DESIGN OPTIMIZATION OF A PHOTOACOUSTIC SYSTEM FOR GAS DETECTION IN EXHALED BREATH

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Abstract Exhaled breath analysis is a promising non-invasive approach for detecting disease-related biomarkers, including nitrogen dioxide (NO_2), which is associated with airway inflammation. A compact photoacoustic spectroscopy (PAS) system was developed using a 405 nm LED source and a resonant acoustic chamber optimized for NO_2 detection. Focused optical excitation enhances localized absorption, generating an acoustic signal detected by a MEMS microphone. The system demonstrated a good response to 50 ppm gas variation, supporting its suitability for low-cost breath analysis applications.

***Keywords*:** Photoacoustic spectroscopy, Biomedical monitoring, Breath biomarkers, Gas sensing, multi-gas detection, Volatile organic compounds (VOCs), Low-cost gas sensor, Environmental monitoring

1. INTRODUCTION

Exhaled breath contains a complex mixture of volatile organic compounds (VOCs), many of which have been identified as non-invasive biomarkers for respiratory and metabolic conditions. Among them, nitrogen dioxide (NO_2) plays a significant role as an indicator of airway inflammation and oxidative stress, particularly in patients with asthma or chronic obstructive pulmonary disease (COPD) [1].

Photoacoustic spectroscopy (PAS) is a powerful technique for detecting trace gases with high sensitivity and selectivity, based on the generation of acoustic waves from modulated light absorption [2–4]. While PAS systems commonly employ laser sources for their narrow spectral bandwidth and high excitation efficiency, their use often involves significant costs, increased power consumption, and reduced portability. Moreover, they are frequently combined with lock-in amplifier-based readout systems, which further limit their practicality. As a result, most commercially available devices are designed for laboratory use and are not easily portable [5, 6]. To address these limitations, light-emitting diodes (LEDs) have been investigated as alternative excitation sources. In particular, LEDs offer advantages in terms of cost, size, and integration potential, making them suitable for compact and low-power PAS platforms. However, their broad emission profile and lower optical power density introduce challenges in achieving efficient, localized excitation within resonant acoustic chambers.

This work investigates the design and performance of a LED-based PAS system tailored for NO_2 detection in exhaled breath. The system aims to combine low cost, compactness, and adequate sensitivity through the integration of optimized optical and acoustic subsystems. The following sections present the detailed design methodology, simulation framework, and experimental validation of the proposed approach.

2. METHODS AND PROCEDURES

The optical source used is the Roithner SMB1N-405V, a high-power violet LED emitting at 405 nm, with a typical optical power of 710 mW at 500 mA. The PAS chamber, showing a resonance frequency (for the 1st eigenmode) of 4.120 kHz, was equipped with a MEMS microphone for acoustic signal detection. The system architecture was validated through computational simulations [7, 8].
Computational Fluid Dynamics (CFD) analyses ensured optimal gas flow uniformity through the chamber, while Finite Element Method (FEM) simulations confirmed the acoustic resonance properties. The toroidal PAS chamber was designed to confine the gas and ensure optimal acoustic resonance to enhance the photoacoustic signal [7]. The gas inlet and outlet were placed at the nodes of the standing wave to reduce airflow disturbances, while the optical source and microphone were aligned with the antinodes to maximize the photoacoustic signal amplitude. Numerical simulations emphasized also the importance of maintaining point-like excitation [7], as diffuse light distribution within the chamber might lead to significant signal degradation. To enable accurate, localized excitation, an optical system was developed to focus the light into a 3mm diameter aperture located 180° opposite the microphone, as shown in Figure 1.

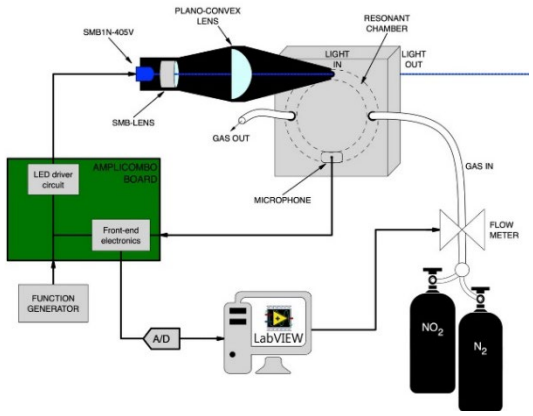

Figure 1. Experimental PAS setup with detail of the optical system with SMB1N-405V LED, SMB-LENS, focusing optics, 3 mm entry hole, and exit window.

The LED broad beam (±63°) was first collimated using a Roithner SMB-LENS (10° FWHM divergence) and then

focused by a plano-convex lens (Thorlabs LA1951) with a focal length of 25 mm and a diameter of 1 inch. The resulting optical setup produced a beam waist of approximately 4 mm, as measured using the knife-edge technique. Although this represents an improvement over unfocused LED excitation, a portion of the optical power is lost due to the aperture constraint, indicating considerable potential for further optimization. To prevent stray light reflections and mitigate distributed gas excitation, a dedicated exit window was implemented on the chamber, enabling the transmitted light to leave the system after passing through the gas sample. This design choice ensured that only the gas within the focused interaction volume contributed to the photoacoustic signal, improving the signal-to-noise ratio.

The system was driven by a custom LED driver enabling sinusoidal modulation at the resonant frequency, while signal acquisition was managed through a custom designed frontend electronics module (*AmpliCombo* board developed by University of Siena), responsible for amplifying and band-pass filtering the detected photoacoustic signal [9, 10]. To minimize ambient noise, the experimental setup was enclosed in an acoustically isolated enclosure. The gas flow during the measurements was kept constant at 200 mL/min, and the different gas concentrations were achieved using an accurate system of flow meters, remotely controlled by the user. The various target gas concentrations were obtained by certified gas cylinders by mixing a 50 ppm NO_2 flow with N_2 as carrier gas flow at the desired concentrations.

3. Results and Discussion

The system response was evaluated at two driving currents (peak-to-peak values): 250 mA (estimated optical power ~366 mW) and 300 mA (~431 mW). In both cases, the PAS signal amplitude was consistent with the step changes in NO_2 concentration in the 0–50 ppm range. The output signal from the microphone was processed by a demodulator integrated into the front-end electronics, allowing observation of a final DC output response from the system [7]. No saturation effects were observed, confirming the robustness of the system under both operating conditions. As expected, increasing the driving current from 250 mA to 300 mA led to an enhancement in the absolute signal amplitude. However, this also resulted in a greater variability around the mean value, mainly due to an increased noise floor associated with diffuse gas excitation. This trade-off underscores the importance of balancing optical power and electronic gain to achieve adequate gas sensitivity while preserving linearity and staying within the ADC's dynamic range.

In Figure 2, the traces represent the average of 9 repeated measurements for each condition, with the baseline offset at 0 ppm subtracted. The signal-to-noise ratio (SNR), computed using the full set of real-time acquisitions, was 32.93 dB at 250 mA and 33.36 dB at 300 mA. To assess measurement repeatability, the coefficient of variation (CV) at 50 ppm was found to be 3.14% for 250 mA and 4.68% for 300 mA. Corresponding 95% confidence intervals were ±10.0 mV and ±15.9 mV, respectively. These values indicate good precision and reproducibility of the measurements, with slightly increased variability at higher excitation power. The signal fluctuations observed at 50 ppm in Figure 2 are attributed to non-ideal behavior of the electrovalve-based flow mixer.

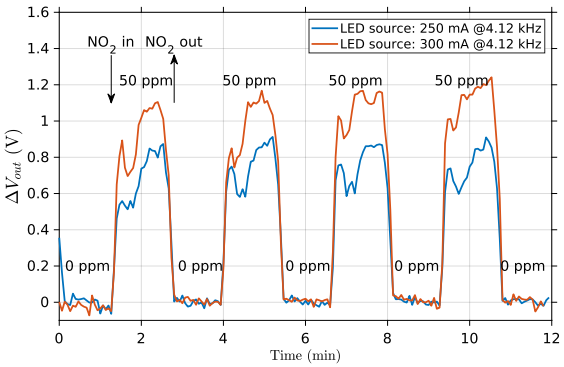

Figure 2: Graph of PAS signal evolution over time with step changes variations in NO_2 concentration (0–50 ppm) evaluated at 250 mA and 300 mA.

4. Conclusions

In this work, we presented a compact photoacoustic spectroscopy system for NO_2 detection in exhaled breath, combining a 405 nm LED source with a custom-designed resonant acoustic chamber. The optical system was optimized to achieve localized excitation. Experimental results confirmed the system's ability to track NO_2 concentrations in the 0–50 ppm range with clear signal variation and without saturation. The trade-off between signal intensity and noise at higher LED currents underlined the importance of optical confinement and careful gain tuning. The modularity and low cost of the setup make it a suitable candidate for portable diagnostic tools. Future work will focus on improving optical coupling efficiency, exploring alternative excitation sources such as laser diodes for enhanced selectivity, and integrating advanced signal processing methods to reduce acquisition time and improve sensitivity.

References

[1] M. Sigrist, "Air Monitoring by Laser Photoacoustic Spectroscopy," in Air Monitoring by Spectroscopic Techniques, Wiley, 1994, pp.163–238

[2] M. Lassen et al., "A versatile integrating sphere based photoacoustic sensor for trace gas monitoring," Opt. Express, vol. 19, no. 3, pp. 3169–3177, 2011.

[3] J. Hodgkinson and R. P. Tatam, "Optical gas sensing: a review," Meas. Sci. Technol., vol. 24, no. 1, p. 012004, 2013.

[4] A. Miklós, P. Hess, and Z. Bozóki, "Application of acoustic resonators in photoacoustic trace gas analysis and metrology," Rev. Sci. Instrum., vol. 72, no. 4, pp. 1937–1955, 2001.

[5] J. Pangerl, P. Sukul, T.Rück, P. Fuchs, S. Weigl, W. Miekisch, R. Bierl, F.M. Matysik, An inexpensive UV-LED photoacoustic based real-time sensor-system detecting exhaled trace-acetone, Photoacoustics,Vol. 38, 2024, 100604,

[6] Trace Gas. "PAS Analyzer product line," 2024. [Online]. Available: http://www.trace-gas.com/gas-analyzers/pas-analyzer/

[7] A. Fort et al., "Highly Sensitive Photoacoustic NO2 Measurement System Based on an Optimized Ring-Shaped Resonant Cell," IEEE Trans. Instrum. Meas., vol. 72, 2023.

[8] E. Panzardi et al., "A Photoacoustic-Based Measurement System for Dual Detection of NO2 and CO2 in Combustion Exhaust Gases," IEEE Trans. Instrum. Meas., vol. 72, 2023.

[9] A. Fort, M. Mugnaini, E. Panzardi and V. Vignoli, "Toward a compact low-cost electronic interface for photoacoustic based gas sensors," *2024 I2MTC*, Glasgow, United Kingdom, 2024, pp. 1-6,

[10] S. M. Cristescu et al., "Laser-based systems for trace gas detection in life sciences," Appl. Phys. B, vol. 92, no. 3, pp. 343–349, 2008.