

Tailoring Acoustic Modes for Ultra-Sensitive Photoacoustic Gas Detection

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Summary:

Photoacoustic gas sensing is experiencing rapid development due to its high sensitivity and selectivity. In this work, we introduce a novel methodology for the design of photoacoustic cells based on a rigorous analysis of acoustic eigenmodes and excitation mechanisms. We demonstrate that the nature of excitation (acoustic versus photoacoustic) strongly influences modal selection and efficiency. A finite element framework is developed to identify optimal resonant modes under realistic conditions. Based on this approach, a photoacoustic system was fabricated and experimentally validated. High sensitivity detection of volatile organic compounds is demonstrated, achieving detection limits in the ppb range.

Keywords: photoacoustic spectroscopy, acoustic resonators, gas sensing, VOC detection

Background, Motivation and Objective

Trace gas detection is crucial for applications ranging from medical diagnostics to environmental monitoring. Photoacoustic spectroscopy (PAS) offers high sensitivity and background-free detection, further enhanced by resonant cells operating above 1 kHz to reduce noise. Various geometries have been proposed, including cylindrical [1], T-type [2], H-type [4], TT-type [5], differential Helmholtz designs [6], and other advanced configurations mainly based on geometric optimization. However, while these designs exploit acoustic eigenmodes, the choice of mode is rarely physically justified. In this work, we address this gap by identifying, from a modal perspective, the modes most favorable to photoacoustic excitation. We show that the fundamental mode is not always optimal and introduce a physics-based approach, based on eigenmode analysis and optical–acoustic overlap, to select resonant modes maximizing the photoacoustic response, enabling more efficient and sensitive cell designs.

Material and Method

We propose a multi-physics finite element framework combining acoustic and photoacoustic modeling. The acoustic field is described by the linearized wave equation with either boundary-driven excitation (pressure or velocity) or volumetric photoacoustic generation proportional to absorbed optical energy.

Eigenmodes are first computed from the homogeneous Helmholtz problem, and the frequency response is obtained by introducing excitation terms under realistic boundary conditions, including thermoviscous losses.

A key contribution is the direct comparison

between excitation mechanisms. Acoustic excitation mainly couples through boundary conditions, while photoacoustic excitation preferentially excites modes with strong spatial overlap with the optical absorption profile.

This leads to the emergence of dominant resonant states, including modes approaching quasi-bound states in the continuum (quasi-BIC), which enhance acoustic confinement and signal amplification.

Results and discussion

The finite element model is first validated under acoustic excitation using a surface boundary condition mimicking a loudspeaker. The system exhibits classical resonator behavior with a dominant fundamental mode under rigid-wall conditions, but the response is strongly affected by boundary conditions and losses, which redistribute energy among higher-order modes (Fig. 1(b)).

The analysis is then extended to the photoacoustic regime, where a volumetric heat source induced by a Gaussian laser beam in stubs d_2 and d_3 drives the excitation (Fig. 1(a)). In this case, modal selection is governed by spatial overlap between optical absorption and acoustic eigenmodes. Simulations show that the strongest photoacoustic coupling is obtained for the second eigenmode, rather than the fundamental one (Fig. 1(b)). This mode is particularly interesting, as it corresponds to perfect absorption under excitation from infinity at the entrance of d_3 , and becomes a bound state in the continuum (BIC) when $d_1 = d_2$. In this regime, variations of d_3 have negligible impact on the modal response, making this configuration highly attractive for photoacoustic spectroscopy, since d_3 can be

used as a gas inlet or reduced without affecting the measurement, ensuring both flexibility and robustness.

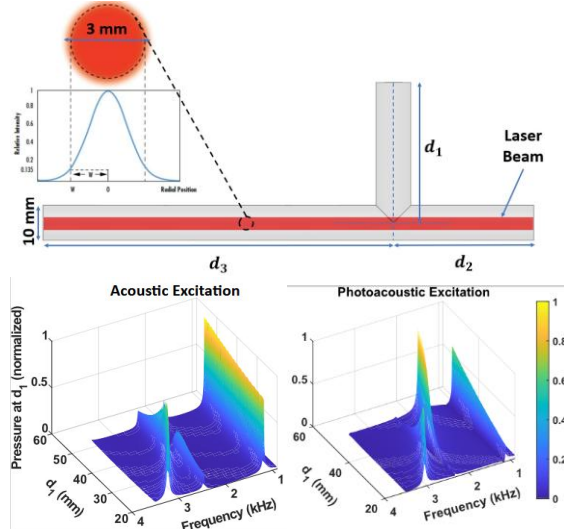


Fig. 1: a) Schematic of the Gaussian laser injected into stubs d_3 and d_2 , with its intensity profile. b) 3D map of the simulated pressure versus d_1 and frequency under photoacoustic and acoustic excitation.

For experimental validation, we developed an aluminum photoacoustic cell composed of three stubs (Fig. 3.a). The geometry was selected to excite the BIC state, with $d_1 = d_2 = 40$ mm. Pressure field at the frequency of BIC state is shown on Figure 3.b. Sensitivity measurements were performed by injecting isopropanol vapor with calibrated generator through the d_3 stub, which also serves as the gas outlet. The system employs a MIRCAT QCL laser (Daylight Solutions) emitting at $8.73\ \mu\text{m}$ (maximum absorption of isopropanol), with modulation provided by a mechanical chopper tuned near the acoustic resonance frequency. A TDK membrane microphone is positioned at the end of the d_3 stub for pressure measurement.

Figure 3 shows the measured photoacoustic signal for different isopropanol concentrations. The signal was acquired using a high-resolution system (200 kHz sampling rate, 24-bit resolution), and the square root of the PSD is plotted in linear scale, revealing a high signal-to-noise ratio. In pure air, the background level is extremely low. Wavelength-dependent tests (not shown here) confirm good agreement with the isopropanol absorption spectrum. The system exhibits good linearity, with an estimated sensitivity of about 6 mV/ppm, enabling a projected detection limit in the few-ppb range.

Acknowledgements

This work was funded by the region Hauts de France and the INSERM through the project SNOOP-I. The authors thank RENATECH, the French national nanofabrication network.

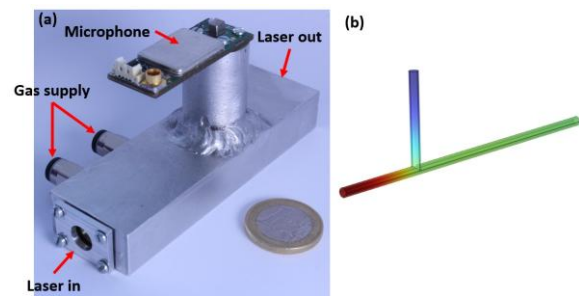


Fig. 3: a) Photograph of the fabricated acoustic cell. b) Pressure field distribution at the frequency of the BIC mode.

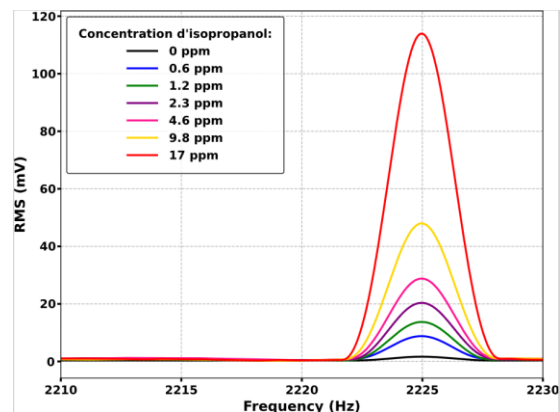


Fig. 4: Measured photoacoustic signal for different isopropanol concentrations.

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