Mathematical Modeling for the Next Generation of Trace Gas Sensors

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Anatoliy Kosterev, Frank Tittel, James. H. Doty III, and David Thomazy (Rice University)

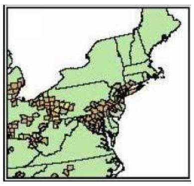
NSF Engineering Research Center: Mid–InfraRed Technologies for Health and the Environment (MIRTHE)

MIRTHE Goals: To develop trace gas sensors using two new technologies:

- Quantum Cascade Lasers (QCL's) – see exhibit by Claire Gmachl (Princeton)
- Quartz-Enhanced PhotoAcoustic Spectroscopy (QEPAS) developed by Kosterev and Tittel at Rice University.

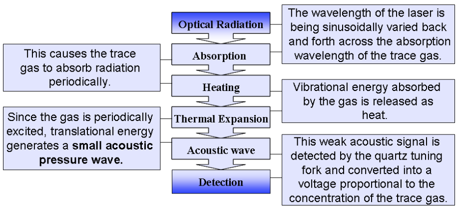
Applications

- Non-invasive disease diagnosis (e.g., liver disease and lung cancer) using breath biomarkers.
- Environmental and industrial monitoring using networks of sensors (e.g., monitoring of atmospheric carbon dioxide levels).
- Homeland security (e.g., chemical weapon detection at airports, train stations, etc).



Photoacoustic Spectroscopy (PAS)

- In 1888 Alexander Graham Bell discovered the photoacoustic effect:
  - ∗ Specifically that periodic absorption of light by matter produces sound.
  - ∗ He used this phenomenon to develop a wireless communication device.
- Since light is only absorbed by the gas at particular wavelengths the photoacoustic effect can detect trace gases.
- In the 1970's PAS was used to detect nitric oxide in the stratosphere which was proof of ozone depletion by man-made chemicals.



Optical Radiation

The wavelength of the laser is being sinusoidally varied back and forth across the absorption wavelength of the trace gas.

Absorption

This causes the trace gas to absorb radiation periodically.

Heating

Vibrational energy absorbed by the gas is released as heat.

Thermal Expansion

Since the gas is periodically excited, translational energy generates a **small acoustic pressure wave.**

Acoustic wave

This weak acoustic signal is detected by the quartz tuning fork and converted into a voltage proportional to the concentration of the trace gas.

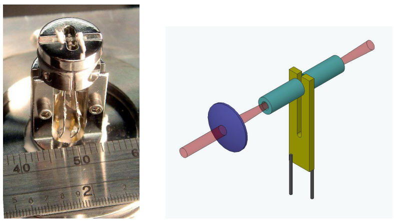
Detection

QEPAS

QEPAS Sensors detect the sound produced in PAS using a quartz tuning fork (like the one in your watch) to amplify and detect the sound wave.

Advantages of QEPAS with QCL's over Previous Techniques

- Greater sensitivity due to the strong absorption by simple molecules in the infrared spectrum and the power of QCL's.
- Rugged and small in size → portable
- Cost Effective → can be deployed in sensor networks.



Left: Actual QEPAS sensor device. Right: Schematic diagram of QEPAS device for simulation.

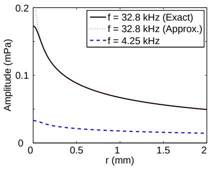
A Mathematical Model for QEPAS Sensors

Goals:

- Increase physical understanding of QEPAS,
- Optimize design of sensors.

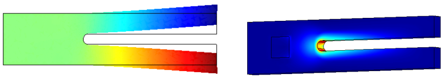
Outline of Model

- The interaction of the laser and the trace gas generates a sound wave which we model using a forced acoustic wave equation.



Simulated acoustic pressure wave as a function of radial distance from laser beam.

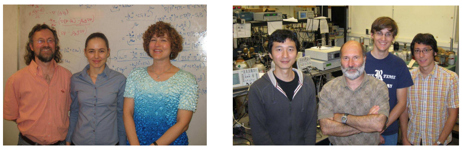
- The sound wave excites a vibration of the quartz tuning fork.



Left: The displacement of the 32.8 kHz tuning fork. The red and blue colors show the maximum and minimum displacement, respectively. Right: The first principal stress. The stress is largest (red) where the tines of the tuning fork meet the base.

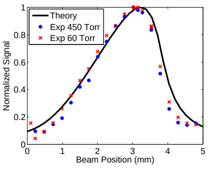
- The photoelectric effect in quartz converts this vibration to an electric current whose strength is proportional to the concentration of the trace gas.

Project Participants



Left: Mathematical Modeling Group (John Zweck, Noemi Petra, Susan Minkoff). Right: Experimental Group (Lei Dong, Anatoliy Kosterev, Jim Doty, Christian Zaugg; Not shown: Frank Tittel and David Thomazy).

Sensor Optimization

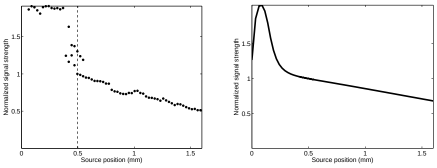


Normalized amplitude of the piezoelectric current as a function of the vertical position of the laser beam for a QEPAS sensor with a 32.8 kHz tuning fork.

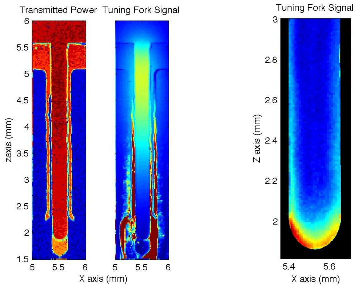
- We used experiments and computer simulation to find the position that produces the largest current.
- These results validate the model and confirm the optimal placement of the laser beam.

Resonant Optothermoacoustic Detection (ROTADE)

- The heat generated by absorption of light can be directly detected using a tuning fork.
- ROTADE and QEPAS are complementary techniques operating in different pressure regimes.
- Experiments and simulations show that the laser must be positioned close to the walls of the tuning fork and near the base of the tines.



Left: The normalized experimental signal strength vs the position of the laser beam. Right: the numerically computed signal strength vs laser position.



Experimental Results. Left: tuning fork image depicting transmitted power and signal as a function of beam position for 300 torr of pure CO_2. Observed signal primarily due to photoacoustic effect. Right: tuning fork (in black) shows the signal due to ROTADE as a function of beam position at a reduced pressure of 20 torr of pure CO_2 .

- We plan to use the models to improve performance of both methods by optimizing the geometry of the tuning fork.

Acknowledgement

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