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Fluid Flow Simulation of Preconcentration Membranes Using Finite Elements Tools

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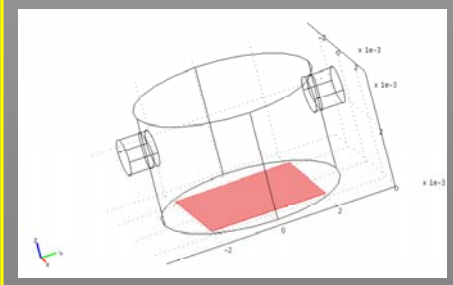
GOALS

Preconcentration is necessary to sense traces of toxic gases that are found in air at very low concentrations. We study the fluid flow behaviour in order to :

✓Optimise chamber geometry to maximize the preconcentration factor

INITIAL CHAMBER

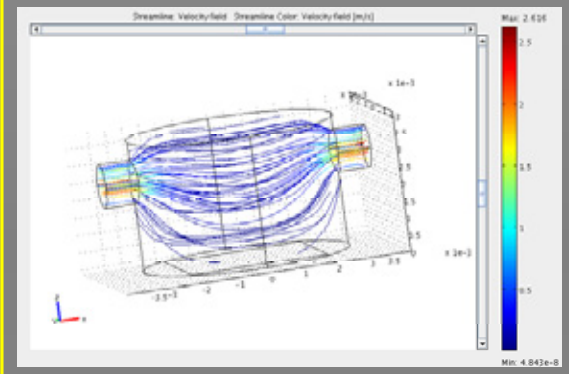


Preconcentrator is located at the base. This is a 4 mm side square of porous alumina substrate with activated carbon deposited on top.

Weakly Compressible Navier-Stokes model is used for fluid flow because velocity of fluid depends on density variations.

We introduce laminar velocity as input and constant pressure as output boundaries constrains.

With the **Convection and Diffusion model** we simulate the concentration variations.



In the preconcentrator there is a two-way reaction which converts free analyte (A_f) to analyte in the wall (A_W). This is governed by the velocity of reaction.

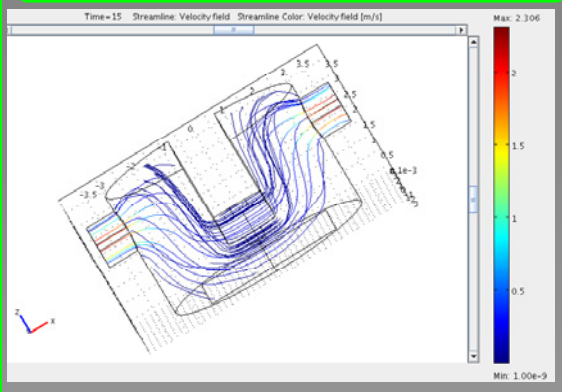
$$A_W \underset{k\_on}{\overset{k\_off}{\rightleftarrows}} A_f$$

Next function which represents the amount of concentration in the preconcentrator must be fulfilled in as boundary condition:

$$\frac{\partial C_{A_W}}{\partial t} = -k\_off \cdot C_{A_W} + k\_on \cdot \left(C_{\max} - C_{A_f}\big|_W \right)$$

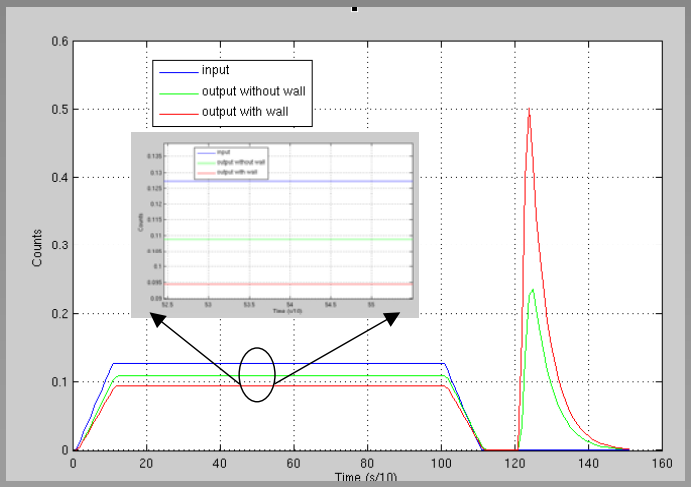
Most part of the air crosses the chamber without affecting the preconcentrator because the main flow is at relatively large distance of it. Using finite elements simulations a problem that experimentally was impossible to measure has been detected.

CHAMBER MODIFICATION



In order to improve this, we will use a "wall" which forces the air to go down near the preconcentrator surface.

We compare the amount of benzene adsorbed without wall and with the wall placed in the middle of the chamber.



	Analyte (u.a.)	Δ Analyte input-output (u.a.)	Amount of analyte adsorbed (%)	Retention factor improvement
Input	0.127			
Without wall	0.109	0.0185	14.53 %	1
With Wall	0.094	0.0329	25.84 %	1.78

Using simulations we have seen that the concentration factor improve 1.78 times. Experimentally, we have obtained an improvement of 1.85 factor . This value is really near to our simulations and it validate this.

So, thanks to simulations we have seen that using this wall, we are able to adsorb more analyte in the same period of time.

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