Numerical Analysis of a ‘T’ Type Resonant Photoacoustic Cell
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Keywords: Resonant photoacoustic cell, Photoacoustic response, Simulation.

Abstract. In this work, we have numerically studied the effect of geometrical parameters on the photoacoustic response of a ‘T’ type resonant photoacoustic cell, in which laser passes through one cylinder, known as absorption cylinder and the resonance is targeted in another cylinder, which is called as resonator, arranged perpendicular to the absorption cylinder. For the study, we solve linearized forms of the continuity equation, Navier-Stokes equation, energy equation, and equation of state using a finite element method (FEM) based software. It is found that the simultaneous excitation of resonance in both resonator and the absorption cylinder reduces the amplitude of acoustic response at the position of microphone. To avoid this, the length of absorption cylinder should not be an exact multiple of the length of resonator.

Introduction

Photoacoustic spectroscopy, because of its non-destructive nature and versatility, has a wide range of applicability, ranging from soft tissues to liquid and gases. It is recognized as an effective and inexpensive method to investigate and characterize the properties of matter. Since the amount of energy absorbed by the gas is miniscule, strength of photoacoustic response also will be low. However, using the concept of constructive interference caused by the boundaries at acoustic resonance, it is possible to achieve amplitude of acoustic pressure detectable by microphone. It would be accurate to model the photoacoustic response using continuity, momentum, and energy and state equations. In this work, we model the acoustic response of resonant cells, based on linearized Navier stokes equation, continuity equation, energy equation and equation of state, which are solved by an FEM software.

Theoretical Background

The photoacoustic response, characterised by the acoustic pressure at a position of microphone, can be predicted by solving for the pressure field of acoustic waves generated by the photoacoustic phenomenon. Assuming the fluid to be viscous, compressible and Newtonian, the acoustic waves triggered by the photoacoustic effect are governed by the continuity, momentum, energy and state equations. For the acoustic wave propagation in a fluid medium, magnitude of variation in velocity, pressure and temperature is much smaller than their background values. Hence, each of the velocity, pressure and temperature can be expressed as small harmonic oscillations about the steady equilibrium values. With the above assumption, aforementioned variables can be decomposed into an equilibrium part and a fluctuating part. In frequency domain, the velocity field can be rewritten as

\[ u = u_0 + u'e^{i\omega t}, \]

where \( u_0 \) and \( u' \) are, respectively, the equilibrium and fluctuating parts of the velocity field. \( \omega \) is the angular frequency of the laser and \( i \) is the imaginary unit. The pressure and temperature fields and the heat source can also be rewritten in the same form. During the wave propagation inside a photoacoustic cell, the mean velocity is assumed to be zero. Since we are interested in only the acoustic parts related to the wave propagation, linearization and further simplification of governing equations provides the following set of equations:

\[ u = u_0 + u'e^{i\omega t}, \]
\[ i\omega \rho' + \rho_0 (\nabla \cdot \mathbf{u}') = 0, \quad (2) \]

\[ i\omega \rho_0 \mathbf{u}' = \nabla \cdot \left( -p' \mathbf{I} + \mu \left( \nabla \mathbf{u}' + (\nabla \mathbf{u}')^T \right) - \left( \frac{2\mu}{3} - \mu_B \right) (\nabla \cdot \mathbf{u}') \mathbf{I} \right), \quad (3) \]

\[ i\omega \rho_0 C_p T' = -\nabla \cdot (-k \nabla T') + i\omega \rho_0 T_0 \alpha_0 + Q', \quad (4) \]

\[ \rho' = \rho_0 (\beta_T p' - \alpha_0 T'). \quad (5) \]

where \( \mathbf{u}' \), \( p' \), \( \rho' \), \( T' \) and \( Q' \) are the fluctuating parts of the velocity, pressure, density and temperature fields and the heat source, respectively, \( \mu, \mu_B, C_p, \alpha_0, \beta_T \) and \( k \) are the coefficients of dynamic viscosity and bulk viscosity, specific heat at a constant pressure, coefficient of thermal expansion at \( T_0 \), isothermal compressibility and thermal conductivity respectively, \( \phi \) is the energy dissipation, \( t \) is the time and \( \mathbf{I} \) is the identity matrix. Eqs. (2-5) are solved using the thermo acoustic module of COMSOL Multiphysics software. The heating of the gas by the absorption of laser can be modelled using the source term, \( Q' \). Assuming a Gaussian profile for the laser beam, source can be approximated as

\[ Q' = a I_0 \exp \left[ -2 \left( \frac{r^2}{w^2} \right) \right], \quad (6) \]

where \( r \) is the radial distance from the centre line of laser beam, \( w \) is the radius of laser beam and \( a \) is the absorption coefficient and \( I_0 \) is the power of the laser.

**Computational Model**

In the present work, we numerically analyse a T-cell, shown in Figure 1, in which laser passes through one cylinder, known as absorption cylinder and the resonance is targeted in another cylinder. The gaseous medium is butane at a temperature of 300K and at atmospheric pressure. Photo acoustic response is measured in terms of the acoustic pressure at the position of microphone. The responses are actually measured as amplified microphone signals, an arbitrary value can be assigned for the term \( a I_0 \) in Eq. (6). In numerical modelling of the sound waves, a rule of thumb is to have at least 5 elements per wavelength. However, the meshing should have sufficient number of elements to incorporate the heating effect by the laser beam passing through the longitudinal axis of the cylinder. In the present work, the range of frequencies is from 100Hz to 3000 Hz. We use the maximum element size of 2 mm, so that the minimum number of elements per wavelength is around 35, which ensures high degree of accuracy. Isothermal and no slip boundary conditions are applied on all boundaries.

**Results and Discussion**

In order to understand the effect of geometrical parameters on the photo acoustic response, two different sets of simulations were performed. In the first set, the diameter of the absorption cylinder was kept constant at 12mm; \( L_a \) and \( L_r \) were varied for different simulations. Figure 2 shows acoustic pressure at the location of microphone, which is at the closed end of resonator in this case, plotted against length of absorption cylinder, for various lengths of resonator. In general, it can be seen that the acoustic pressure increases initially with increasing length of absorption cylinder, then reaches a peak value, then decreases. This trend is clearly visible in the cases where lengths of resonator are 40mm & 25mm. For resonator length of 30mm, the acoustic pressure value drops drastically at an
absorption cylinder length of 60mm. Similar trend is seen for the case where $L_r=30\text{mm}$ and $L_a=30\text{mm}$. In both these cases, the length of resonator, which is a cylinder open at one end, is half that of the length of absorption cylinder, which can be approximated as a cylinder closed at both ends. In such cases, frequency of first longitudinal resonance mode will be same for both resonator and the absorption cylinder. If both cylinders are excited at the same frequency, standing waves will be generated in both simultaneously, thereby spreading the net acoustic energy over a larger volume, which would result in lower amplitude of acoustic pressure at the location of microphone. Figure 3 shows pressure profiles at the longitudinal axis, for both resonator and absorption cylinder. So, it can be inferred that the combination of sizes of resonator and absorption cylinders, which triggers resonance in both cylinders simultaneously, needs to be avoided, since it would reduce the amplitude of photo acoustic response. This should be an important design consideration in the case of T cells.

In the second set of simulations, length of resonator was kept constant at 40mm; simulations were performed for various values of $L_a$ and $D_a$. It is found that the acoustic pressure drops drastically with increase in $D_a$, which implies the need to keep the diameter of absorption cylinder to the lowest possible value. Any increase in the diameter of absorption cylinder above the value of the diameter of the Laser beam would not be beneficial as far as heating effect is concerned. But the practical considerations with regard to welding of the resonator in to the absorption cylinder need to be taken care, and a ratio of $D_a/D_r=2$, which is considered in the present work would be an optimal ratio.

Figure 1. Structures of a T cell. $L_r$ and $D_r$ are the length and diameter of the resonator and $L_a$ and $D_a$ are those of the absorption cylinder.

Figure 2. Acoustic pressure at the position of microphone corresponding to different combinations of $L_a$ and $L_r$, at constant $D_a$ and $D_r$, for T cell.
Conclusions

In this work, we demonstrated that photoacoustic response in resonant photoacoustic cells can be modelled using linearized forms of Navier-Stokes equation, continuity equation, energy equation and equation of state. Since the simultaneous excitation of resonance in both resonator and the absorption cylinder reduces the amplitude of acoustic response at the position of microphone, the length of absorption cylinder should not be an exact multiple of the length of resonator. Considering the non-linear relationship between geometrical parameters and the photoacoustic response, development of a sophisticated surrogate model such as Kriging would be really useful to optimize the cell geometry, which could be an interesting topic for future research.

Acknowledgement

This work has been supported by the Human Resources Development of the Korea Institute of Energy Technology Evaluation and Planning (KETEP) grant funded by the Ministry of Knowledge Economy, Korea (No. 20114030200030).

References


