Fluid Flow Simulation of Preconcentration Membranes Using Finite Elements Tools.

R. Inglés[1*], J. Pallarés[2], J. L. Ramirez[1], E. Llobet[1]

[1]Dept. of Electronic, Electrical and Automatic Control Engineering, ETSE, Universitat Rovira i Virgili, Tarragona, Spain
[2] Department of Mechanical Engineering School of Chemical Engineering Universitat Rovira i Virgili, Tarragona, Spain

*Av Paisos Catalans, 24-26, 43007 Tarragona, Spain. E-mail: roser.ingles@urv.cat
Phone number: 0034.977.25.65.72 Fax: 0034.977.55.86.66

Abstract: We use finite elements simulations in order to study the fluid flow behaviour in a chamber of a preconcentrator. We realised that most part of the fluid does not affect our preconcentrator because it is going out the chamber at high distance above it and parallel to the preconcentrator. So, we are wasting most part of our fluid and we need a lot of time to have a good concentrator factor. We propose a chamber modification that forces the fluid to go near the preconcentrator and perpendicular to it, thus, improving concentration factor almost twice. With this new design we are able to concentrate more analyte in the same period of time.
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Keywords: Preconcentrator, fluid flow simulation, concentration simulation, microsensor system.

1. Introduction

Several toxic gases such as benzene are dangerous at low concentrations. At present, gas sensors are not able to detect concentrations on the limits required. That is why the design and implementation of preconcentrators is an important task. [1-4]

A preconcentrator is used to adsorb these traces of toxic gases during a period of time. Then, the full amount of adsorbed gas is released by means of a temperature step in the absorbent material, thus obtaining an increased concentration detectable by gas sensors.

We decided to simulate the chamber that we were using in experimental measurements in order to see the fluid flow behaviour. Thanks to simulation we realised that the gas sample to be sensed flew parallel to the preconcentrator surface, so most part of the analyte to be detected did not affect the absorbing material. We propose a new chamber design, by means of simulations, which was more efficient and economic that developed different chambers. Our proposal improves the chamber design forcing a larger amount of the sample flow to interact with the absorbent material increasing the concentration factor almost twice more.

In section 2 is explained the experimental chamber and the experimental set up used. In section 3 the fluid flow simulation is explained and results using the initial chamber are shown. In section 4 a new design is proposed and the comparison with previous design is developed. Finally, in section 5, conclusions are tipped.

2. Experimental Chamber

We have a cylindrical 6-mm diameter 3.8-mm height chamber. It has input and output 1.27-mm diameter tubes situated at 2 mm above the base (See Figure 1a).

Preconcentrator is located at the base. This is a 4 mm side square of porous alumina substrate with activated carbon deposited on top (See Figure 1b).

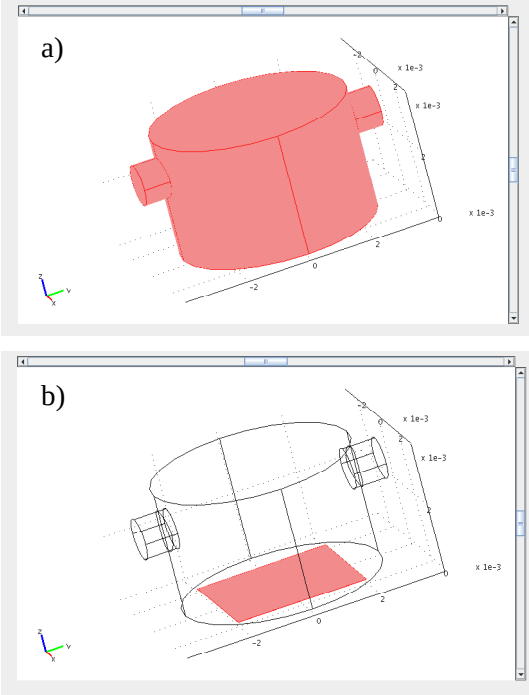

Figure 1: Preconcentrator Chamber: a) Chamber morphology b) Preconcentrator location

In the experimental set up, we introduce the preconcentrator in this chamber; a 100 ml/min flow of 150 ppb of benzene diluted in CO_2 is injected during 10 minutes at ambient temperature, so the preconcentrator is adsorbing the analyte.

Then we force a 100 ml/min flow of helium and we heat the preconcentrator to desorb all the benzene adsorbed in the material. Nowadays, we are using a gas chromatograph mass spectrometer (GCMS) to measure the desorption peak.

3. Fluid Flow Simulation

In order to study fluid flow behavior inside the chamber, we are coupling different models of Comsol Multiphisics: Weakly Compressible Navier-Stokes model for fluidic and Convection and Diffusion model for concentration.

We use the Weakly Compressible Navier-Stokes model for fluid flow because velocity of fluid depends on density variations (Formula 1). We introduce laminar velocity as input and constant pressure as output boundary condition.

$$\nabla \bullet (\rho u) = 0 \qquad (1)$$

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 on the wall (A_W). This is governed by the velocity of reaction which also depends of temperature.

$$A_W \underset{k\_on}{\overset{k\_off}{\rightleftharpoons}} A_f \qquad (2)$$

In the literature, the adsorption and desorption process is modeled using a linear function. [4-6]. Next function must be fulfilled in our preconcentrator:

$$\frac{\partial C_{A_W}}{\partial t} = -k\_off \cdot C_{A_W} + k\_on \cdot \left(C_{\max} - C_{A_f}\Big|_W \right) \qquad (3)$$

In our model, we use this function as preconcentrator boundary. During the adsorption phase we use a concentration in the chamber inlet and we measure the concentration in the outlet.

In Figure 2 we can see the streamline of velocity field. Most part of the air crosses the chamber without affecting the preconcentrator because the main flow is at a relatively large distance of the preconcentrator.

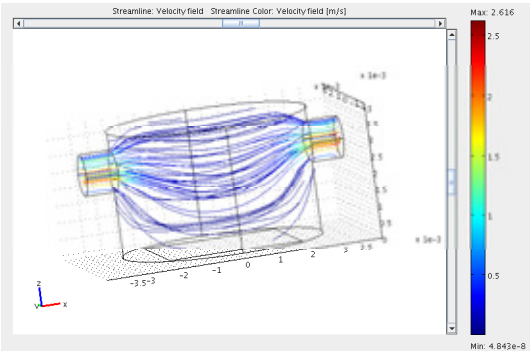

Figure 2: Simulation results in the initial chamber

4. Chamber modification

Most part of the air is crossing the chamber without affecting the preconcentrator. In order to improve this, we will use a "wall" which forces the air to go down near the preconcentrator surface.

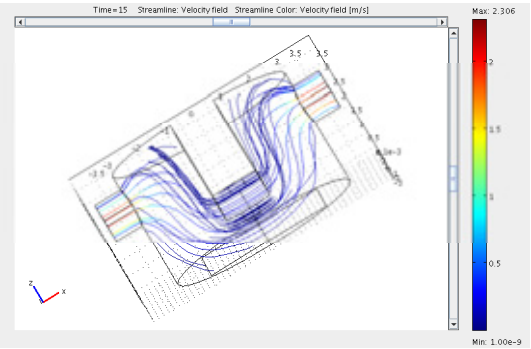

Figure 3: Simulation results with a wall

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

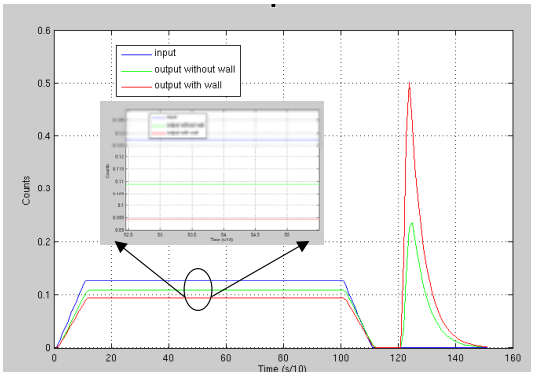

Figure 4: Comparison results

In Figure 4 we can see with a blue line the concentration that is going inside the chamber. From 0 to 11 seconds we are introducing benzene. At 11 seconds we stopped the adsorption phase. At 12 seconds we heat the preconcentrator in order to desorb the analyte concentrated. With green and red lines we can see the concentration going out the chamber without and with the wall respectively. We can see, in the adsorption phase, that using the wall we are adsorbing more analyte in the same period of time. This is also visible in the desorption peak. Now we will see the comparison in a table.

Table 1: Comparison of simulation results without and with wall for a 0.1273 u.a. input

	Analyte out (u.a.)	ΔAnalyte input-otput (u.a.)	Amount of analyte adsorbed (%)	Retention factor improvement
Without wall	0.1088	0.0185	14.53 %	1
With wall	0.0944	0.0329	25.84 %	1.78

In Table 1 we can see the value of counts during the adsorption phase. This is the amount of analyte going out of the chamber. Δ Counts is the difference between input and output analyte, so, with this value we extract the percentage adsorbed and the improvement is related to this.

This wall improves the preconcentrator adsorption capability in a 1.78 factor. So, using this wall, we are able to adsorb more analyte in the same period of time.

Experimentally, we have obtained an improvement of 1.85 factor, which is near to the simulation result.

5. Conclusions

We have used Comsol Multiphysics to simulate our preconcentrator chamber and we have detected a problem which was unknown. By using a new design developed with Comsol Multiphysics we are able to absorb more analyte in the same period of time than with our previous design.

Experimental measurements realised with the GCMS have validated our simulations, This simulations more economic, faster and simpler than experiments have contributed to understand the problem and to propose solutions.

6. References

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7. Acknowledgements

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