Modelization of Photoacoustic Trace Gases Sensors

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Introduction: Photoacoustic (PA) detection is a technique that can be used to detect trace levels of gases using optical absorption and subsequent thermal perturbations of the gases. PA sensors generally use acoustic resonances to enhance the signal level and to improve the minimum detectable concentration. A cell design based on two identical cells connected by thin capillaries that use the Helmholtz resonance was developed. This design allows noise reduction by performing differential measurements between the two cells. (Figure 1) presents the design of the cell and the pressure wave amplitude associated with the Helmholtz resonance

As the technique has favorable detection characteristics when the system dimensions are scaled down, the realization of a micro-cell design would be of great interest to generalize the use of such sensors. In order to optimize the cost of development for such sensors, we must be able to accurately predict the response of the sensor.

We describe here our first results about a macroscopic cell using two different methods : eigenmodes determination using the Pressure Acoustics module and Frequency dependent study using the Thermoacoutics module.

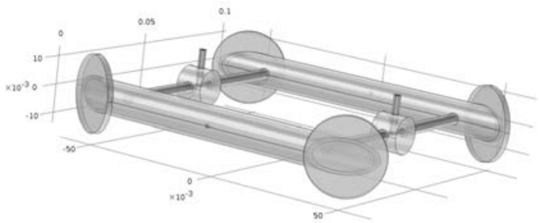

Figure 1 3D view of the glass PA cell

Computational Methods:
Photoacoustic devices use acoustic resonance to enhance signal to noise ratio. In order to determine the resonant frequencies of a complex-shape cell the homogeneous Helmholtz equation has to be solved [1-3].

$$\nabla^2 p(\vec{r}) + k^2 p(\vec{r}) = 0 \qquad \frac{\partial p}{\partial n} = 0$$

We use the Acoustics module in the Pressure acoustics interface to determine the eigenmodes of our cell. The response of the cell is the expressed as the expansion on the eigenmodes

$$p(\vec{r},\omega) = \sum_j A_j(\omega) p_j(\vec{r}) \qquad A_j(\omega) = i\frac{A_j\omega}{\omega^2 - \omega_j^2 + i\omega\omega_j/Q_j}$$

Coupling between acoustic mode and cell excitation

$$A_j = \frac{\alpha(\gamma-1)}{V_c}\int_{V_c} p_j^* I dV$$

Losses

$$1/Q_j = 1/Q_j^v + 1/Q_j^{s_\kappa} + 1/Q_j^{s_\eta}$$

$$1/Q_j^v = \frac{\omega_j}{c}\left[l_\eta + (\gamma-1)l_\kappa\right]$$

$$1/Q_j^{s_\eta} = \frac{1}{2}\left(\frac{c}{\omega_j}\right)^2 \frac{d_\eta}{V_c}\int_{S_c} \left|\nabla_t p_j\right|^2 dS$$

$$1/Q_j^{s_\kappa} = \frac{1}{2}(\gamma-1)\frac{d_\kappa}{V_c}\int_{S_c} \left|p_j\right|^2 dS$$

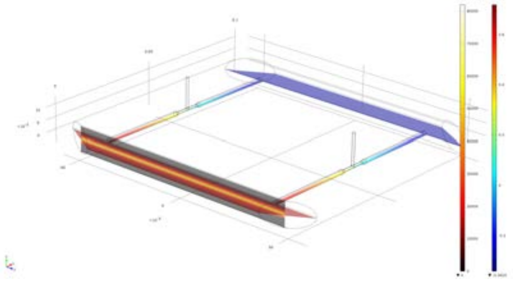

Figure 2. Laser beam intensity and pressure distribution of the Helmholtz mode

In order to optimize the design of a miniature photoacoustic cell another approach was used using Frequency dependent study in the Thermoacoustics interface of the Acoustics module. This interface is designed to accurately model acoustics in geometries with small dimensions. Tthe interfaces simultaneously solve for the acoustic pressure *p,* the particle velocity vector **u,** and the acoustic temperature variations *T* [4].

$$\begin{aligned}
&\nabla.\frac{1}{\rho_c}(\nabla p_t - \vec{q}) - \frac{k_{eq}^2 p_t}{\rho_c} = Q \\
&i\omega\rho_0\vec{u} = \nabla.\left(-p_2\vec{I} + \mu\left(\nabla\vec{u} + (\nabla\vec{u})^T\right) - \left(\tfrac{2}{3}\mu - \mu_B\right)(\nabla.\vec{u})\vec{I}\right) \\
&i\omega\left(\frac{\partial\rho_0}{\partial p_2}p_2 + \frac{\partial\rho_0}{\partial T}T\right) + \rho_0\nabla.\vec{u} = 0 \\
&i\omega\rho_0 c_p T = -\nabla.(-k\nabla T) - i\omega p_2\frac{T_0\partial\rho_0}{\rho_0\partial T}
\end{aligned}$$

Results: The simulation with the Pressure acoustics interface has been compared to experimental determination of the photoacoustic cell response : Quality factors and resonance frequencies were compared with experimental ones demonstrating a very good agreement.
Similar results where obtained using the Thermoacoustics interface.

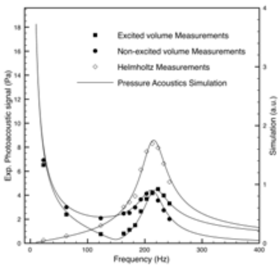

Figure 3. Comparison between Measurements and simulation using Pressure acoustics interface

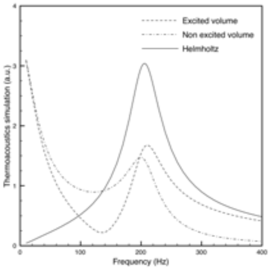

Figure 4.Frequency response of the macroscopic cell determined with the Thermoacoustics interface

Conclusions: Resonant frequencies, eigenmodes and quality factors of a Differential Helmholtz resonant photoacoustic celle were determined using the “Acoustics” module of the Comsol Multiphysics 4.2. An excellent agreement was found with experimental points.
In order to prepare future work on miniaturized photoacoustic cells where an acoustic boundary layer with significant losses appears, the “Thermoacoustics” interface was also used and gave similar results.

References:

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