Modeling for Design Optimization of Quartz Enhanced Photoacoustic Spectroscopy-Based Sensors

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Introduction

Our goal is to measure the flux of environmentally relevant gases in and out of the ocean. The flux will be determined using the Eddy Correlation method, which requires high temporal and highly variable (ppb) measurement of gas concentrations. We are exploring Quartz Enhanced Photoacoustic Spectroscopy (QEPAS) as a possible solution.

In photoacoustic spectroscopy, the optical source is modulated at an acoustic frequency. If the optical wavelength corresponds to an absorbance line in the gas, the periodic optical signal will launch an acoustic signal that can be detected with a microphone. In QEPAS, a quartz tuning fork is used instead of a microphone. Compared to other PAS methods, this promises great simplicity and sensitivity.

The Laser Science Group at Rice University has observed that the addition of an acoustic resonator tubes about the tuning fork dramatically increases the current output. But determining the optimal tube geometry is analytically difficult. Numerical modeling is essential in order to fully test various design options at an acceptable cost.

System modeled in COMSOL Multiphysics

Perfectly Matched Layer (PML) used to prevent acoustic reflections at boundary

Design space divided in half to reduce computation time

Absorption modeled as line source

Anatomy of a Model

Source and surrounding gas modeled in acoustic module

Fork modeled in piezoelectric module

In the piezoelectric domain, the time surface boundaries are loaded by the pressure determined in the acoustic module. Viscous damping is added on the surface as an oppositional force that is parameterized using an oscillating sphere model fit to experimental data on the effect of pressure on the tuning fork quality factor.

In the acoustic domain, the time surface boundaries are set at normal acceleration, with their acceleration value taken from the acceleration determined in the piezoelectric module.

Comparison to Data

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<th>COMSOL</th>
<th>Experiment</th>
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<td>Q, mm</td>
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<tr>
<td>32,764</td>
<td>86,402</td>
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</tbody>
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Optimal tube length is a local maximum due to interaction between the fork and the structure.

Results

Pressure profile evolution with acoustic resonators illustrates this interaction.

We are now working to experimentally validate these modeling results, and to extend the model to examine the effect of changing the radius on the system.

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