A long-wave infrared spectrometer based on an external-cavity quantum cascade laser and a hollow silica waveguide

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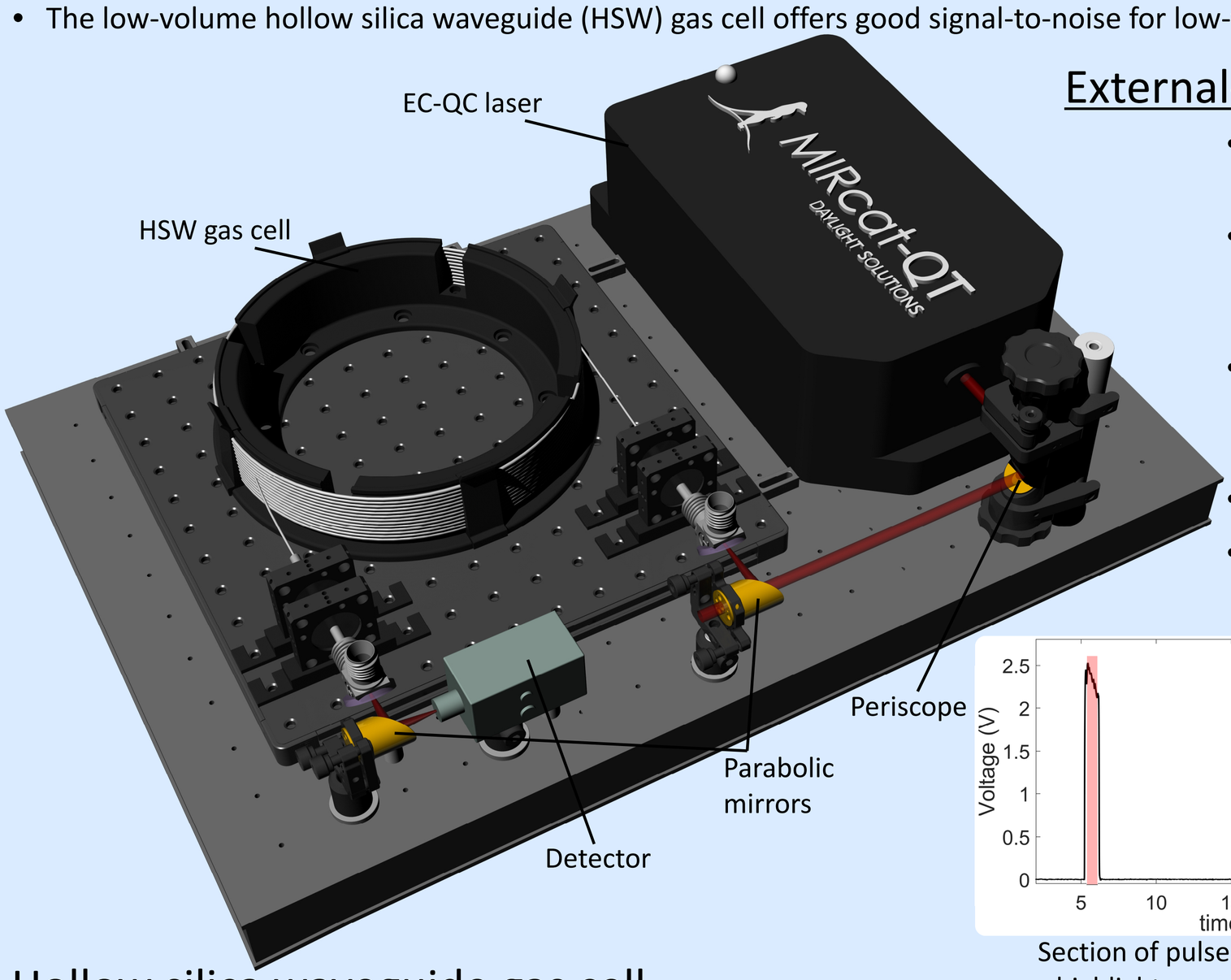
Introduction and background

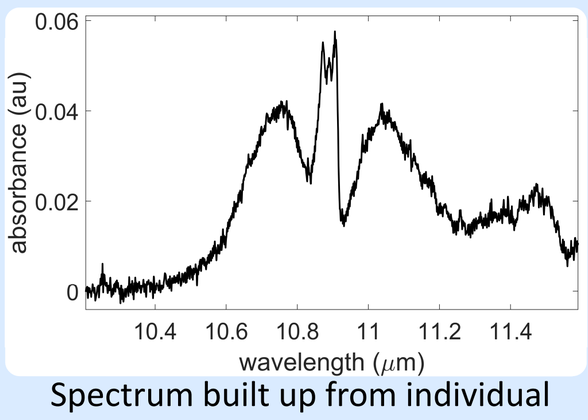
- Diagnosis of disease can be achieved through quantification of volatile organic compounds (VOCs) in headspace gas of patient matrices (e.g. faeces, urine, or breath).
- This can be done using gas chromatography/mass spectrometry (GCMS) at centralized laboratories.
- Aim to develop spectroscopic instrumentation to perform VOC quantification at point-of-care.
- An external-cavity laser provides a large tuning range allowing measurement of a wide range of absorbing species with broad spectral features.
- The low-volume hollow silica waveguide (HSW) gas cell offers good signal-to-noise for low-volume samples.



External-cavity QCL spectrometer

- Pulsed quantum cascade laser source offers tuning from 10-13 μm, covering many VOC absorptions.
- 250 MSs^{-1} (max) 14-bit digitization resolves individual pulses, which are averaged to build up spectra.
- Laser sweep triggering stabilizes spectral position and allows real-time spectrum refresh (3-4 Hz per μm typical).
- Typical spectrum constructed from ~40,000 pulses.
- The detector is a four-stage cooled Hg-Cd-Te photodetector.

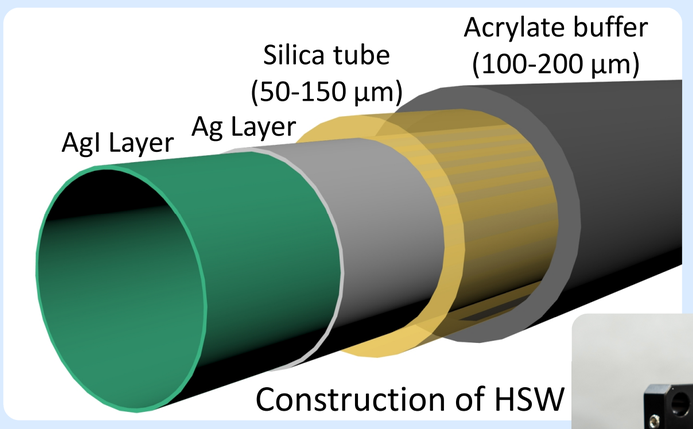
Section of pulse train. Shading highlights averaged regions



Spectrum built up from individual pulse data. (Propane at 1,000 ppm)

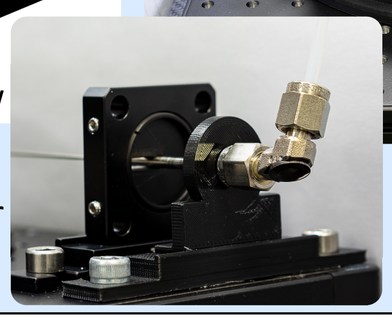
Hollow silica waveguide gas cell

- HSW consists of a silica tube internally coated with silver/ silver halide.
- Gas cell built using a 5 m length of HSW.
- Gas cell constructed using elbow gas compression fittings. (patent WO/2016/181100).
- Diamond windows offer wide transmission across IR spectrum. Brewster alignment suppresses interference fringes.



Construction of HSW

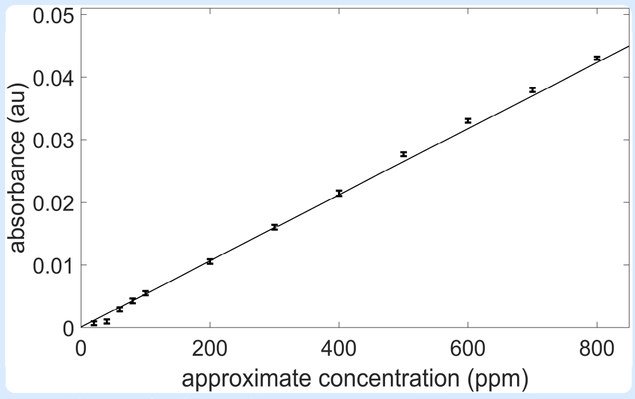
Photograph of HSW gas cell on 3D printed mount



Photograph of Brewster aligned window

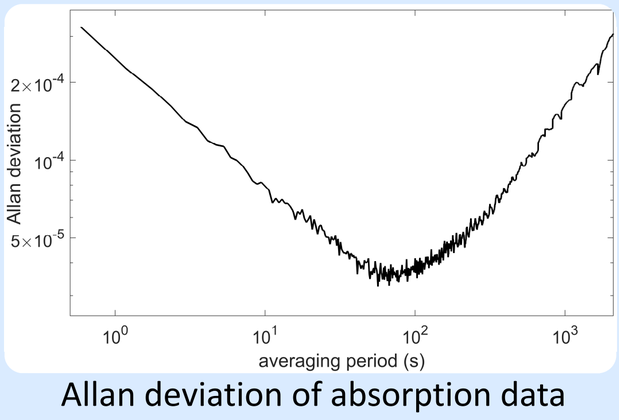
Results using propane test gas

- Accurate flow rates achieved using a network of mass-flow controllers.



Plot of absorbance vs. concentration

- Allan deviation of absorption data acquired from propane spectra recorded at ~0.75 Hz.
- Minimum value of ~3×10^{-5} obtained at an integration time of ~100 s.



Allan deviation of absorption data recorded over a ~2 hr period

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