FEM analysis of cylindrical resonant photoacoustic cells

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Abstract. Using a mathematical model on photoacoustics that includes both temperature and pressure effects explicitly, we analyze the behaviour of resonances of a cylindrical photoacoustic cell consisting of two buffer volumes and a resonator. We excite the cell at a certain frequency and find the ratio of resonator versus buffer diameter needed to obtain resonance. The results show that the resonance ratio depends on the absolute cell size. Also the amplitude of the acoustic signal measured in the middle of the resonator does not necessarily decrease when the total cell volume is increased. If the resonator diameter is sufficiently small, decreasing its diameter will increase the acoustic signal, although the total cell volume has to be increased to obtain resonance. This gives the advantage of being able to obtain a comparably large signal and at the same time use large buffer diameters to suppress window absorption signals. Finally we also compare the quality of the above-mentioned model and the lossy Helmholtz equation. We find that there is a shift in resonance ratio and the signal damping differs slightly. Albeit these differences are not large, and in many cases negligible, the model can be easily coupled with a solid absorption model in order to investigate the importance of thermal and pressure coupling between two acoustic media subject to heat absorption.

1. Introduction

Due to the general simplicity and low cost of photoacoustic devices, this measurement technique has received more attention in recent years. There exists a broad range of application for these devices, mainly photoacoustic spectroscopy for fluids and solids to be used in, e.g., environmental, biological or medical applications [1,2,3].

Despite the general simplicity of these devices, there are still some noise issues to be solved when measuring very small gas concentrations [4]. These issues include environmental noise as well as background signaling from the windows and cell walls [2,4]. Both windows and walls absorb heat and thus add to the signal induced by absorption in the gas. An important factor in optimizing both the signal amplitude and the signal to background ratio is the geometric design of the cell. It has been found that the acoustic pressure amplitude decreases when the total cell volume increases [4], while the window background signal decreases when the buffer diameter increases [2]. To find the desired geometry properties, a mathematical model for simulating the cell behavior is employed.

There exist various mathematical models for these cells, the most common being the transmission-line (TL) model [2,4] and the direct solution of the monofrequency wave equation, i.e., the Helmholtz equation [3,5,6]. The TL model is based on the Helmholtz equation and basically assumes separability or constant cross-section albeit small changes in the cross section can be handled. The direct numerical...
solution does not require separability, however, this method is computationally more demanding. Both models only allow boundary conditions to be imposed on the pressure which might be a problem when the coupling from fluid to solid materials is to be modelled. So far it has been assumed that the coupling is dominated by the temperature and that this can be approximated as a thermal piston in the fluid [1,7,8], while it has been shown that both pressure and temperature couplings can be important[9]. In this work, a more general model, including both pressure and temperature explicitly, is presented and solved for a photoacoustic cell consisting of a resonator and two buffer volumes. With this model the ratio between the resonator and buffer diameters to obtain resonance is investigated. This is then used to find out which parameters are of main importance in obtaining larger acoustic pressure amplitude at resonance; the total cell volume or the resonator diameter. It has been suggested that the total cell volume is the important part [4].

2. Theory

The fundamental equations for acoustics including heat and viscous losses read[10]

\[
\frac{\partial \rho}{\partial t} + \rho_0 \nabla \cdot \vec{u} = 0, \tag{1}
\]

\[
\rho_0 \frac{\partial \vec{u}}{\partial t} = -\nabla p + \left( \eta + \frac{4}{3} \mu \right) \nabla \nabla \cdot \vec{u} - \mu \nabla \times \nabla \times \vec{u}, \tag{2}
\]

\[
\frac{\rho_0 T_0}{\partial s} = K \nabla^2 \tau + \rho_0 \epsilon, \tag{3}
\]

\[
\epsilon = \epsilon_0 \exp \left( -\frac{r^2}{2a^2} \right) \cdot \exp(i\omega t), \tag{4}
\]

where the quantities \( \rho, \vec{u}, p, \tau, s, \sigma, \eta, \mu, r \) denote density, particle velocity, pressure, temperature, entropy, Gaussian spreading, the coefficient of shear viscosity, the coefficient of bulk viscosity, and the distance from the z-axis in the cylinders, respectively. The changes in quantities with respect to equilibrium values are denoted as follows

\[
\tilde{\rho} = \rho_0 + \rho, \tag{5}
\]

\[
P = p_0 + p, \tag{6}
\]

\[
\tilde{T} = T_0 + \tau, \tag{7}
\]

\[
\tilde{S} = S_0 + s, \tag{8}
\]

where the equilibrium values are denoted by a subscript zero. In the former equations only first order terms of viscosity and heat conductivity are taken into account and furthermore it is assumed that there is no background flow. The function \( \epsilon \) is the heat input function given by the laser beam and is modeled as a Gaussian beam that is aligned to the z-axis of the photoacoustic chamber, thus there will be no azimuthal excitation. Here only the time varying part of the heat input is taken into account. When combining equations (1) and (2) and rewriting equation (3), using the thermodynamic relationship

\[
s = \frac{2p}{\rho_0} \left( T - \frac{1}{\gamma - 1} \right), \tag{11}
\]

where \( \alpha = P_0/T_0, C_p \) is the heat capacity at constant pressure and \( \gamma \) is the ratio of specific heats, we obtain a set of coupled differential equations in \( \tau \) and \( p \), namely

\[
\nabla^2 p = \frac{\gamma}{c^2} \left( \frac{\partial^2}{\partial t^2} - l_h c \frac{\partial}{\partial t} \nabla^2 \right) (p - \alpha \tau), \tag{9}
\]

\[
l_h c \nabla^2 \tau = \frac{\partial}{\partial t} \left( \tau - \frac{\gamma - 1}{\alpha \gamma} \frac{p}{C_p} - \frac{\epsilon}{C_p} \right), \tag{10}
\]

where \( l_h = \frac{K}{\rho_0 c_p c} \) and \( l'_h = \frac{\eta + 4/3 \mu}{\rho_0 c} \) with \( c \) being the speed of sound.

The boundary conditions for these equations have to be specified for both \( p \) and \( \tau \). They read

\[
\frac{\partial p}{\partial n} \bigg|_{\partial \Omega} = 0, \quad \tau \bigg|_{\partial \Omega} = 0, \tag{11}
\]

where the pressure condition is based on the assumption that the acoustic impedance of the cell material is much higher than the acoustic impedance for the inside gas, and the temperature condition is based on the assumption that the cell material has a much higher heat conductivity than the inside.
gas and as such suppresses any temperature fluctuations on the boundary. The solutions are expected to be time harmonic with angular frequency $\omega$, so $\partial / \partial t \to i\omega$. The equations (9) and (10) are solved numerically using finite element analysis. The finite element tool we employ is Comsol Multiphysics 3.5 and volumetric sweeps have been run on a single input frequency. The modelled geometry can be seen in Figure 1. It was found that a frequency of 1660Hz is a convenient choice for obtaining resonance in the given geometry intervals. For comparison purpose, equations (9) and (10) can be linearized in $l_p, l_h$ to one differential equation in pressure (by taking the zero order of (10) and inserting into (9)). This gives the inhomogeneous Helmholtz equation

$$\nabla^2 p + k^2 p = -i\omega \frac{\alpha y \epsilon}{c_p c^2}$$

$$k^2 \approx \frac{\omega^2}{c^2} \left( 1 - i\frac{\omega}{c} l_p - i(\gamma - 1) \frac{\omega}{c} l_h \right).$$

(12)

Since the latter equation is an equation in acoustic pressure only, no explicit boundary conditions for the temperature can be specified here. The boundary condition for pressure remains the same as in equation (11).

Figure 1. Geometry of the modeled cell. The microphone position is indicated by the gray line in the middle of the cell. Here $L=0.2\, \text{m}$, $7\, \text{mm} \leq d_{\text{resonator}} \leq 10\, \text{mm}$ and $2 \cdot d_{\text{resonator}} \leq d_{\text{buffer}} \leq 5 \cdot d_{\text{resonator}}$.

2.1. Results
The position of the different resonance peaks can be seen in Figures 2 and 4 for solutions of equations (9)+(10) and (12), respectively. The corresponding total cell volume for resonance at 1660Hz can be seen in Figures 3 and 5.

Figure 2. Buffer radii for resonance at different resonator radii. Note that the resonance peak for the smallest resonator radius is the most powerful.
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Figures 2 and 3 reveal that, contrary to previous assumptions, an increase in the total cell volume does not necessarily mean a decrease in pressure amplitude at the microphone position. Figures 4 and 5.
5 show that the resonance ratios are shifted slightly and that the inhomogeneous Helmholtz peaks are somewhat larger (wider) than the peaks for equations (9) and (10).

3. Conclusions
Using a general model, including pressure and temperature explicitly, we analyzed the behavior of a cylindrical photoacoustic cell with two buffer volumes. We found, in contrast to previous assumptions, that the pressure amplitude does not necessarily decrease when the total cell volume increases. Apparently, for a sufficiently small resonator diameter, the resonator volume is the determining factor. This means that if the resonator diameter is small enough, one can increase the diameter of the buffer volumes significantly, thus increasing the filter function of the buffers.

We also compared the inhomogeneous Helmholtz-equation model with our model and find that the imposed boundary conditions are rather important. There are two consequences of using the inhomogeneous Helmholtz equation, the first being a shift in resonances and the second being the neglect of thermal losses due to temperature boundary conditions. It should be noted, that this model does not take into account viscous losses arising from the boundary, however, it takes into account volumetric viscous losses. The use of this model is a first step to model a full system consisting of heat absorption in solids and in fluids, where both pressure (stress) and temperature distributions are coupled.

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References
[1] C. Haish and R. Niessner, Spectroscopy Europe 14, 10 (2002)
[2] F.H.C. Bijnen, J. Reuss and F.J.M. Harren, Rev. Sci. Instrum. 67, 2914 (1996)
[3] B.T. Cox, S. Kara, S.R. Arridge, and P.C. Beard, J. Acoust. Soc. Am. 121(6), 3453(2007)
[4] A. Miklos, P. Hess, and Z. Boszoki, Rev. Sci. Instrum. 72, 1937 (2001)
[5] B.T. Cox and P.C. Beard, J. Acoust. Soc. Am. 117(6), 3616 (2005)
[6] G.J. Diebold and P.J. Westerveld, J. Acoust. Soc. Am. 84(6), 2245 (1988)
[7] A. Rosencwaig and A. Gersho, Journal of Applied Physics 47(1), 64 (1976)
[8] A.C. Tam, Reviews of Modern Physics 58(2), 381(1986)
[9] F.A. McDonald and G.C. Wetsel, Journal of Applied Physics 9(4), 2313 (1978)
[10] P.M. Morse and K.U. Ingard, Theoretical Acoustics, Princeton Univ. Press, Princeton, NJ (1986)