DESIGN, SIMULATION AND STRUCTURAL OPTIMIZATION OF A LONGITUDINAL ACOUSTIC RESONATOR FOR TRACE GAS DETECTION USING LASER PHOTOACOUSTIC SPECTROSCOPY (LPAS)

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Abstract: An LC circuit model is used to simulate 1D acoustic resonator. It is designed for CO photoacoustic spectroscopy. The effects of the structural parameters, quality factor and resonant frequency are analyzed. The optimized dimension of the buffer volume is investigated and calculated. Also, the effects of the ambient temperature and gas flow velocity on the resonant frequency are simulated.

1. INTRODUCTION

Laser photoacoustic spectroscopy (LPAS) is a widely recognized technique to measure trace gases at parts-per-million (ppm) or parts-per-billion (ppb) level using semiconductor laser in the near infrared range. This technique is based on the generation of an acoustic wave in a gas excited by a modulated laser beam at a wavelength corresponding to an absorption line of the gas species, and on the detection of this sound using a microphone [1].

Modulated light sources mostly apply to gas phase analysis in frequency domain. In this case, performance of an LPAS system can be improved by resonance amplification when the absorption takes place in an acoustic resonator. Thus, a crucial part of a PA gas detection setup is the cell in which the PA signal is generated and detected. The optimized design of acoustic resonator is important for the sensitivity of the PA gas detection in order to reduce the influence of the background noise and improve its signal-to-noise ratio (SNR) [2]. The most frequently applied cavity resonator is the cylinder, with symmetry that coincides well with that of a laser beam propagating along the cylinder axis or one of its eigenmodes. The characteristic features of these different eigenmodes of a cylindrical resonator are illustrated in Fig.1. Only oscillations at the resonant frequencies of these eigenmodes are amplified and they will significantly gain energy.

In this paper, based on the photoacoustic theory, an LC circuit model is used for the simulation of 1D longitudinal acoustic resonator. As an application of the model, a 1D acoustic resonator for CO photoacoustic spectroscopy is studied.

2. THEORETICAL ANALYSIS AND MODELING

The physical quantities characterizing the acoustic and thermal processes in resonators are the temperature $T$, pressure $p$, gas density $\rho$, and the gas flow velocity $u$. The acoustic differential equations of a 1D lossless system can be written as [2]

$$\frac{\partial p}{\partial t} + \rho \cdot c^2 \frac{\partial u}{\partial x} = (\gamma - 1) H$$  \hspace{1cm} (1)

$$\frac{\rho \cdot \partial u}{\partial t} + \frac{\partial p}{\partial x} = 0$$  \hspace{1cm} (2)

Where $S$ is the cross-sectional area of the resonator and $H$ is the heat added per unit volume. These equations are very similar to the corresponding power transmission line equations:

$$\frac{\partial V}{\partial t} + \frac{1}{C'} \cdot \frac{\partial I}{\partial x} = 0$$  \hspace{1cm} (3)

$$L' \cdot \frac{\partial I}{\partial t} + \frac{\partial V}{\partial x} = 0$$  \hspace{1cm} (4)

Where $L'$ and $C'$ are the inductance and capacitance of unit length of the cable, respectively. Based on the similarity of the above pairs of equations sound propagation in pipes can be treated similarly to the propagation of electromagnetic waves in cables [3]. Thus, in equivalent LC circuit
model of transmission line, the sound pressure $p$ and volume velocity $u$ can be replaced with voltage $V$ and current $I$ respectively and the driving source analogous to $H$ can be represented by $I_0$ [4] as follows

$$I_0 = (\gamma - 1) \frac{P_L \alpha \cdot I}{(\rho \cdot c^2)}$$

(5)

Where $P_L$, $\alpha$, $\gamma$ are the power of the laser, absorption coefficient, and the specific heat ratio of the gas respectively, while $c$ and $l$ are the velocity of sound and length of resonator, respectively.

Therefore, we can define the parameters of the LC Circuit as follows

$$L = \rho \cdot l/S$$

(6)

$$C = S \cdot l / (\rho \cdot c^3)$$

(7)

$$R = \omega \cdot [(\gamma - 1) \cdot d_k + d_d] \cdot \frac{\rho \cdot l \cdot D}{2 \cdot S^2}$$

(8)

Where $d_k$ and $d_d$ are the thicknesses of viscous and thermal boundary layers respectively, and $\omega$ is the working frequency. The input impedance $Z_{in}$, resonant frequency $\omega_0$, and quality factor $Q$ can be determined as follows

$$Z_{in} = \frac{1}{i \omega C} / (R + i \omega L) = \frac{L/C}{R + i(\omega L - 1/\omega C)}$$

(9)

$$\omega_0 = 2\pi \cdot f_0 = \frac{\pi \cdot c}{l} = \frac{1}{\sqrt{LC}}$$

(10)

$$Q = \frac{\omega_0 L}{R} = \frac{2 \cdot S}{D \cdot [(\gamma - 1) \cdot d_k + d_d]}$$

(11)

And the output voltage proportional to PA signal is

$$V_{PA} = [I_0] \cdot [Z_{in}] = [I_0] \cdot \frac{L/C}{\sqrt{R^2 + (\omega L - 1/\omega C)^2}}$$

(12)

If the quality factor is much larger than 1, the acoustic resonator factor is

$$F = (\gamma - 1) \cdot \frac{1/2}{\omega_0} \cdot V \cdot Q$$

(13)

When the resonator works at resonant frequency, we should take the harmonic pressure distribution of the standing wave within the resonator into consideration. Therefore, the resonator length $l$ in equations (5–8) should be replaced by the defined effective length [3]

$$l_{eff} = (1/\pi) \cdot l$$

(14)

If the gas sample has high heat conductivity and dynamic viscosity, the differential equations (1, 2) is not valid, thereby, the LC model is also ineffective.

3. RESULTS AND DISCUSSION

3.1. Design of the 1D Longitudinal Acoustic Resonator for CO Detection

The wavelength of the laser source must be selected to coincide with the absorption line of the gas species [1, 2]. Thus, with consideration of Carbon monoxide (CO) molecules as a target molecule, the typical DFB diode laser with power of $P_{laser} = 10 mW$ and wavelength around $\lambda = 1563.6 mm$ [5] is selected.

The designed PA cell consists of a polished brass resonator ($l = 40 mm$, $r = 2 mm$), with two buffer volumes at each end ($l_h = 20 mm$, $r_h = 10 mm$). The calculated resonant frequency is $f_{res} = 4341.8 Hz$ with quality factor $Q = 42.03$ and PA cell constant $F = 2458 Pa \cdot cm/W$. The simulation is performed based on the resonator with the above parameters and dimensions if not specially mentioned.

3.2. Temporal and Local Variation of Pressure in Acoustic Resonator

The solution of the differential equations (3, 4) is [3, 6]

$$V(x, t) = \left[ \frac{I_0}{\omega_0 C} \cdot Z_C \cdot (A \cdot e^{\beta x} - B \cdot e^{-\beta x}) \right] e^{i\omega t}$$

(15)

$$I(x, t) = (A \cdot e^{\beta x} + B \cdot e^{-\beta x}) \cdot e^{i\omega t}$$

(16)

Where $\beta$ and $Z_C$ are the propagation constant and the characteristic impedance of the transmission line. The amplitudes $A$ and $B$ are determined by the boundary conditions of gas flux $I(x)$ and the pressure $V(x)$ at two ends of resonator. As can be seen in Fig.2, the maximum variation of pressure occurs in the middle of the resonator and it becomes zero at the ends of resonator. Thus the best position of microphone is the middle of the resonator where the maximum of the standing acoustic wave occurs.

![Fig.2. Pressure variation at different position and time.](image)

3.3. Resonator Length and Resonant Frequency

The projection of the peak PA signal at different resonator lengths on the frequency axis in Fig.3 is the resonant frequency at different lengths.

Since noise sources (intrinsic noise of the microphone, amplifier noise and external acoustic noise) have nearly a $1/f$ frequency dependence, low modulation frequencies should be avoided in PA trace detection. In order to minimize the noise, modulation frequencies in the 1–5 kHz frequency region are recommended [2], that result in resonator lengths about 3.4–17 cm. Since the small volume...
results in a short response time and has the additional advantage of realizing compact and portable system, smaller length of resonator is preferred.

![Figure 3: PA signal at different frequencies and lengths.](image)

**3.4. The Effect of Gas Flow Velocity on the Resonant Frequency of Photocoustic Resonator**

To take into account the effect of gas flow velocity, for the first longitudinal mode, resonant frequency can be determined as follows

\[ f_{100} = \frac{c}{2l} (1 - M^2) \]  

(17)

Where \( M \) is Mach number that can be expressed by ratio of gas flux and sound velocity. Therefore, dependence of resonant frequency on gas flow velocity enforces us to control gas flow in PA cell. As shown in Fig.4 if gas flux is very slow, the change of resonant frequency is ignorable and \( M \) can be neglected.

![Figure 4: Relation between resonant frequency and Mach number at various resonator lengths.](image)

**3.5. Role of the Buffer Volume as an Acoustic Filter**

In PA cell design, we consider a buffer volume as an acoustic filter at each end of resonator leading to noise attenuation of absorbed laser beam by PA cell windows and turbulence in gas inlet and outlet (see Fig.5). Absorption of laser beam by PA cell windows generates acoustic waves at the same resonant frequency of resonator. So optimum dimension of buffer volume must be selected to act as a damper at resonant frequency [6].

![Figure 5: Schematic representation of the longitudinal PA cell [1].](image)

**3.6. Resonant Frequency and Ambient Temperature**

The velocity of sound depends on the temperature of air rather than the air pressure.

\[ c = \sqrt{\gamma \frac{R_m T}{M}} \]  

(19)

Where \( R_m, M, T \) are the gas constant, molar mass and ambient temperature respectively. According to equations (10) and (12), the relation between PA signal and frequency under different ambient temperatures can be calculated. Fig.7 shows that ambient temperature has few effects on PA signal, while it can significantly change the resonant frequency of the resonator which may considerably deteriorate the performance of acoustic resonator. It is worth noted that, if the acoustic resonator is designed based on the ambient temperature at \( T = 300K \), while it practically works at the temperature of \( T = 285K \), the PA signal becomes 56.3% smaller than the predicted value. Therefore, in order to avoid non-resonant mode and have the best...
performance of the LPAS, special attention should be paid to the ambient temperature.

![Image](image1.png)

FIG. 7. The temperature dependence of the resonance frequency.

3.7. Quality Factor, PA Cell Constant and Resonator Dimensions

The quality factor \( Q \) is a criterion of resonant frequency broadening that depends on resonator losses (such as viscous and thermal losses). The PA cell constant \( F \) is also depends on designed resonator characteristics (such as dimension, frequency and quality factor).

Now, with theoretical analysis of equations (11, 13), we have:

\[
Q \cdot F = \frac{(\gamma - 1)}{2\pi \left(\frac{\gamma - 1}{\sqrt{2\kappa/\rho C_p + \sqrt{2\mu/\rho}}} \right)^2}
\]  

(20)

Since whole coefficients are parameters of the gas species, we can draw the conclusions that in resonant PA cells, the \( Q \cdot F \) is independent from the resonator dimension and resonant frequency. Comparing Fig.8 (a) with Fig.8 (b), results in same conclusion. Thus, a high quality factor \( Q \) demands a large volume-to-surface ratio and thin boundary layers, which will result in low acoustic cell constant. This causes a drastic decrease of the gas detection sensitivity, which is agreeable with the results in [3]. Therefore, trade-off between the quality factor and the acoustic cell constant is the key issue for the design of resonator. Medium \( Q \) (10 < \( Q < 50 \)) resonators are used frequently in PA detectors built for ultrasensitive trace gas monitoring [2].

4. CONCLUSIONS

LC circuit model is built for the simulation of a longitudinal acoustic resonator. The model is used for the design of a longitudinal acoustic resonator for CO trace gas detection. We focus on the PA signals, quality factor and acoustic cell constant at different working frequencies and various parameters of the resonator as well as ambient temperature. The role of the buffer volume as an acoustic filter is investigated and optimized dimension of the buffer volume, to achieve minimum noise transmission coefficient, is calculated. Also, the effects of the ambient temperature and gas flow velocity on the resonant frequency of photoacoustic resonator are simulated. This new model is commonly suitable to guide the design of a longitudinal acoustic resonator in LPAS for trace gas detection.

![Image](image2.png)

FIG.8. Quality factor (a) and PA cell constant (b) at different resonator dimensions.

REFERENCES