Simulation of Helmholtz Resonators for Optical Gas Sensing: Comparison Between Pressure Acoustics and Thermoacoustics

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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. 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.

The Acoustics Module of COMSOL Multiphysics® has been used to solve the equations of *pressure acoustics* and to predict the response of such a sensor. A very good agreement with experimental determinations has been observed for a macroscopic cell [1]. When the PA cell dimensions are reduced to the millimeter range, pressure acoustics is no longer accurate and another formulation must be used [2]. We present comparisons between experimental determination of the cell frequency response and the two kinds of simulation performed using COMSOL Multiphysics®. Figure 1 presents three different cells with decreasing dimensions. Figure 2 presents the cell geometry used in COMSOL Multiphysics® with laser beam intensity and the pressure distribution.

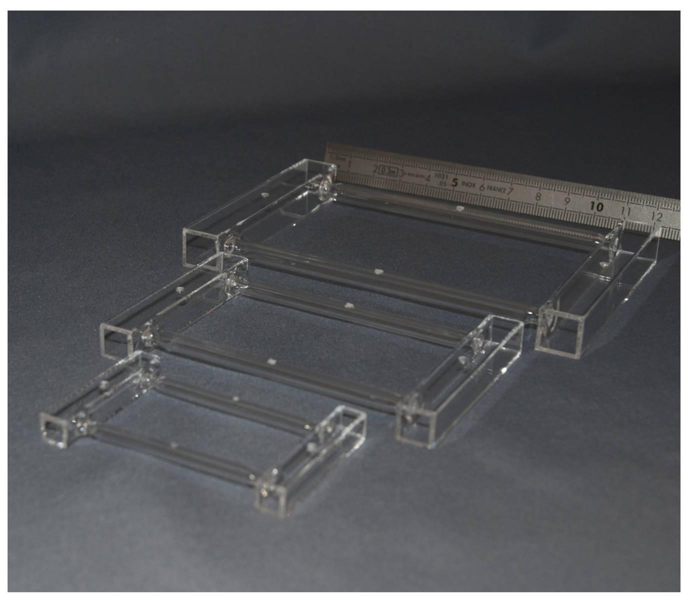

Figure 1 : 3 different cells

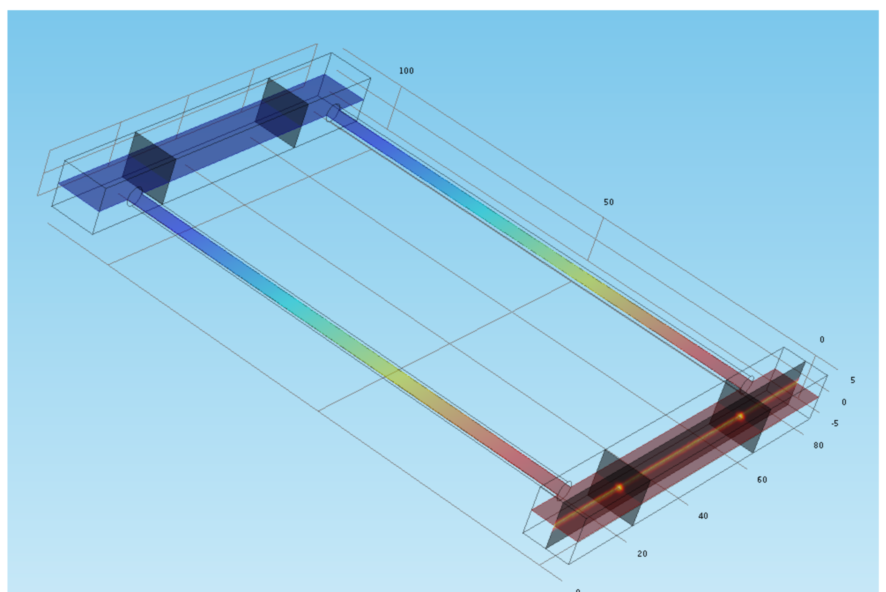

Figure 2. Laser beam intensity and pressure distribution of the Helmholtz mode

Computational Methods:
Two different methods were used : expansion on the eigenmodes of the cell determined using the *pressure acoustics* interface [3,4].

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

The Acoustics Module in the *pressure acoustics* interface was used to determine the eigenmodes of our cell. The response of the cell is the expressed as the expansion on the eigenmodes

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

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

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

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

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

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

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

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

Results: For the largest cell (8 cm optical path length, ϕ=4 mm capillary), the simulation with the *pressure acoustics* interface has been compared to experimental determination of the photoacoustic cell response : Quality factors, resonance frequencies and response of the cell were compared with experimental ones demonstrating a good agreement (Figure 3). In a second step, the cell response has been studied using the *thermoacoustics* interface. Figure 4 presents the compared value for resonance frequencies using the different interfaces. The agreement is highly dependent on mesh quality for the *thermoacoustics* interface.

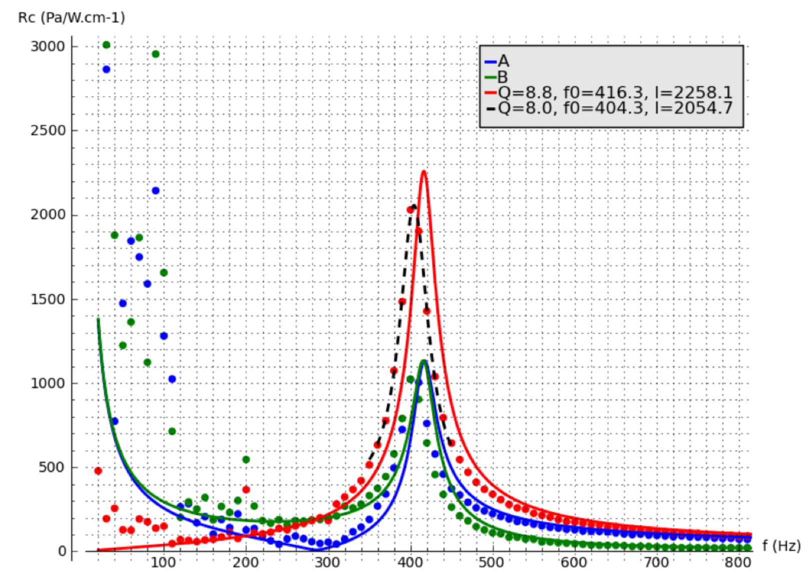

Figure 3 : Experimental response vs simulated response *(pressure acoustics*, 8 cm cell)

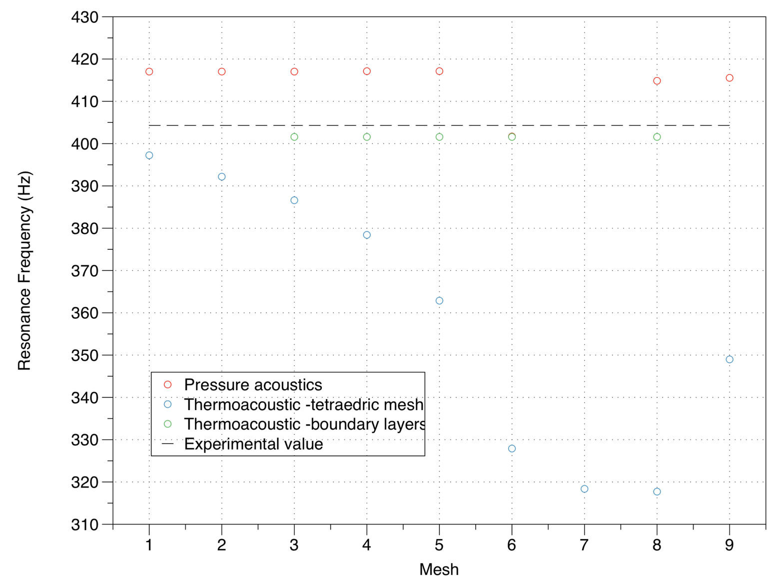

Figure 4 : Comparison between experiments, *pressure acoustics* and *thermoacoustics*

The same simulations were performed for the smallest cell (2 cm optical path length, ϕ=1 mm capillary). Figure 5 presents the compared values for resonance frequencies using the different interfaces. Figure 6 presents the calculated response (Frequency study, *thermoacoustics* interface).

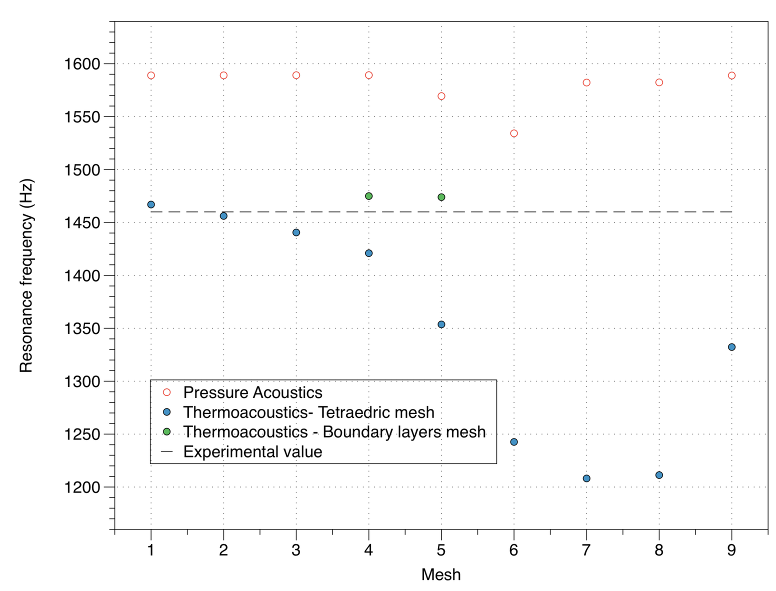

Figure 5 : Comparison between experiments, *pressure acoustics* and *thermoacoustics*

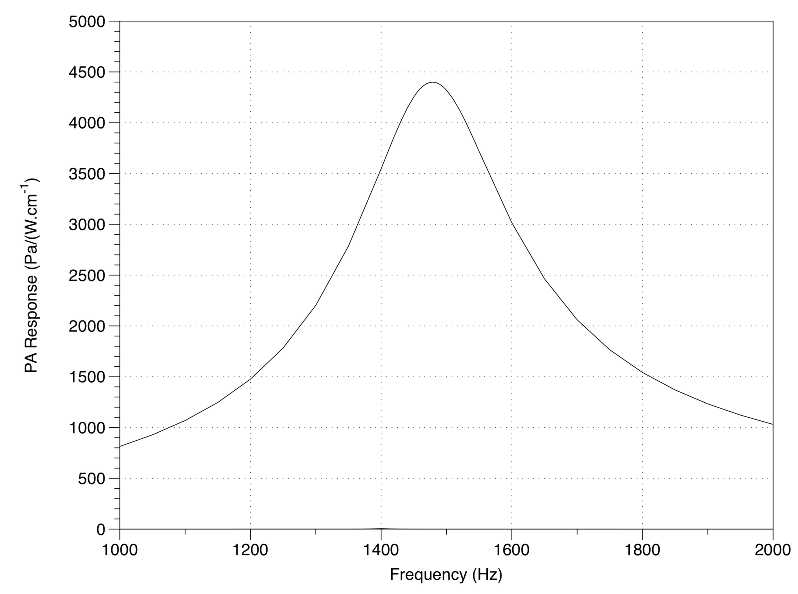

Figure 6 : Simulated response (*thermoacoustics*, 2 cm cell)

Conclusion: We performed comparison between experimental characterization and numerical simulations using *pressure acoustics* and *thermoacoustics* formulations of PA cells of various dimensions. When decreasing the cell dimensions, the *thermoacoustics* formulation gives more accurate values for the main characteristics of the PA cell (Resonance frequency, quality factor and response). For the studied cells, the *pressure acoustics* formulation overestimates the resonance frequency (~3% for the 8 cm cell, ~8 % for the 2 cm cell) whereas the *thermoacoustics* formulation gives a resonance frequency within 1% of the experimental determination.

References:
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