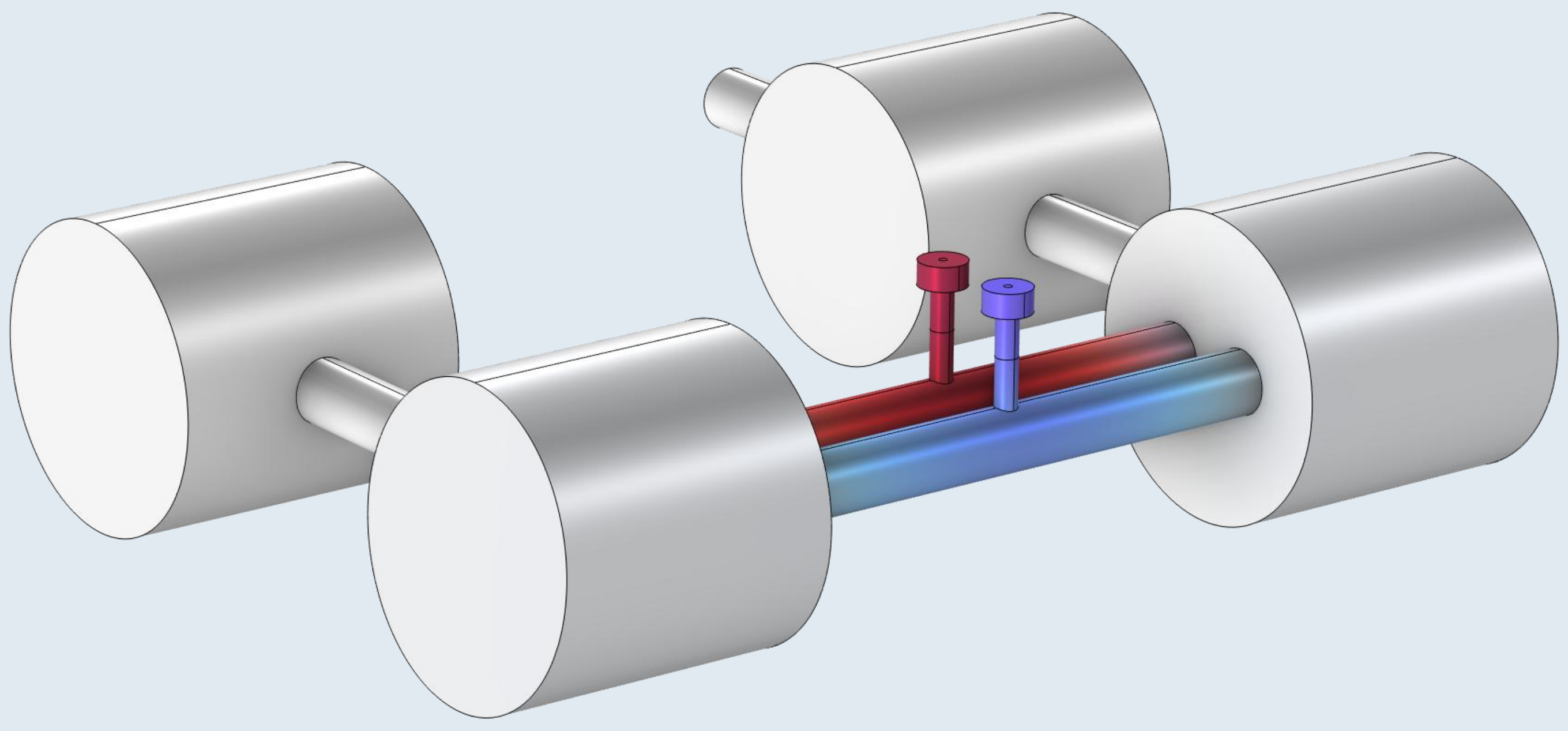

Validated Numerical Model and Simulation-Based Design Optimization of a Photoacoustic Cell

We developed and validated a finite element model of a photoacoustic cell and applied it to optimize the geometry for improved performance.

Á. Csókási[1, *], P. Végh[1], I. Magashegyi[1], Z. Bozóki[1]

1. Centre of Excellence for Interdisciplinary Research, Development and Innovation of the University of Szeged, Szeged, Hungary.

Introduction

Photoacoustic spectroscopy (PAS) enables highly sensitive gas detection by directly measuring the sound generated from light absorption, and it has found applications in environmental monitoring, medical diagnostics, and the oil and gas industry. The performance of PAS systems strongly depends on the acoustic design of the photoacoustic cell (PAC), with background signals from laser–window interactions being a significant limitation. Building on methods documented in the literature, we used finite element modeling for our existing differential, longitudinal PAC. The model was validated against experimental data. Based on this, we performed a simulation-based design optimization, varying buffer dimensions to study their effect on the signal-to-background ratio (SBR). The workflow shows how COMSOL Multiphysics® can help design more efficient photoacoustic sensors and reduce the number of prototyping iterations.

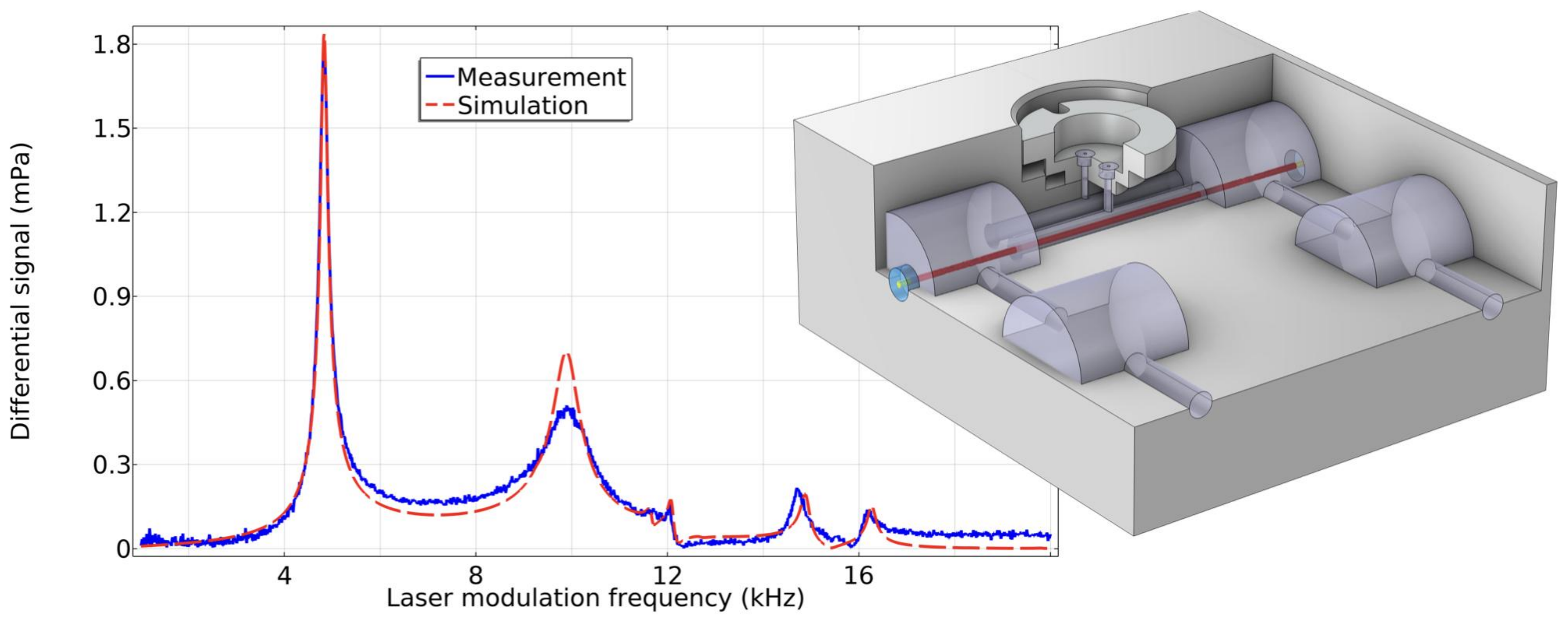

Figure 1. Left: Measured and simulated (FEM) differential signal. Right: The CAD of the used PAC in the simulation.

Methodology

The geometry of the chamber was reconstructed from CAD files and modeled as a fluid domain filled with N_2–H_2O mixture. Simulations were performed using the *Pressure Acoustics, Frequency Domain* interface. Losses were included through an equivalent fluid model and thermoviscous boundary conditions. The microphones were modeled as impedance boundaries, and the laser excitation was implemented as a Gaussian heat source.

The frequency response was calculated by the Helmholtz equation:

$$\left(\nabla^2 + \frac{\omega^2}{c^2}\right) p(\boldsymbol{r}, \omega) = \frac{\gamma - 1}{c^2} i\omega Q_{heat}(\boldsymbol{r}, \omega)$$

Results

Simulations with separate excitation sources showed that sample heating excites both the ring and longitudinal modes, while window heating excites the longitudinal mode significantly, which contributes to the background signal. Increasing buffer length caused a phase manipulation effect: in the longitudinal mode, the in-phase pressures in the two resonators nearly cancel in differential operation, strongly suppressing the background signal. Parametric optimization revealed that the PA signal from sample heating remained roughly constant, whereas the background decreased. At $l_b = 0.75 \cdot l_r$ and $d_b = 12$ mm, the SBR improved from 1.56 to 57.7, corresponding to a ~ 37-fold enhancement.

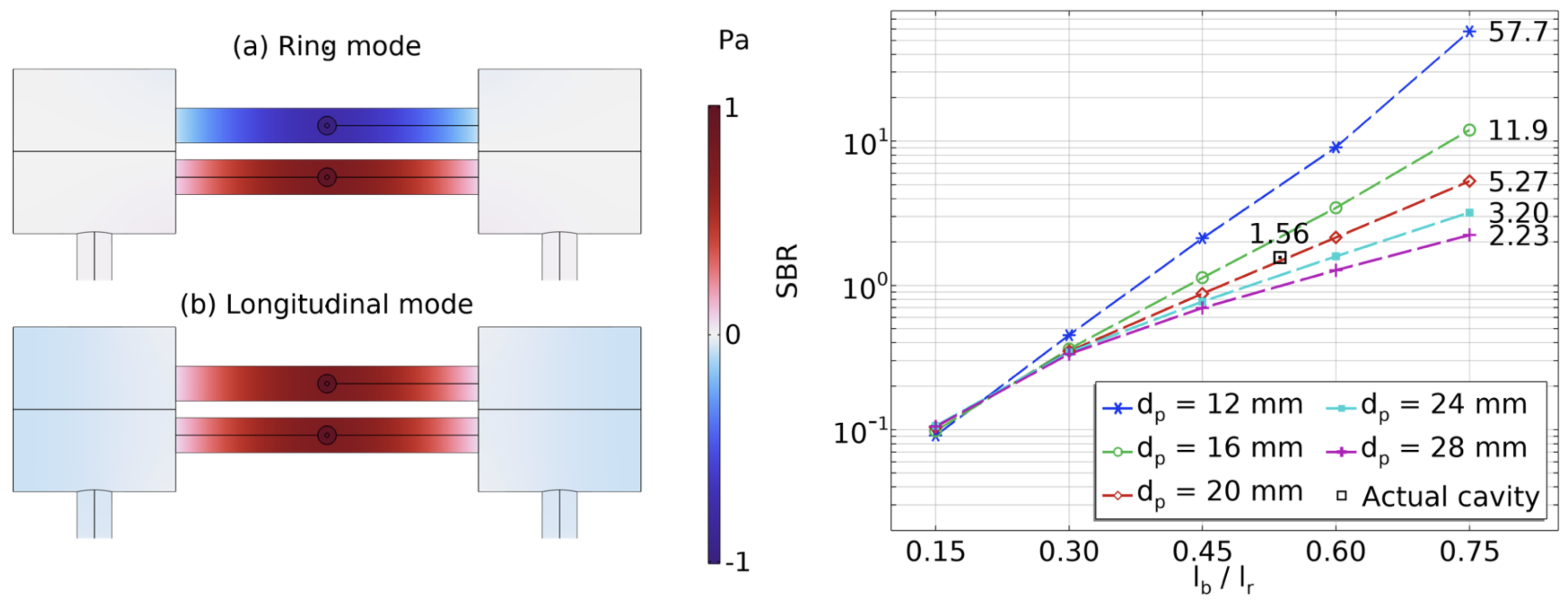

Figure 2. Left: Fundamental PAC modes in the 4.5–5.5 kHz frequency range. Right: The SBR vs. buffer length for different buffer diameters.

REFERENCES

1. A. Miklós et al., "Application of acoustic resonators in photoacoustic trace gas analysis", *Rev. Sci. Instrum.*, vol. 72, pp. 1937-1955, 2001.
2. B. Baumann et al., "Finite element calculation of photoacoustic signals", *Appl. Opt.*, vol. 46, pp. 1120-1125, 2007.
3. M. I. Cotterell et al., "Optimizing the performance of aerosol photoacoustic cells using finite element model. Part 2: Application to a two-resonator cell", *Aerosol Sci. Technol.*, vol. 53, pp. 1128-1148, 2019.

Excerpt from the Proceedings of the COMSOL Conference 2025 Amsterdam