Topology Optimization of an Acoustical Cell for Gaseous Photoacoustic Spectroscopy using COMSOL® Multiphysics

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Abstract

This paper presents the optimization of the acoustic cell of a gaseous photoacoustic spectroscopy setup using COMSOL Multiphysics software. A thermo-acoustic model is used to properly simulate the multiphysics problem appearing in the cell. Indeed, a pulsed laser is heating the analyte present in the gas and this heating generates an acoustic wave measured by a microphone. The goal of the work presented here is to maximize the sound pressure received at the microphone. The 3D topology optimization of COMSOL is then used to propose innovative shape of the cell. Finally, the performance obtained with the new optimized cell is compared to conventional cylinder cell.

1. Governing physics concepts

Due to its ability to detect traces of analytes up to the part per billion range or less, gaseous photo-acoustic spectroscopy presents a lot of interests in the detection of hazardous compounds, security threats, etc… Its very high signal-to-noise ratio compared to conventional optical spectrometers is mainly due to the detection scheme. Indeed, the analyte is optically excited by laser while an acoustic signal is harvested with -almost- no background noise. However, the generated soundwave can be quite weak. Therefore, the chamber is also used to amplify the signal.

The basic principles of gaseous photoacoustic spectroscopy can be described as following. An analyte is dissolved in a buffer gas -like air, pure nitrogen or a noble gas- and the spectrometer is used to identify it and to measure its concentration. This gaseous mixture is enclosed inside a chamber called cell in which a laser beam is propagating. When laser wavelength corresponds to one of the absorption peaks of the analyte, the analyte will be excited. By modulating the laser intensity periodically in times, a set of repetitive excitation-deexcitation cycles of the analyte is generated. Because the deexcited states lie in rotational and vibrational regime of the molecule, it follows a periodical and local raise of temperature. This heating-cooling cycle of the gas generates a sound wave with an intensity proportional to the laser power, the nature of the analyte and its concentration and with a frequency corresponding to the intensity modulation frequency of the laser. Sweeping the laser wavelength, the analyte spectre can be recover.

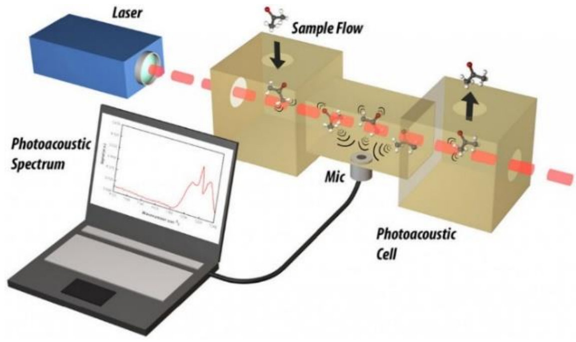

Figure 1. Principle of photoacoustic spectroscopy. An intensity modulated laser beam is shot through the cell. The analyte, presenting an absorption peak at the same wavelength than the laser, will excite-deexcite cyclically. The result will be a local and repetitive heating-cooling process that generates a sound wave. The cell will amplify it if the sound frequency corresponds to its own natural frequency.

(image from https://www.copac.dk/photoacoustic-spectroscopy/)

As explained earlier, this sound wave is quite weak: by choosing a frequency modulation of the laser equal to the natural frequency of the cell, which also plays the role of an acoustical chamber, the generated sound will be amplified. Finally, a strategically placed microphone picks up the signal (see Figure 1).

As any sensor, there is a trend to miniaturize it. Challenges to overcome encompass a more sensitive microphone along with further amplification of the created soundwave. Until now, the geometry of the acoustic chamber itself was not deeply investigated mainly due to manufacturing limitations. However, thanks to the progress of new processes like 3D printing, a new design space is open in order to improve the sensitivity of those -future- miniaturized photoacoustic spectrometers.

2. Setting topology optimization

Topology optimization aims to find a shape that fits a set of given constrains while maximizing -or minimizing- an objective function. Although this technique emerged in the late XIXth century, it benefited speeded-up development since the last two decades thanks to increasing computational power. As any mathematical variational problem, a function to be optimized has to be defined. We typically use a material density function ζ over a domain of interest Ω:

$$\zeta(u) = \begin{cases} 1 & if\ material \\ 0 & if\ void \end{cases} \qquad u \in \Omega \tag{1}$$

As COMSOL uses a gradient-based optimization algorithm and we have a discrete problem, we set this function ζ the ability to continuously take values between 0 and 1. But in order to enforce those two extreme values, a Heaviside based projection scheme [1] is applied on every step of the optimization process:

$$\zeta_P(u) = \frac{\tan(0.5\,\beta)+\tan(\beta(\zeta(u)-0.5))}{2\tan(0.5\,\beta)}$$
(2)

Values above (respectively below) 0.5 will be then pushed to 1 (respectively 0) with a speed depending on the parameter β.

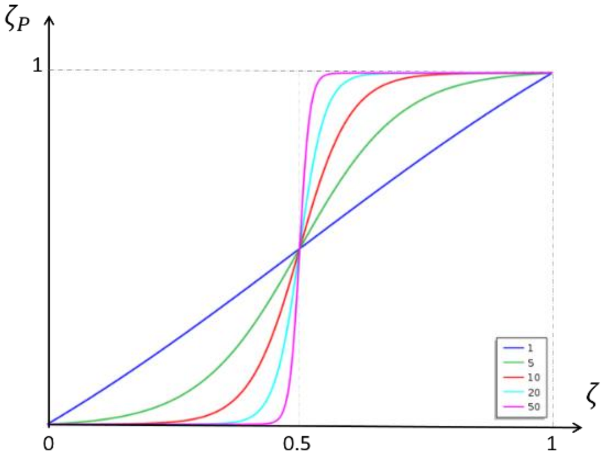

Figure 2. Effect of the modified Heaviside projection for different value of β.

Moreover, this fixes a threshold between air and solid at 0.5. It is the presence (1) -or the absence (0)- of material that will define the shape of our chamber and therefore the acoustical properties of the medium.

In our acoustical chamber, the lossless propagation of a sound wave in a medium is governed by the Helmholtz equation:

$$\nabla.\left(\frac{\nabla \boldsymbol{p}}{\rho}\right) + \frac{\omega^2}{\rho c^2}\boldsymbol{p} = 0 \tag{3}$$

with $\boldsymbol{p}$ the complex pressure field, ρ the volumic mass of the medium and c the speed of sound through it. Since the two latest parameters depend on the nature of the material, they will be impacted by the function ζ. To vary the material properties accordingly we chose to use the SIMP (Solid Isotropic Material with Penalization) technique [2] which use a parameter q as penalization factor:

$$\begin{cases} \rho(u) = \rho_{air} + \zeta_P(u)^q\,(\rho_{solid} - \rho_{air}) \\ c(u) = c_{air} + \zeta_P(u)^q\,(c_{solid} - c_{air}) \end{cases}$$
(4)

Let us note that there should be no sound travelling in the ''solid'' zones: the acoustical impedance mismatch is high enough to suppose that there is no transfer from gas to solid. Therefore, we introduced a material penalization damping or ''pamping''. This prevents the solver to give us unwanted solutions by having any distribution for pressure other than a decay inside the solid. Since we considered before a lossless propagation of sound, we need to add the pamping for the solid region only. An attenuation coefficient for those regions is therefore set:

$$\alpha = \zeta_P(u)^q \alpha_0 \tag{5}$$

where α_0 is set as high as 1 Np/mm, for example, and in the gaseous region, this attenuation drops to zero.

The obtained and optimized ζ function has a checkboard pattern due to the domain discretization. Since we desired a smoothed solution without refining the mesh, we implemented a regularization technique [3] which requires the solving of another Helmholtz equation:

$$-r^2\nabla^2\tilde{\zeta} + \tilde{\zeta} = \zeta \tag{6}$$

where r represents a regularization parameter and is taken -usually- as being 1.5 the mesh size element. which is set to 1/6 of the sound wavelength (a general rule of thumb while simulation propagating waves with Finite Element Modelling). The regularized $\tilde{\zeta}$ function will be taken as our final solution of our topological problem. The advantage to use such regularization technique is the ability to implement and solve it at the same time with the sound propagation equation -while optimizing- in COMSOL Multiphysics. Moreover, by carefully setting the boundary conditions on this smoothed function $\tilde{\zeta}$, we can impose the presence -or absence- of material and then impact the outer surface of the final shape. We can also have a slight control over the "amount" of matter in our shape. This is made by adding a constrain on the function ζ : its average over the design domain can be set to be higher or lower than a specific value k:

$$\frac{\int_\Omega \zeta\, d\Omega}{\int_\Omega\ d\Omega} \lesseqgtr k$$
(7)

with k between 0 and 1.

3. Implementation with COMSOL Multiphysics

We show here how we implemented the technique described previously in COMSOL Multiphysics. A 3D model was defined and we used the Pressure Acoustic module in order to solve lossless propagation of sound. The laser beam is simplified here to a linear sound source. An air-filled cylinder, with the axis along the laser beam is out of the optimization domain. The

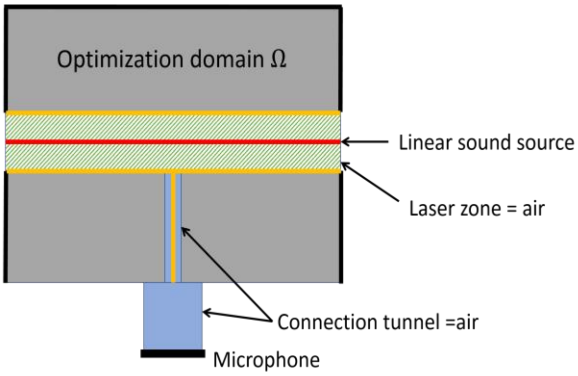

*Figure 3 Schematic of the optimization. The green zone where the laser shines is left as plain air. A tunnel junction between the cell and the microphone is also set as plain air. To ensure an acoustical path from the laser to the microphone, another ''air-path'' is set. The laser can be simplified acoustically speaking as a linear sound source. The remaining domain **Ω** in grey is where the topological optimization is undertaken. The bold lines indicate the boundary conditions for the function $\tilde{\zeta}$, enforcing that way the material: 1 for black (solid) and 0 for yellow(air).*

microphone is assumed to be circular, plane and its position is set wherever it is desired. As we would like to retrieve the highest sound pressure intensity as possible over this disk, our objective is set as:

$$\max_{\tilde{\zeta}\ over\ \Omega} \quad \frac{\int_S |p|^2 dS}{A} \tag{8}$$

we maximize the average pressure squared over the disk regarding the regularized density function ζ which is defined over the domain of interest **Ω**.

As we can notice, our configuration presents a symmetry with respect to the plane defined by the line source and the centre of the microphone. Half of the space will be then used for computation. We set the Heaviside projection function (2) as a global function in COMSOL and the SIMP model (4) as a variable in the Component definition. Material are defined as regular air in the areas in blue and we use the SIMP hybrid material (4) for the green one (see Figure 4).

The Pressure Acoustic module, which solves equations (3), is set to consider an acoustically elastic material in the plain air region, whereas we set the pamping (5) in the green region. The axis of laser is set as the linear sound source. The outer surface is considered as hard (and reflective) walls. The Optimization module regroups the definition of the density function ζ as a variable (with an initial value of 0.5 in **Ω**), the objective to maximize (8) and the material quantity constrains (7). This module will actually implement the topology optimization scheme.

The design space is defined as the cube around the ''laser'' cylinder. And finally, we set the Coefficient Form PDE to solve the equation (6) in the same region. Boundary conditions for ζ are accordingly defined to impose air and solid: the ''laser'' cylinder interface and the microphone impose a 0 value for ζ, whereas the surface of the cube will be set to 1 (see Figure 3).

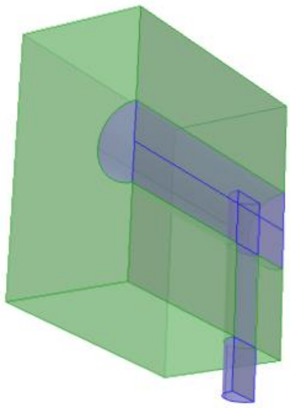

Figure 4. Example of 3D geometry implemented in COMSOL. Half of it is plotted due to symmetry. Notice the horizontal cylinder representing the laser beam; the axis is the linear sound source. Another vertical cylinder on top of the microphone location is considered air-filled in order to ensure an acoustic path. The part highlighted in green is the actual zone where the topological optimization was undertaken.

Finally, we chose to use the SNOPT (Sparse Nonlinear OPTimizer) algorithm over the MMA (Method of Moving Asymptote) one because it converges more efficiently.

4. Results

We set the volume of the cube to 1 cm^3 and the frequency to 25 kHz. This frequency was chosen because it is out of the audible range -hence most of the acoustic pollution. In addition to that, as shown in equation (9), the lower the frequency, the higher the signal. For this work, we considered PMMA as the solid. Density and sound speed are respectively: 1180 kg/m^3 and 2500 m/s. We studied the obtained shapes depending on the evolution of several parameters on which we can impact. The first one is the microphone position: its impact is quite obvious. The reason of such an investigation is to first verify the good operation of the algorithm and also to make comparison on the impact of other parameters that we will vary (defined afterwards). The other parameters are those defined for: the Heaviside projection β (2), the penalization parameter q in (4), the initial

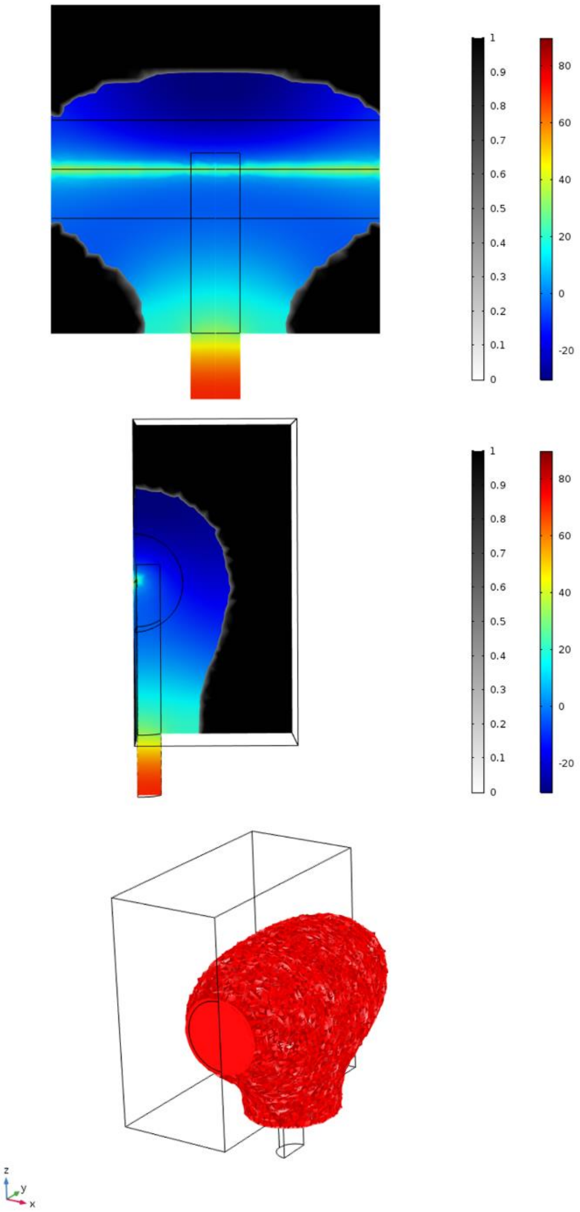

Figure 5. Profile, transverse and 3D reconstructed view of the optimized shape. The microphone location is located at the bottom of the cylinder tunnel. In the two first, the color represents the pressure amplitude while the black and white (set to transparent here) represent the material presence. For a power of 10^{-5}W sound wave input power, we retrieve a 71 Pa pressure average on the microphone.

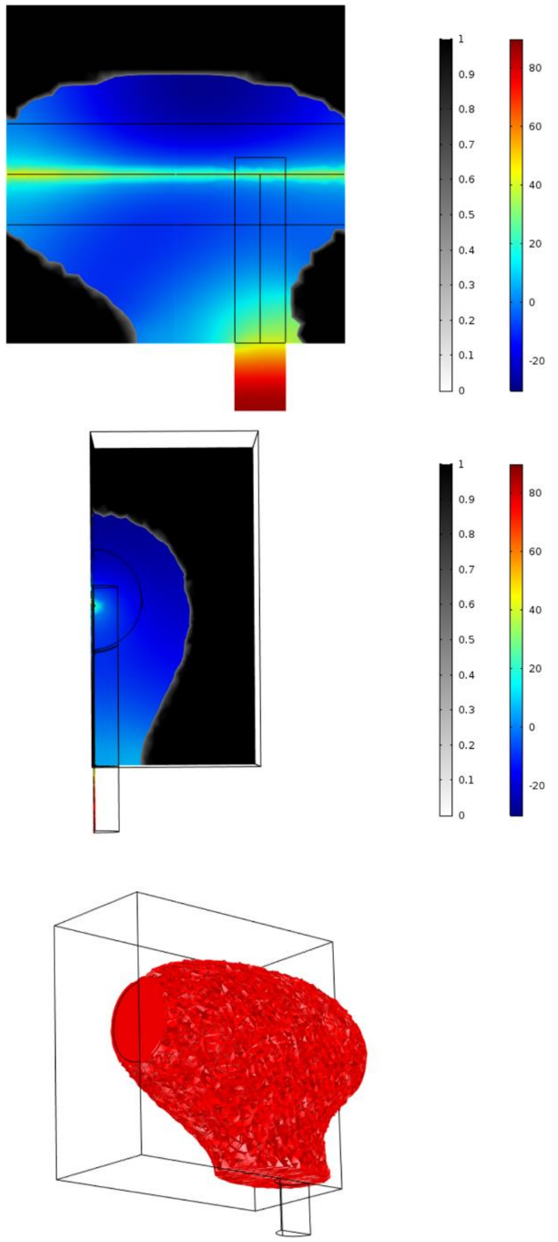

Figure 6. Profile, transverse and 3D reconstructed view of the optimized shape. The microphone location was excentred on purpose and is located at the bottom of the cylinder tunnel. In the two first, the color represents the pressure amplitude while the black and white (set to transparent here) represent the material presence. For a power of 10^{-5}W sound wave input power, we retrieve a 86 Pa pressure average on the microphone.

attenuation α_0 in (5) and the regularization parameter r in (6).

As a first thing, we can notice that the main shape around the laser beam is quite the same (Figure 5 and Figure 6): we have a kind of ellipse (more a ''potato'') that presents the same revolution symmetry around the laser beam. The only difference will be around the microphone location: we have a kind of collector that concentrates the soundwave into the tunnel. After several simulations, we noticed that the opening of that collector depends on the wavelength. Variation of either of parameters β, α_0 and q (from equations 2, 4 and 5) has no impact on the final shape but influences the convergence speed of the optimization algorithm. Simulations with smaller values are faster to compute but requires more steps and might not converge while higher values require more time and computational power but converges in a few steps. Finally, variation of the regularization parameter r has an impact on the final shape. It was expected since equation (6) averages the ζ function with values within a sphere of radius r. The bigger this value, the smoother the retrieved surface. However, by averaging, we lose the details from small features that might impact the performance of the cell. An optimum should be found in order to use and not misuse this feature. Keeping it around 1.5 times the size mesh seems to be reasonable.

The shape was then retrieved by exporting the function $\tilde{\zeta}$ data into MATLAB. A small code was used to retrieve points of $\tilde{\zeta}$ that are around 0.5 (through a 0.05 window) and interpolates then a surface. That surface is then reimported into COMSOL as a 3D geometry. Using the Thermo-acoustic module, defining boundary layers [4] on that surface and a modulated heat source, the photoacoustic effect is then simulated (see Figure 7).

In order to compare the final performance of our optimized ''potato'' cell and a conventional cylinder, we used a simplified formula [4] that links the pressure p at the microphone, the absorbed power of the laser by the analyte and the dimensional parameters of a cell:

$$p = K_{geom} \frac{(\gamma-1)\, L\, Q}{\omega\, V} \alpha P_L \tag{9}$$

where V is the volume of the chamber, ω its natural frequency, L the path length travelled by the laser, αP_L the absorbed power by the analyte from the laser, γ the specific ratio of the buffer gaz, K_{geom}, a geometric constant and Q, the quality factor which is the ratio between stored energy and losses during one cycle. Only the two last parameters are shape dependent. Therefore, in order to compare two cell shape, we need to fix a same volume, path length, absorbed power and buffer gaz. We set up then the buffer gas as being air, the path length as 1 cm, the volume as 24 mm³ (volume of the optimized shape) and the laser beam having a power of 1 MW/m³ with a waist of 0.5 mm. Moreover, the tunnel connecting the cell to the microphone needs to have the same length (2 mm) since it plays the same role as an additional resonator.

Applying all these constraints, the frequency response of the two chambers, from 10 to 40 kHz, is compared in Figure 7. We can see that the optimized cell presents a higher amplification capability around 24kHz, its resonance frequency, while the cylinder reaches its maximum at 30kHHz. At their resonances, the potato cell will provide 2 time more output pressure compare to the cylinder cell.

If we take a closer look to the cell geometry, we can explain why this shape presents better amplification capabilities. It is mainly due to lower losses at the cell walls. On the cross section picture in Figure **Erreur ! Source du renvoi introuvable.**5 and Figure 6, we can approximate the upper part of this shape to a circle. The sound emitted by the laser is a point source at the centre of the circle and is

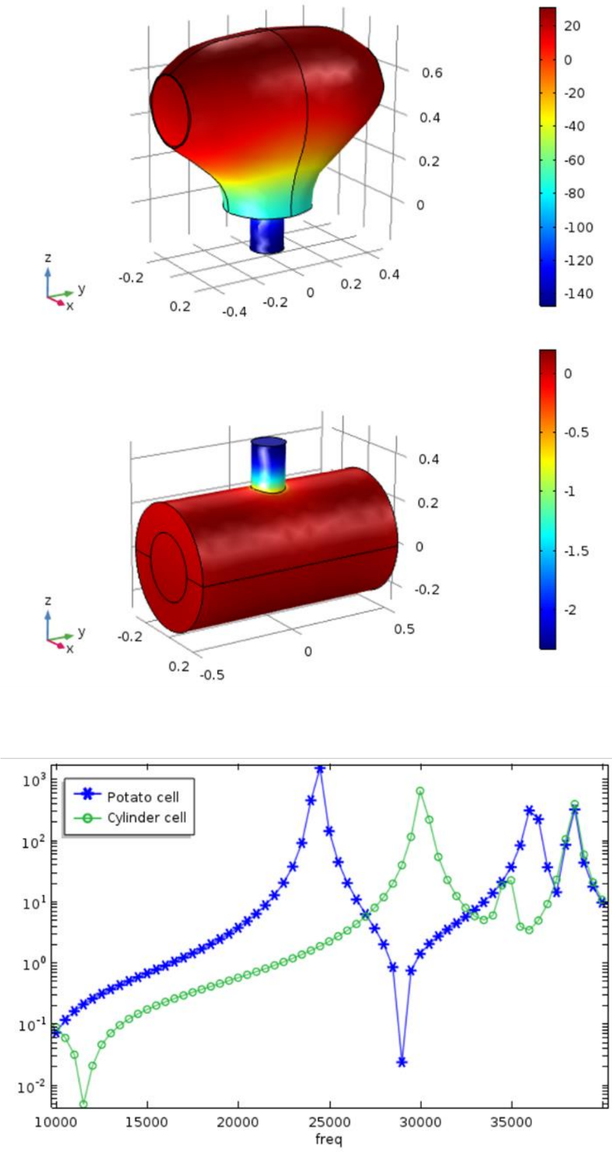

Figure 7 Simulated pressure repartition at 25 kHz on the designed cell (first one) and a conventional cylinder (second one). Colors represent the repartition of pressure in Pascals. At the bottom, frequency response (in a logarithmic scale) of the two chambers, from 10 to 40 kHz. We notice the higher amplitude of the signal and the highest resonant amplitude is retrieved on the ''potato'' cell.

propagating with radial waves. The interaction of such a wave with a circular wall will present no friction and therefore no losses.

5. Conclusion

We presented the topology optimization of an acoustic chamber for gaseous photoacoustic spectroscopy. Knowing the direction of the laser beam and the position of the microphone, we derived a unique shape that consists on a kind of ellipse with its revolution axis along the laser beam and a collector facing the microphone. COMSOL Multiphysics allowed us to both implement the topology optimization technique and to do some smoothing on the retrieved shape. This regularization technique should be used carefully though in order to not ‘’crop’’ on the retrieved shape. A simulation of the photoacoustic effect on that chamber was also made and its performance was compared with a conventional cylinder. It is shown, while both chambers fit in a $1cm^3$ cube, that the newly developed shape has 2 times better sound amplification capabilities than the one currently used.

Further work should focus on developing a topology optimization scheme using thermo-acoustic equations and also experimental confirmation of this simulation work.

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