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# Modeling the Response of Photoacoustic Gas Sensors

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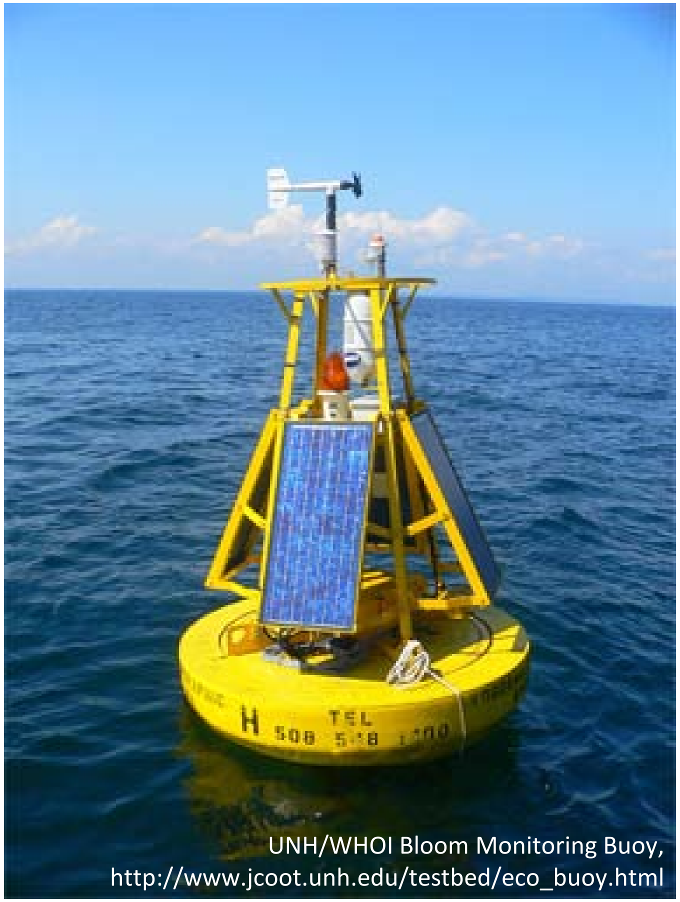
# Motivation

- There is a need for improved measurements of the ocean-atmosphere fluxes of trace greenhouse gases from ships and buoys.

- Flux measurements require sensing wind velocity and gas concentration at 5 – 10 Hz, and at O(ppb) levels.



UNH/WHOI Bloom Monitoring Buoy,
http://www.jcoot.unh.edu/testbed/eco_buoy.html

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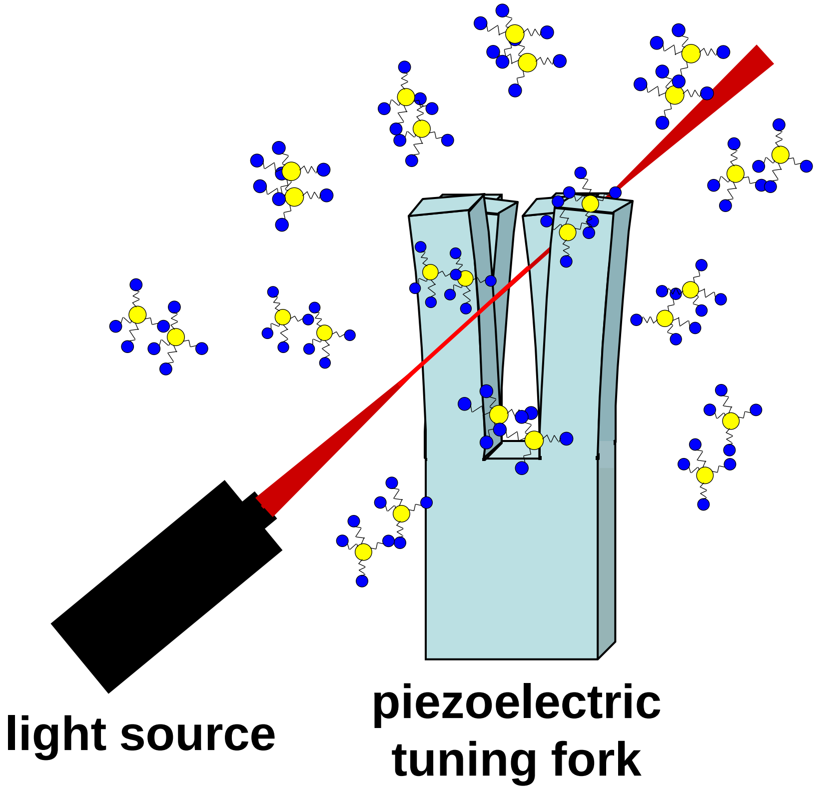
# Photoacoustic Spectroscopy (PAS)

- An infrared spectroscopic technique where light, modulated at acoustic frequencies, excites the molecules vibrationally.
- Collisional de-excitation produces an acoustic wave that (conventionally) is detected with a microphone.
- The resulting laboratory sensors are compact, robust, and can sense ppb gas concentrations.
- "Quartz EnhancedTuning Fork PAS", pioneered by Kosterev *et al.* at Rice University, replaces the microphone with a more sensitive piezoelectric tuning fork (*i.e.* resonant) detector.



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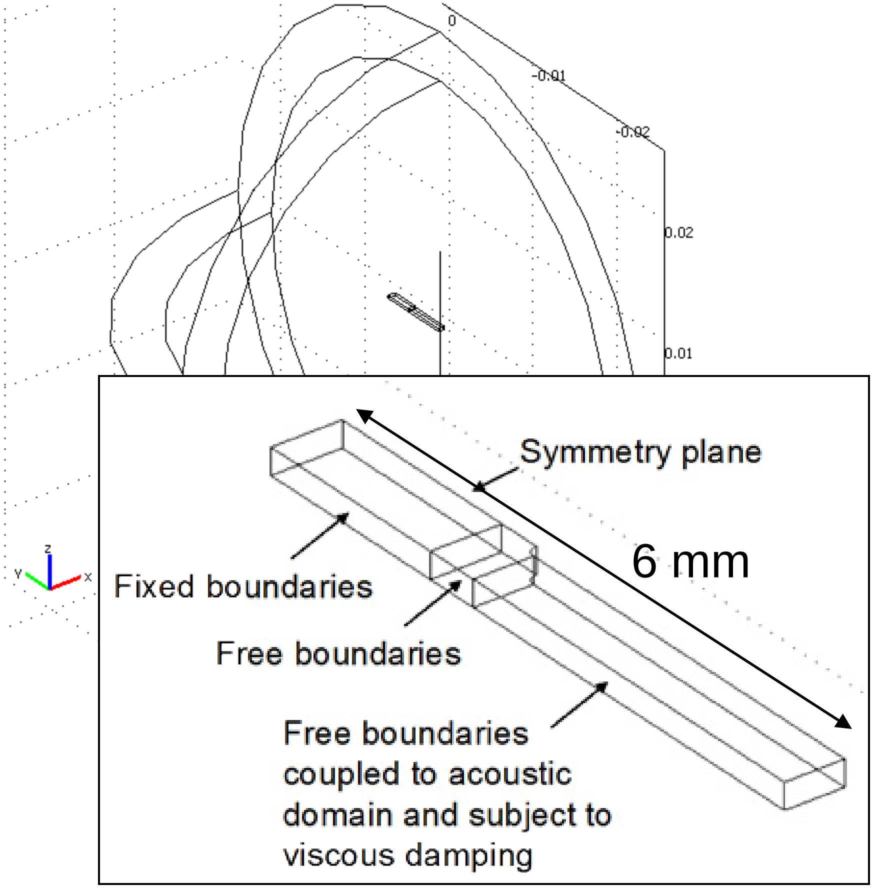
# A Multiphysics Problem

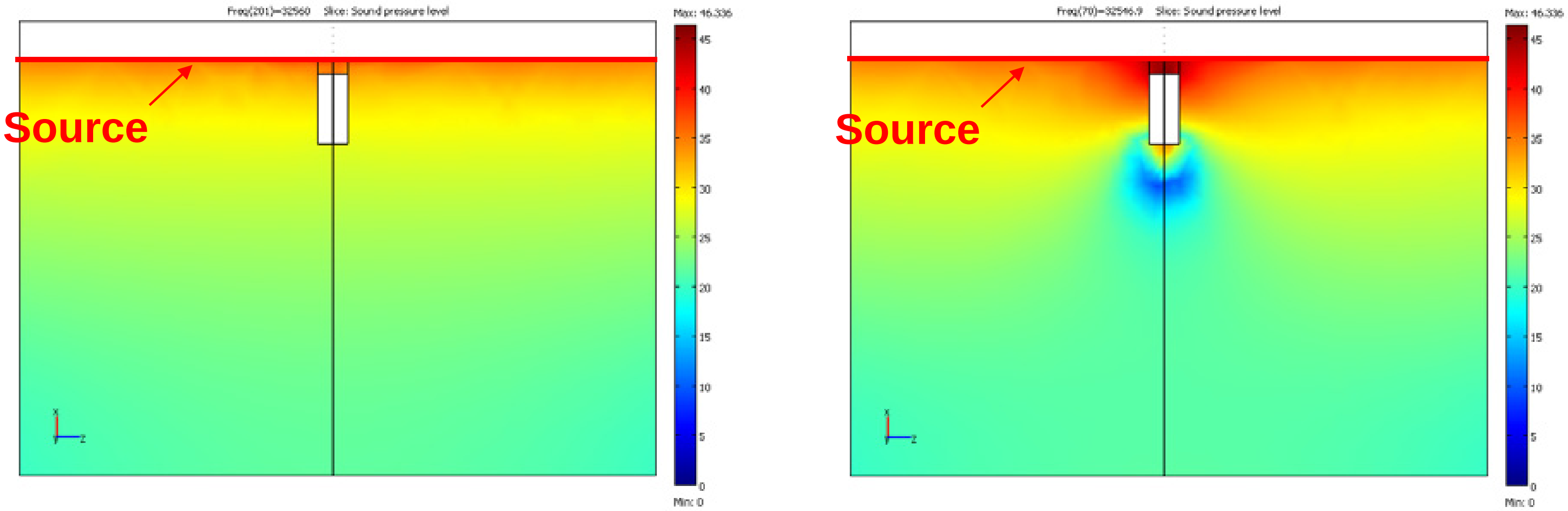
- Numerical modeling is used to test design options efficiently.
- PAS is a true multiphysics problem:
  - Infrared molecular absorption and collisional de-excitation…
  - Launches an acoustic wave…
  - Which travels through the system…
  - Coupling to the piezoelectric tuning fork structure…
  - Resulting in an electrical signal…
  - While the primary source of energy loss is viscous damping!

# COMSOL Model

- Uses 3D Pressure Acoustics and Piezo Solid modules.
- Takes advantage of symmetry plane.
- Absorption and de-excitation is modeled as a line source with a specified strength.
- Viscous damping is added explicitly as a velocity-dependent term in the dynamical equations of the fork, and is parameterized using an oscillating sphere model.
- Output current is calculated from the charge on the tine surfaces.
- A PML is used to prevent reflection of acoustic waves back into the system.



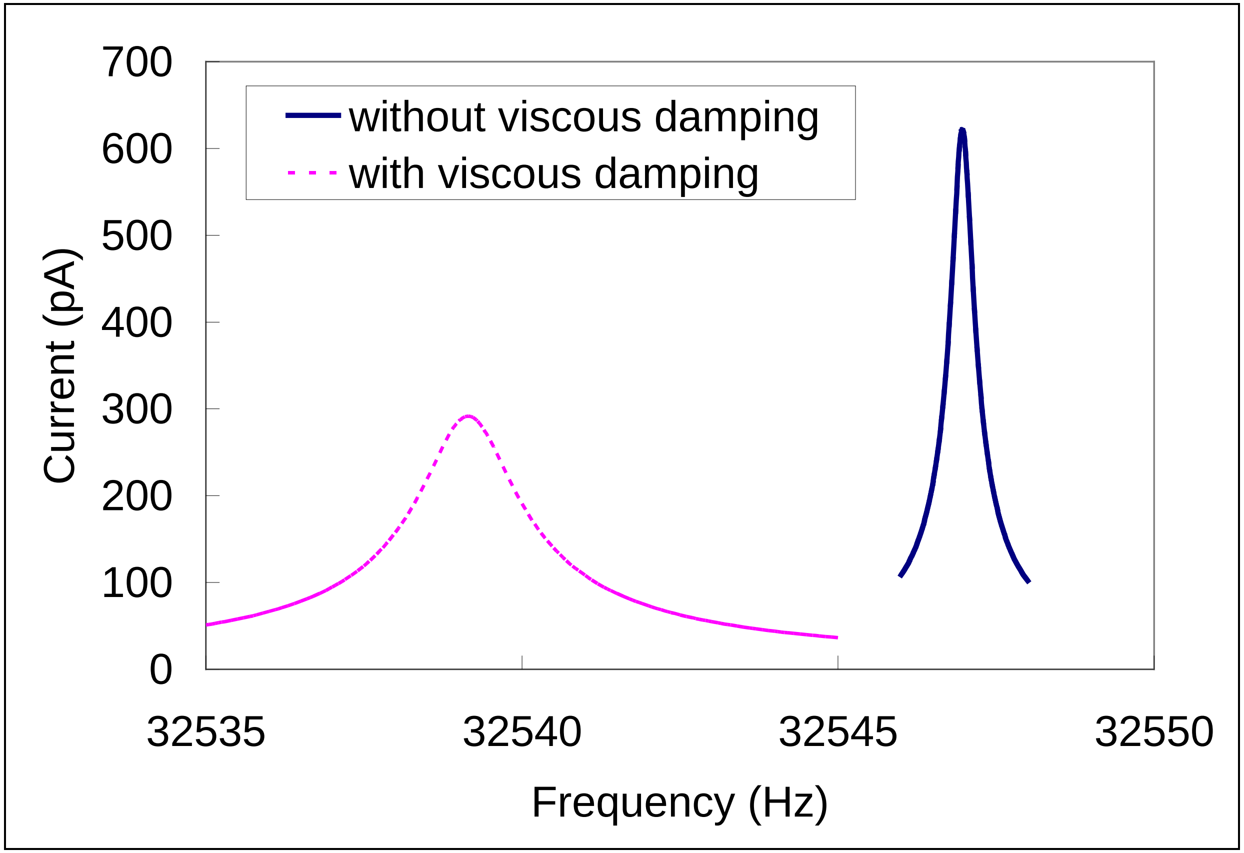
# Results: Pressure Field



- Top view of a tuning fork tine in plane with the line source.
- Left panel: pressure field for off-resonance excitation of the fork.
- Right panel: pressure field on-resonance. The pressure field is consistent with the radiation pattern from a linear quadrupole (D.A. Russell, “On the Sound Field Radiated by a Tuning Fork”, *Amer. J. Phys.* **68**, 2000)

# Results: Damping Effects

- The length of the free boundary part of the stem was used as a fitting parameter for the resonant frequency in vacuum.
- The “equivalent sphere radius” in the damping model was adjusted to give the observed frequency shift for forks in a vacuum and in the atmosphere.



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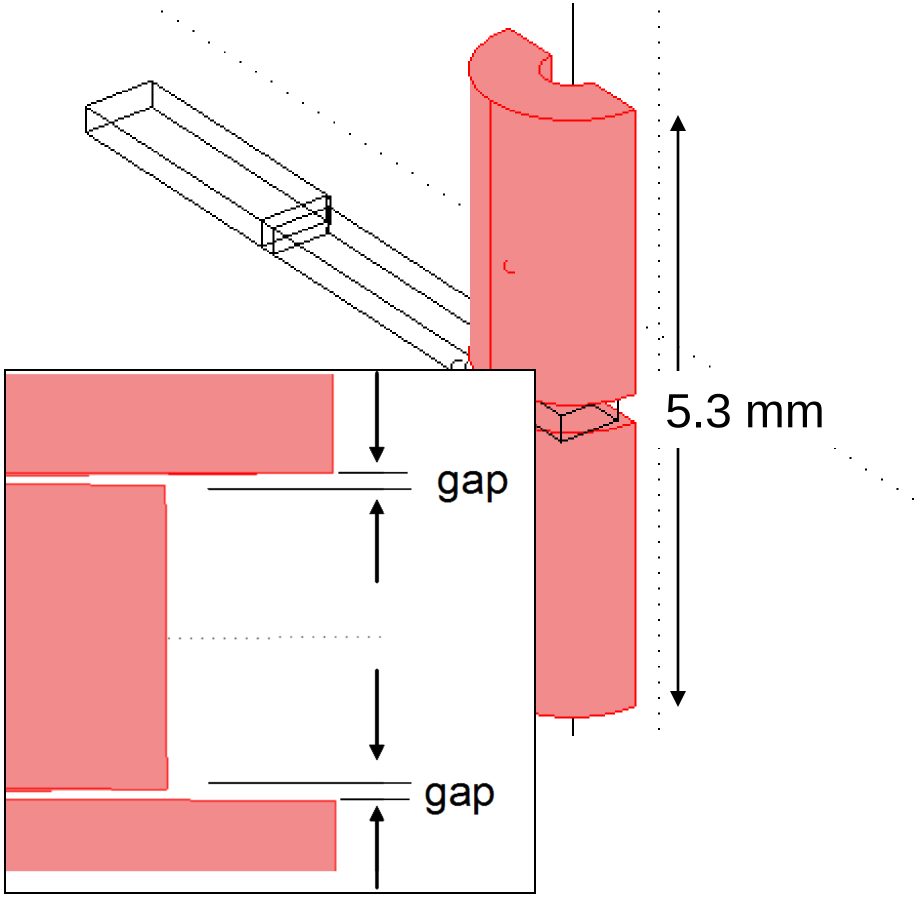
# Results: Comparison to Experimental Data

| | COMSOL Model | Experiment |
|---|---|---|
| $f_0$ and Q in vacuum | 32.547 kHz, 95726 | 32.764 kHz, 93456 |
| $f_0$ and Q at 760 Torr | 32.539 kHz, 23242 | 32.756 kHz, 13271 |
| Signal for 6.7% $CH_4$ at 375 Torr | 0.54 V/(W/cm) | 1.24 V/(W/cm) |

- Compared against observations reported in:
  - A. A. Kosterev *et al.*, "Applications of Quartz Tuning Forks in Spectroscopic Gas Sensing", *Rev. Sci. Instrum.*, **76**, 043105 (2005).
  - A. A. Kosterev *et al.*, "Quartz-Enhanced Photoacoustic Spectroscopy", *Optics Lett.*, 27, pp. 1902-1904, (2002).

# Signal Enhancement Studies

- Tubes added around the beam to confine the acoustic energy.
- They are sized so that their longitudinal resonance matches the TF resonance.
- The gap between the tubes and fork is a necessary evil.



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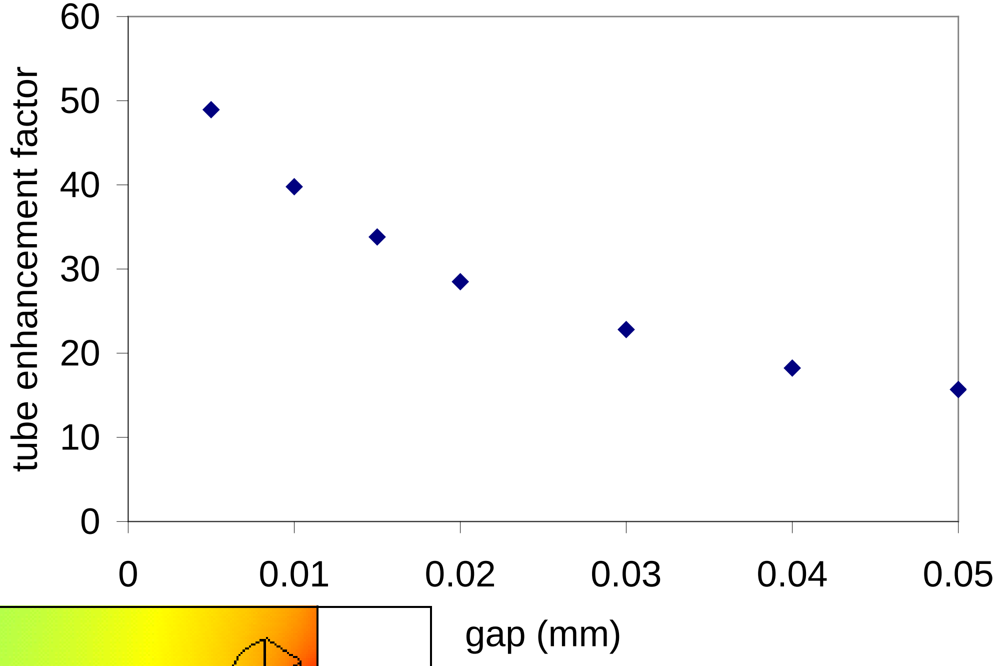
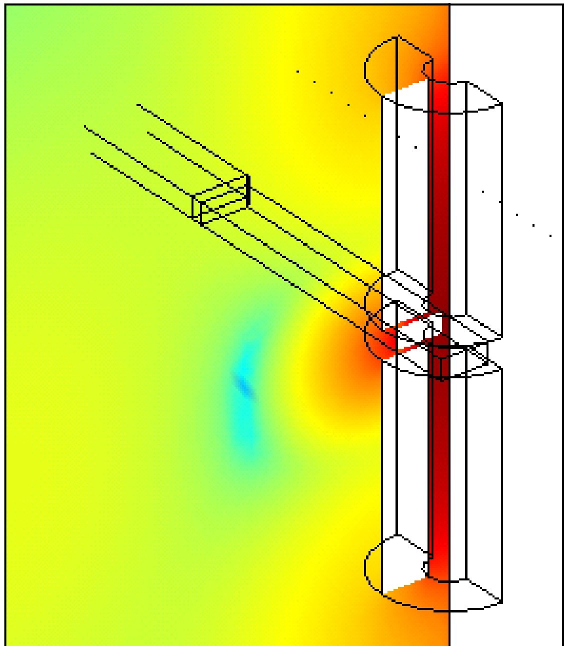
# Signal Enhancement Results

- Resonator tubes enhance responsivity by a factor of 15 – 50 depending on the gap.
- Experimentally, enhancements of 8 to 20 have been observed, for gaps between 30 and 50 μm.
- These results suggest design variations that may result in greater signal gains.





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# Summary

- COMSOL was used to develop a numerical model for a photoacoustic spectroscopic system, which poses a complex multiphysics problem.
- We obtained good preliminary agreement between model results and experimental data.
- The model will be a useful tool for evaluating alternative PAS designs.
- Future work will focus on evaluating new designs, and developing a better understanding of the fluid mechanics of the viscous damping.

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