Topology Optimization of a 3D-printed Acoustic Chamber For Photoacoustic Spectroscopy with COMSOL Multiphysics®

by RACHID HAOUARI
PhD Candidate
OVERVIEW

STRUCTURE OF THIS PRESENTATION

- Principles of photoacoustic spectroscopy
- What is topology optimization?
- Problem definition and simulation set up
- Results, comparison and confirmation
- Conclusion
PHOTOACOUSTIC SPECTROSCOPY

BASIC PRINCIPLES OF GASEOUS PHOTOACOUSTIC SPECTROSCOPY AND MAIN ADVANTAGE

1. Laser emitter
2. Chopper (amplitude modulation)
3. Gas with analyte inlet/outlet
4. Buffer
5. Resonator
6. Microphone

Gas chamber = cell
Pressure response of a PAS cell

\[ p = K_{\text{geom}} \frac{(\gamma - 1) L Q}{\omega V} \alpha P_L \]

Ways for improvement

- Downsizing \((V)\)
- Multiple laser beam crossing (mirrors) \((L)\)
- Noble gas as a buffer \((\gamma)\)
- Higher laser power \((P_L)\)

\[ K_{\text{geom}} \]

Geometry of the cell?
CAN WE SIGNIFICANTLY IMPROVE THE RETRIEVED SIGNAL BY JUST TAILORING THE CELL SHAPE?
SIMULATION OF THE PHOTOACOUSTIC EFFECT
DESCRIPTION OF BOUNDARY CONDITIONS

- Use Thermoacoustic module to take into account thermal and viscous losses

Harmonic excitation $\Rightarrow$ Frequency domain study

- Gaussian radial repartition of heat power = laser heating
- Air bulk modulus : 17 $\mu$Poise
- Boundary layer = $\max(d_{th}, d_{visc})$
## Impact of the Cell Shape

All shapes fit a 1 cm³ volume

<table>
<thead>
<tr>
<th>Buffered cylinder Ø 4 mm</th>
<th>Heart + res.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Target eigenfrequency (kHz)</td>
<td>26</td>
</tr>
<tr>
<td>Q factor</td>
<td>67,877</td>
</tr>
<tr>
<td>Cell constant (Pa.cm/W)</td>
<td>6100,9</td>
</tr>
<tr>
<td>Average pressure at mic's location (Pa)</td>
<td>4,0266</td>
</tr>
</tbody>
</table>

24,7
95
17062
11,26
PURPOSE OF TOPOLOGY OPTIMIZATION

FIND THE BEST SHAPE OPTIMIZING ITS FUNCTION WHILE COMPLYING TO A SET OF CONSTRAINS

Bridge

- **Function**: withstands the weight
- **Constrains**:
  - limited amount of material
  - light
MATERIAL DEFINITION

THE OPTIMIZED SHAPE IS AN OPTIMISED DISTRIBUTION OF A MATERIAL PROPERTY

We are looking for material distribution
\[ \zeta(r) \equiv \begin{cases} 1 & \text{if material 1} \\ 0 & \text{if material 2} \end{cases} \quad \text{over } \Omega \]

\( q \) penalization parameter:
pushes toward 0 or 1

Material property will depend on the position

SIMP model
(Solid Isotropic Material with Penalization)

\[ \rho(r) = \rho_{\text{mat1}} + \zeta(r)^q (\rho_{\text{mat2}} - \rho_{\text{mat1}}) \]
PENALIZATION FUNCTIONS

SET OF FUNCTIONS TO FORCE THE CONVERGENCE TOWARD DESIRED SOLUTIONS

Heaviside projection

- Slow convergence of $\zeta$ values toward 0 & 1
- Gradient based optimization techniques
  $\Rightarrow$ continuous function $\zeta_P = P(\zeta)$

Penalized damping = Pamping

- $\sim$ no sound in the solid (impedance mismatch)
- $\Rightarrow$ artificial damping
- damping coefficient
  $$\alpha\left(P(\zeta(r))\right) = \begin{cases} 0 & \text{if air} \\ K \gg 1 & \text{if solid} \end{cases}$$

Set the threshold between 2 materials @ $\zeta = 0.5$
Solution presents a checkboard pattern

Averaging $\zeta$ the over an $r_0$ radius circle

Can be done by solving

$$-r_0^2 \nabla^2 \tilde{\zeta} + \tilde{\zeta} = \zeta$$

Smoothed solution $\tilde{\zeta}$

 Typical value for $r_0 \approx 1.5$ mesh size

BC : convenient to set material on desired boundaries
OBJECTIVE AND CONSTRAINTS DEFINITION
SETTING UP THE GEOMETRY AND OBJECTIVES FOR OPTIMIZATION

Objective

\[
\text{Maximize the average pressure retrieved @ microphone}
\]

\[
\max \int_{\Omega} |p|^2 \, dS
\]

Constraints

- Relative positioning
- Guaranteed acoustical path
- Amount solid in \( \Omega \)

\[
0 < k_{down} \leq \frac{\int_{\Omega} \zeta \, dV}{V} \leq k_{up} < 1
\]
BOUNDARY CONDITIONS
SCHEMATIC VIEW AND PARALLEL BETWEEN BC AND MATERIAL TOPOLOGY

- Dirichlet BC for air: $\xi = 0$
- Dirichlet BC for solid: $\xi = 1$
- Linear sound source: $p_0e^{i\omega t}$
- Laser volume
- Sound connection
- Topo opt SIMP material

Linear sound source
Laser zone = air
Connection tunnel = air
Microphone

Lossless sound propagation
Pamping
Lossy sound propagation
COMSOL® IMPLEMENTATION

KEY VARIABLES AND PARAMETERS TO BE IMPLEMENTED

- Heaviside projection
- SIMP model
- Topo Opt
  - def
  - bounds
- Objective
- Constrains
- Regularization
  - BC

Solvers available:
- SNOPT
- MMA

No damping

Pamping
OPTIMIZED CHAMBER @ 25 kHz
MICROPHONE LOCATION SET @ THE CENTRE
OPTIMIZED CHAMBER @ 25 kHz
MICROPHONE LOCATION SHIFTED FROM THE CENTRE
COMPARISON BETWEEN PAS CELLS

CRITERIONS TO COMPLY TO MAKE CORRECT COMPARISONS OF TWO CELLS

Pressure response of a PAS cell

\[ \frac{p}{QK_{geom}} = \frac{(\gamma - 1) L Q}{\alpha P_L} \]

2 PAS cells are equivalent if they have the same

- Volume \( V \)
- Laser path length \( L \)
- Buffer gas \( \gamma \)
- Absorbed laser power \( \alpha P_L \)

The rest is shape dependent
CONFIRMATION OF SIGNAL IMPROVEMENT THANKS TO TOPOLOGY OPTIMIZATION

COMPARISON OF SIMULATED PHOTOACOUSTIC SIGNAL FROM TWO CELLS

Frequency domain analysis

the optimized shape shows extended amplification capabilities
CONCLUSION
CONCLUSION

- Topology optimization of PAS cell was undertaken
- Building and setting up the COMSOL model
- Definition of equivalency between cells for improvement signal assessment
- Comparison and confirmation of improved signal simulated