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AEROSPACE ENGINEERING

Computation of rotational vibrational spectra for use in supersonic flow spectroscopy

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Overview

Scramjet (Supersonic Combustion Ramjet) technology could potentially allow for the creation of hypersonic passenger flights, capable of traversing continents in just a few hours. Scramjets work very much like ramjets, save for the fact that the combustion powering the engine takes place during supersonic flow.

Combustion within supersonic flow is extremely complicated – The flow must be treated as compressible, and energy created from ongoing combustion must be considered. Thus, to develop a better understanding of supersonic combustion flows, it is necessary to experimentally simulate and analyze them.

To analyze the temperature and composition of these flows, Raman spectroscopy is used.

During the last two semesters, I have compiled a program capable of simulating the Raman spectra of an arbitrary mixture of gases at an arbitrary temperature. The output of this program can potentially be used to do the reverse in the future, the calculation of composition and temperature from the spectrum.

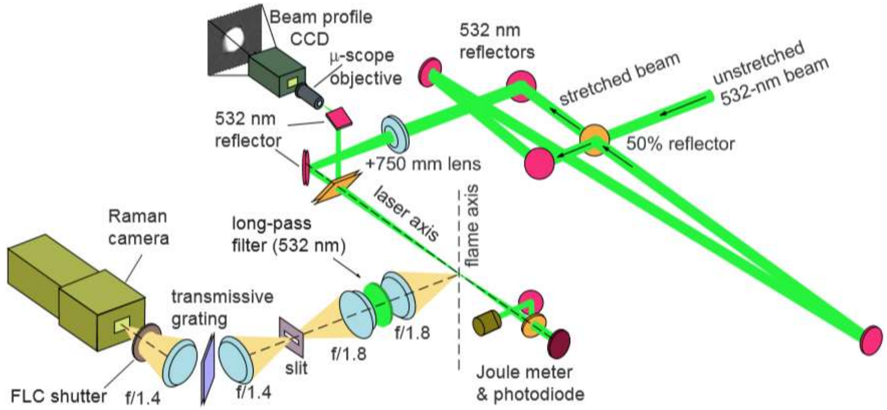
Raman Spectroscopy

Raman Spectroscopy is a method of measuring the temperature and chemical composition of a sample, and the primary method used in this laboratory. In this method of analysis, a laser is shot through the supersonic flame, and the scattering of the laser off the molecules in the flame is measured to determine the temperature and composition at that point in the flow.

Photons from a monochromatic source (like a laser), when interacting with the molecules in a sample, can change frequencies by causing a transition between rotational or vibrational states, exchanging energy with the molecule in question, and creating a distinct pattern of output frequencies. This process is extremely rare, though, and almost all of the scattered light is of the same frequency as the source (this is known as Rayleigh scattering), making the use of filters necessary to remove unwanted signals.

To simulate the Raman spectra per-detection, physical chemistry and quantum mechanics were used to determine the viable rotational and rovibrational transitions in the sample.

The Apparatus



- 2nd harmonic of a Nd-YAG laser is used
- High power output (1 J) necessitates the use of an Interferometric Pulse Stretcher, lest the air be ionized from the high irradiance, which could harm the detector. The Interferometric Pulse Stretcher stretches the duration of the pulse from 10^{-8} seconds to $2.5x10^{-5}$ seconds.
- The laser is then focused by a lens to a radius of 125 μm and passed through the test section containing the supersonic flame. After the laser passes through the test section, part of it is measured by a photodiode to determine the intensity of the beam, and, by extension, the expected intensity of the Raman spectrum produced.
- The Rayleigh and Raman scattering observed from the side is passed through a number of lenses and a long pass filter before entering the Raman camera, to focus light on to the detector and remove extraneous Rayleigh scattering.

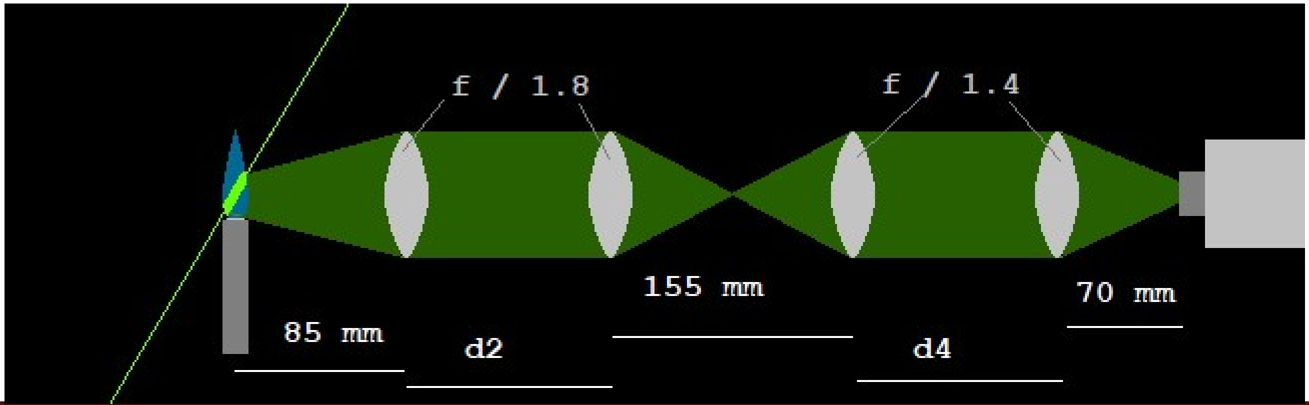
Figure is sourced from Dr. Alex Bayeh's PhD thesis (2013)

Optics

The optical apparatus between the flame and the Raman camera is used to collect as large of a portion of the scattering as possible (thus low f-number lenses are used), separate different wavelengths of the light, and refocus it into the Raman camera. In order to create an accurate simulation of the spectrum's result, the optics of the detector had to be understood.

The detector was analyzed through a process known as optical ray-tracing, which represents optical components as matrices and light as vectors.

It should be noted that a long-pass filter is used to block unwanted Rayleigh scattering.



Diffraction gratings and the Detector

Diffraction gratings are optical components taking advantage of the effects present during the interaction of light with a material with repeating features on scales comparable to the wavelength of the light. This causes scattering in directions dependent on the frequency of the light.

This effect can be used in a spectrometer, as different wavelengths of light can be separated in a manner nominally linear to their frequency. This allows for the imaging of Raman spectra in two dimensions, one spatial and one relating to the frequency of the light.

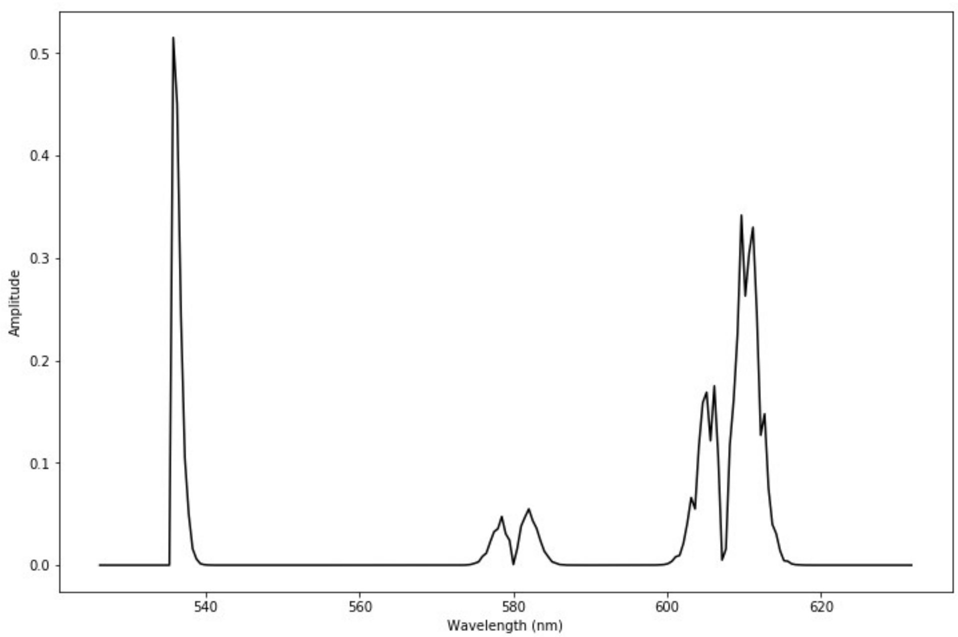
The detector in the Raman camera then collects the light from the optical apparatus in a 512x512 pixel camera, which outputs the spectrum.

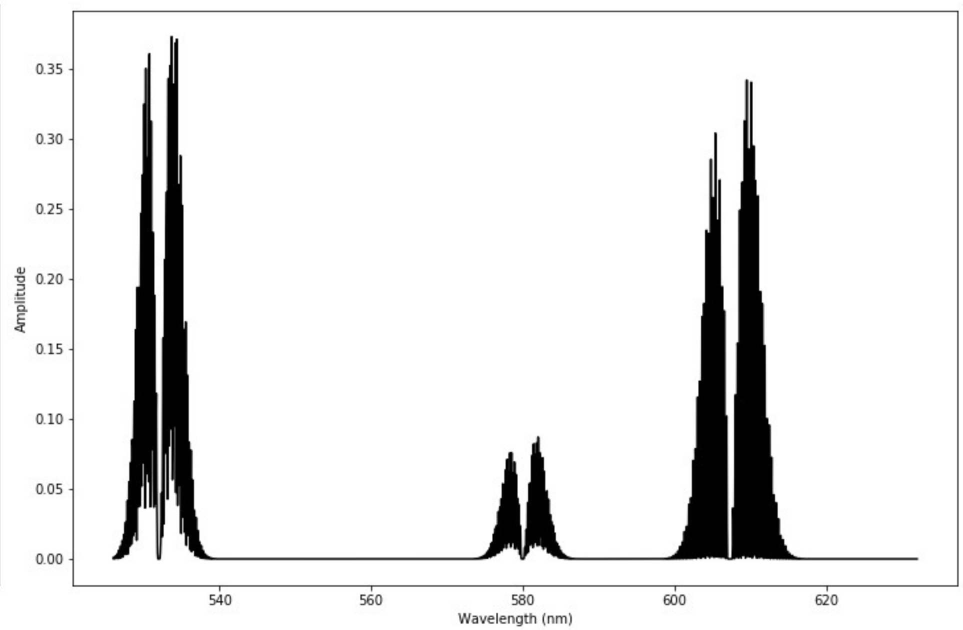
By using a combination of ray-tracing and diffraction grating analysis, the spectrum generated can be discretized through a virtual detector to facilitate comparison with experimental data.

The Program

Using the methods outlined on the previous slides, and using the Python programming language, a program was developed to simulate both the rotational and rovibrational Raman spectra of an arbitrary mixture of gases at an arbitrary temperature.

An example of the end product is shown below – A spectrum of air at 300 K; both what the detector shows, and the true spectrum.





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Questions?

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