{\partial x}(0,t) = k_{g,CO_2}\left(p_{CO_2} - c_{CO_2} H_{CO_2}\right)$$

Mass transport coefficient — **Partial pressure in gaz phase** — **Henry constant**

Average velocity: 0.0033 m/s

Partial pressure OH°_g in gaz phase: 1620Pa

Partial pressure p_{CO2} in gas phase: 0, 10 and 20 Pa

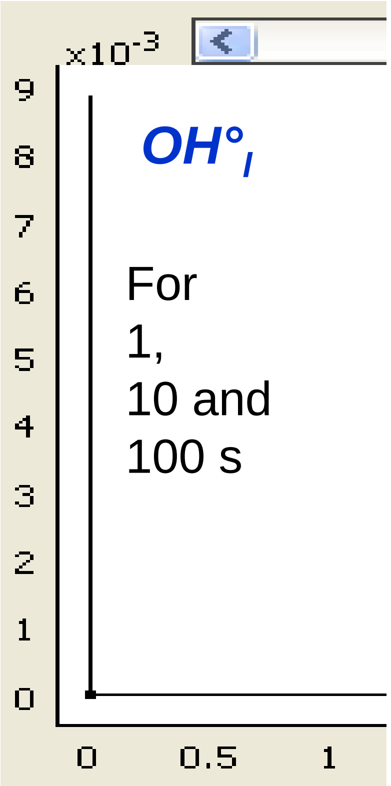
Calculations were performed for 1, 10 and 100 seconds.

⇓

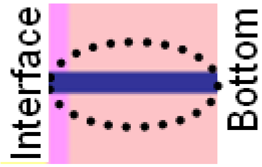
Concentrations of OH°_l, $HO_2{}^\circ{}_{,}$, H_2O_2, O_{2l}, mred, CO_{2l} as a function of time and depth

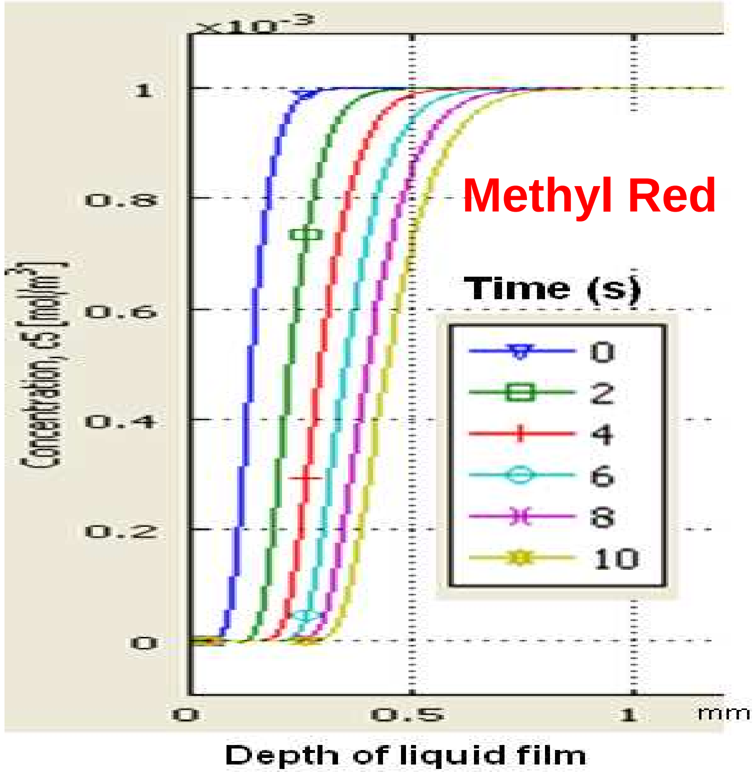
UPMC PARISUNIVERSITAS — enscp chimie paris

1D diffusion model (results)



Depth of liquid film





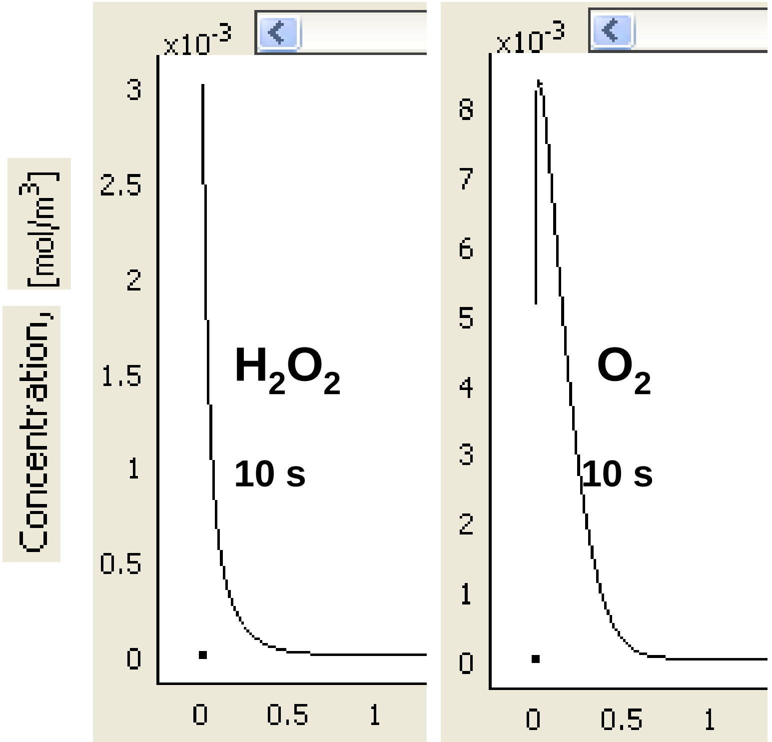
Hydroxyl radicals are consumed immediately by reaction 5

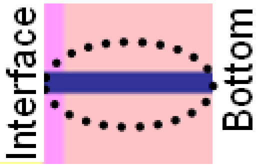
$OH°$ + mred → **$\sim 10^{10}$ *l/mole.s*** → **$H_2O + CO_2$**

probably with H_2O_2 as an intermediate species

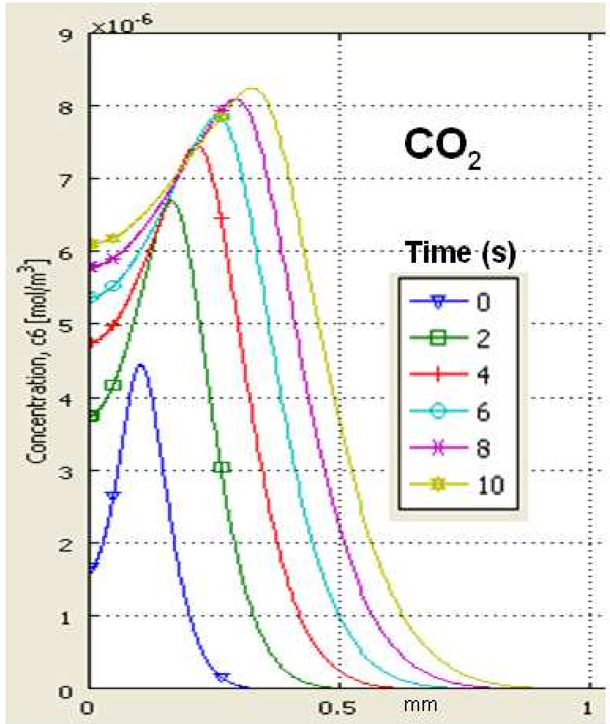
For contact times of about 10 s everything happens in the first 0.5 mm!

1D diffusion model (results)





Depth of liquid film (mm)



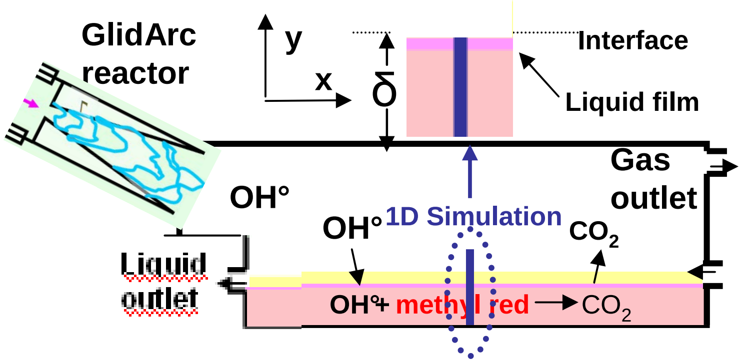
Depth of liquid film (mm)

H_2O_2 is formed very rapidly near the interface : $OH°_l + OH°_l \rightarrow H_2O_2$ then

CO_2 is formed by the reaction 6 but is not consumed since there is no reaction for this. Normally CO_2 should be released in the gas phase.

2D model

2D model setup



$OH°_g$ is formed by by e^- - M_2 collisions in the GlidArc interelectrode region.

$OH°_g \rightarrow OH°_l \rightarrow$ diffusion, reaction liquid phase

$OH°_l$ + mred $\rightarrow CO_{2l} + H_2O$

$CO_{2g} \leftarrow CO_{2l}$ **Diffusion in the liquid phase**

Models used:

1/ Navier-Stokes incompressible (chns)

Subdomain Settings - Incompressible Navier-Stokes (chns)

Equations

$$\rho \mathbf{u}\cdot\nabla\mathbf{u} = \nabla\cdot[-p\mathbf{I} + \eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] + \mathbf{F}$$

$$\nabla\cdot\mathbf{u} = 0$$

Velocity and Pressure fields

2/ Convection and Diffusion **(chcd and chcd2)**

Subdomain Settings - Convection and Diffusion (chcd)

Equation

$$\nabla\cdot(-D\nabla c2) = R - \mathbf{u}\cdot\nabla c2,\ c2 = \text{concentration}$$

chcd

Concentration of gaseous species

$OH°_g$ CO_{2g}

chcd2

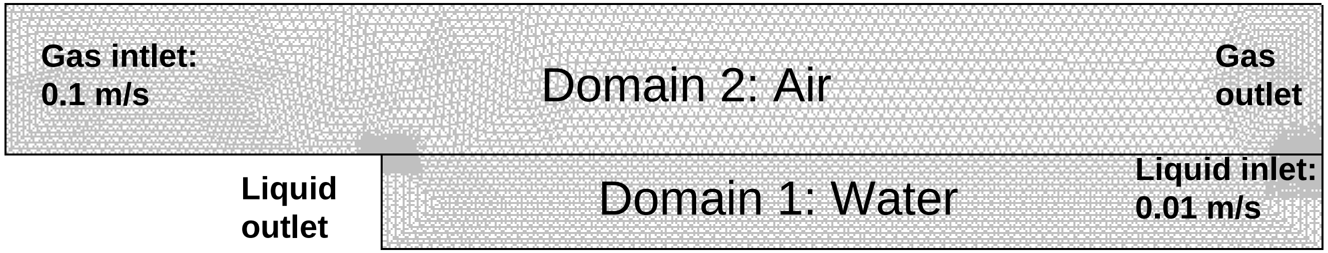
Concentration of liquid species

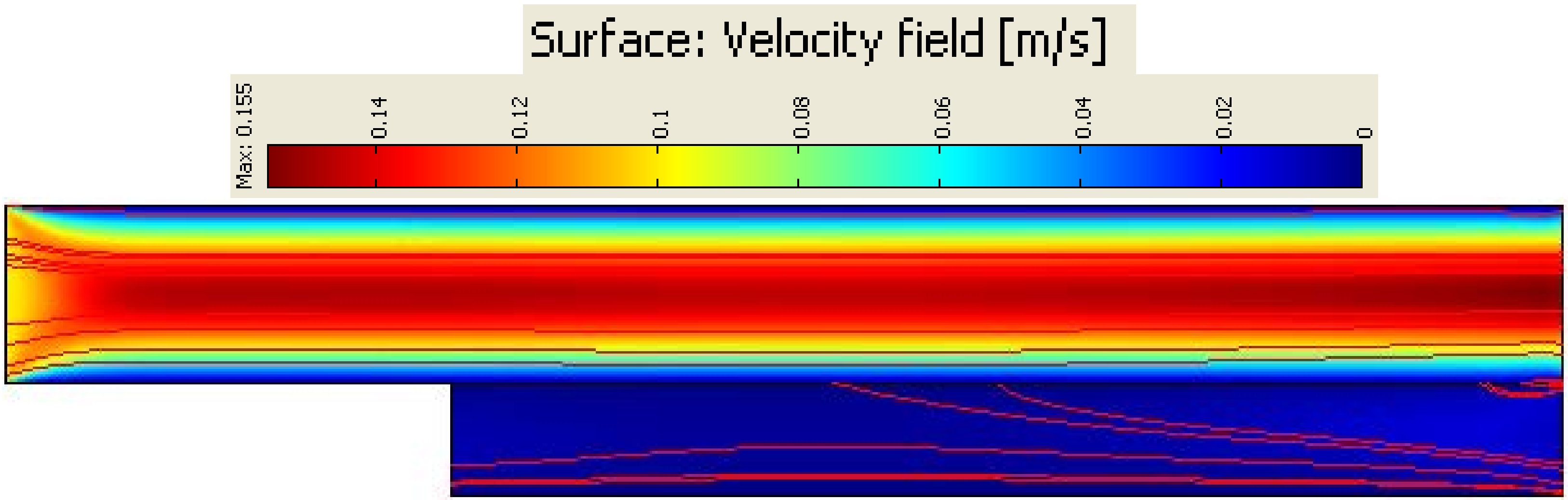
$OH°_l$ mred CO_{2l}

Flow simulation

1/ Navier-Stokes incompressible (chns)

Triangular Mesh





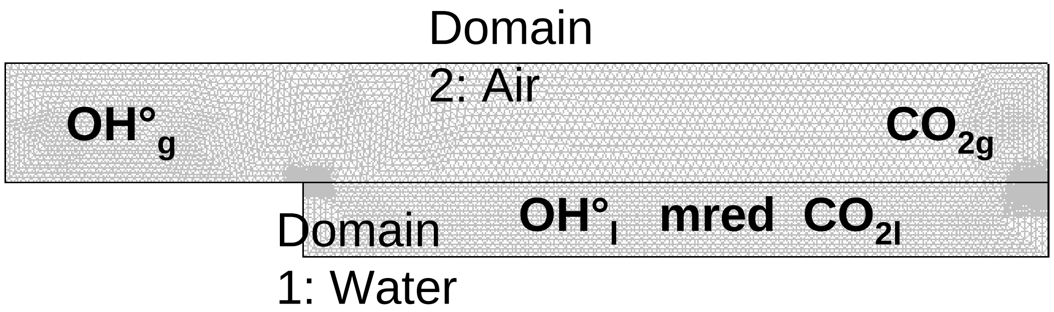
Liquid phase can be considered as immobile compared to the gas phase

Streamlines indicate an interaction between the two phases in the right end

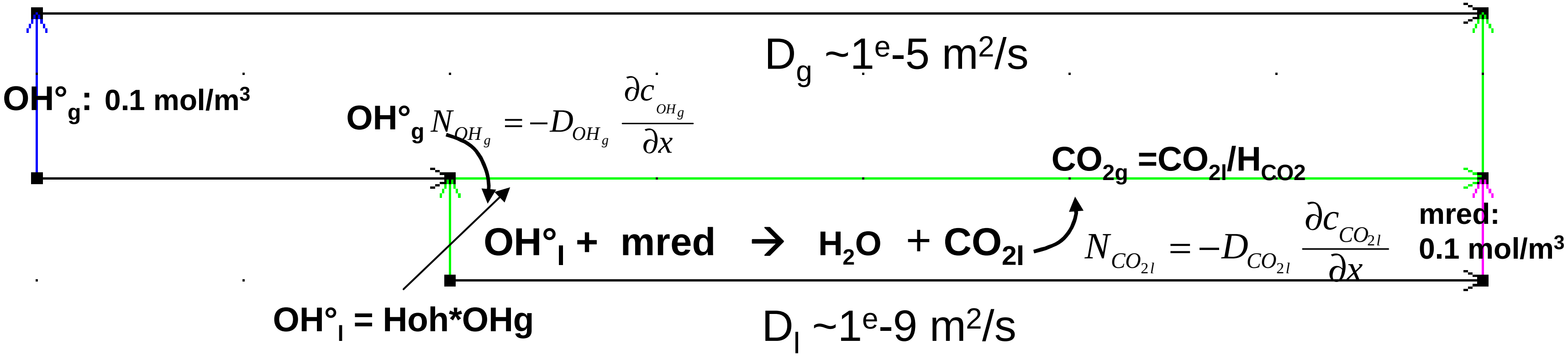
2/ Convection and Diffusion (chcd and chcd2)

Domains

active		
	chcd	~~chcd2~~
	~~chcd~~	chcd2

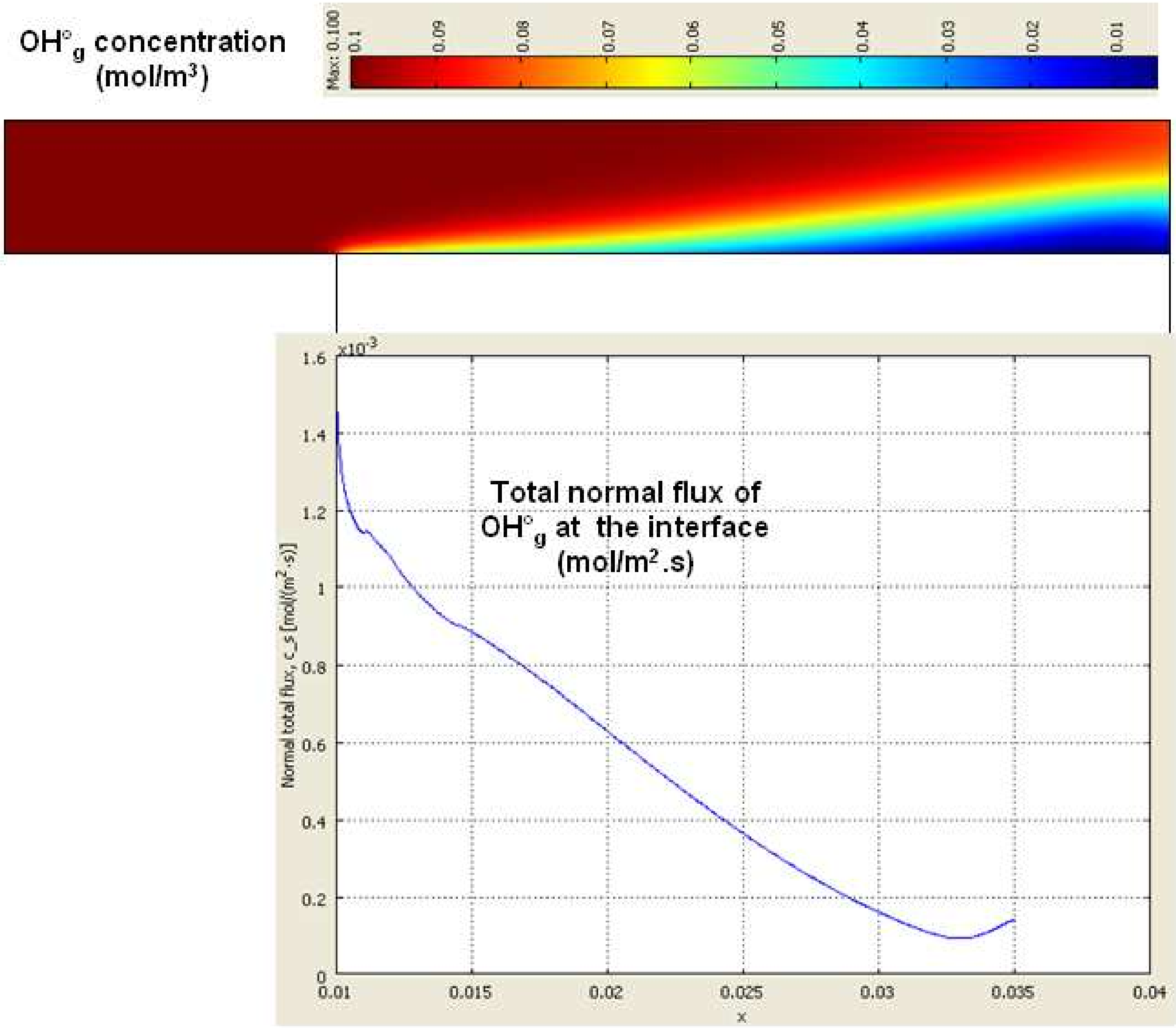


Boundary Limits



Henry constant

2/ Convection and Diffusion (chcd and chcd2)

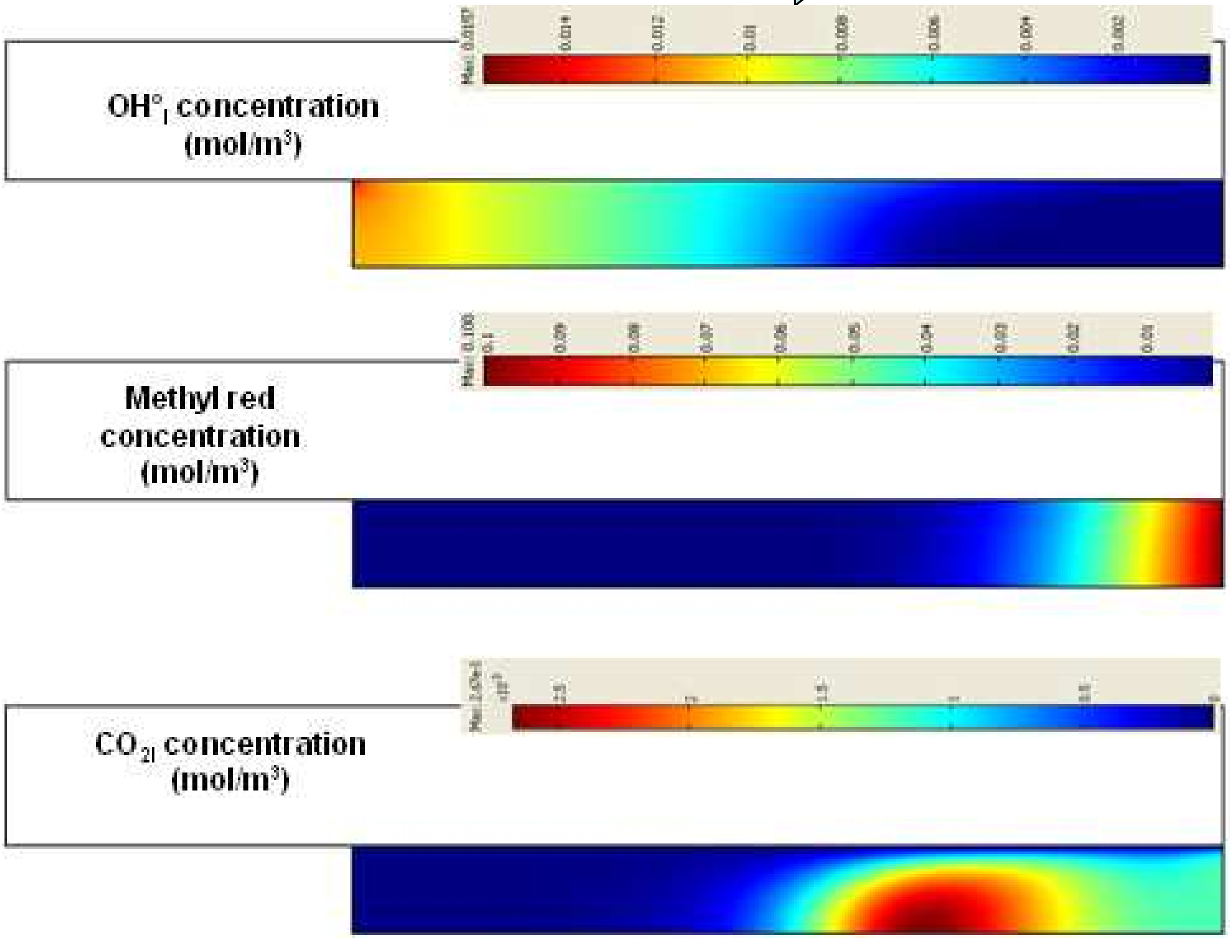


Convection diffusion simulation

Convection diffusion simulation

2/ Convection and Diffusion (chcd and chcd2)

Liquid phase reaction: $OH°_l$ + mred $\xrightarrow{\sim 10^{10}\ l/mole.s}$ $H_2O + CO_{2l}$



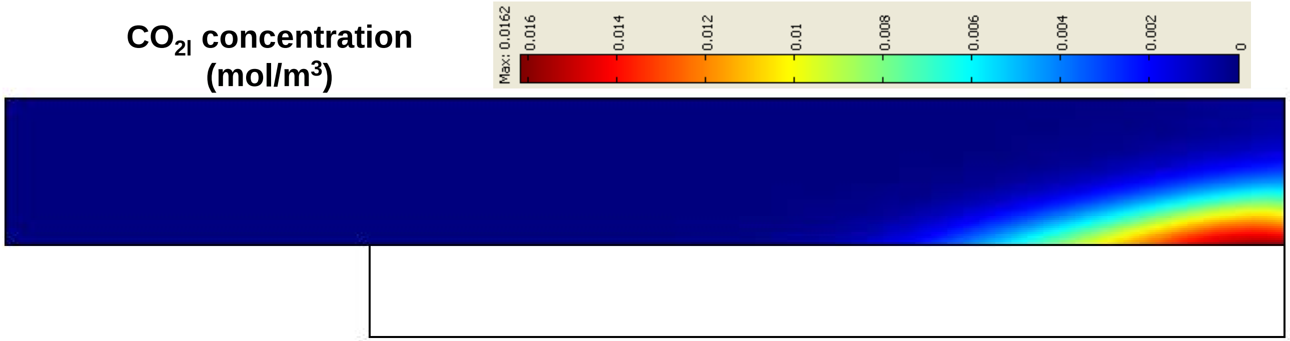
As in the 1D simulation hydroxyl radical are consumed immediately

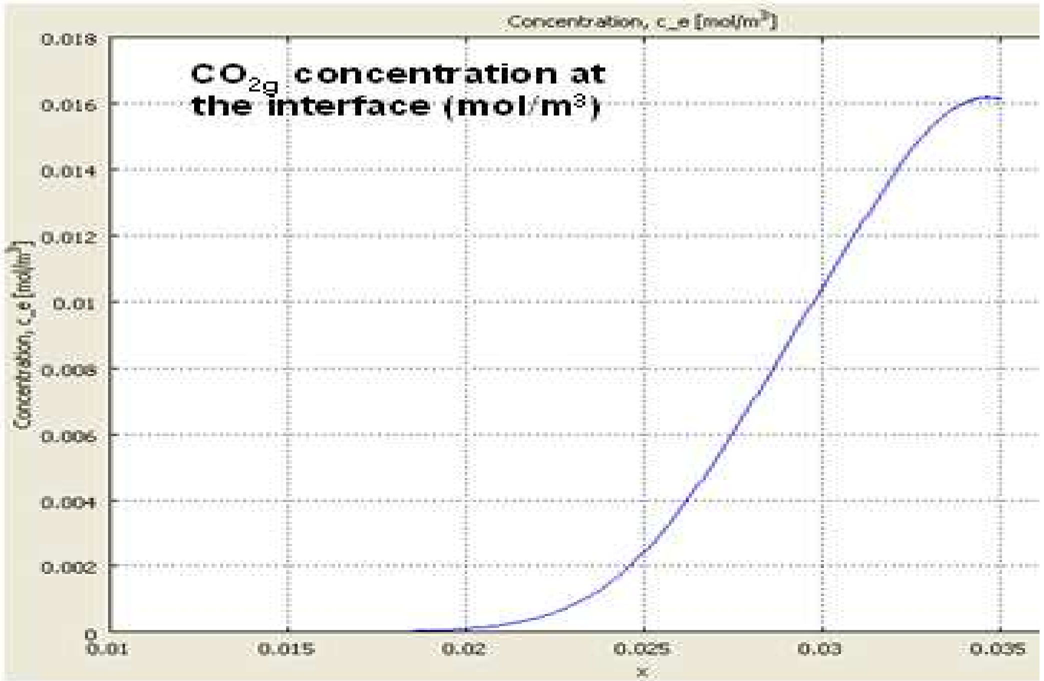
Convection diffusion simulation

2/ Convection and Diffusion (chcd and chcd2)

CO_2 production and diffusion in the gas phase

CO_{2l} concentration (mol/m^3)





Carbon dioxide enter in the gas phase domain mainly from the right end of the reactor. Under the action of the convection, the concentration increases near the outlet.

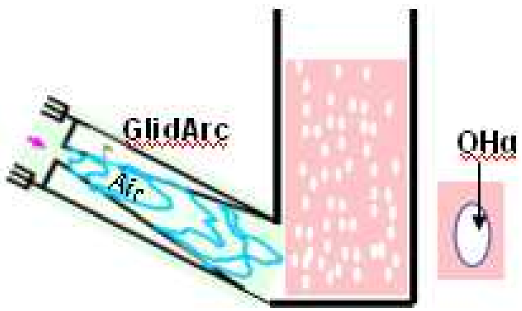
Conclusion

- It is possible to simulate in 2D, a continuous two phase horizontal counter-current reactor, the convection- diffusion process for the treatment of water charged with organic pollutants.
- Simulation shows a fast absorption of OH°, formed by the electrical discharge, in a few tenths of mm from the interface gas- liquid.
- However, even if this new reactor is better, compared to the existing batch reactor because is continuous, the contact area remains always low.

So the contact area should be improved.

Future Work

Setup of a bubble reactor or a three phase reactor



A lot of work for modelling

Thank your for your attention

Questions?