Development of an Infrared Laser Absorption Tomography Technique

Meghan Colleen Snyder
University of Virginia, Charlottesville, VA 22904
Advisor: Dr. James McDaniel
Mechanical and Aerospace Engineering, University of Virginia

Abstract

The non-intrusive, laser-based technique of Tunable Diode Laser Absorption Tomography (TDLAT) is a combination of infrared laser absorption spectroscopy and tomographic image reconstruction. The tomographic experimental design, setup and reconstruction algorithm are discussed, as well as the line-of-sight water vapor absorption measurements. This research will lead to spatially resolved measurements of water vapor concentration and temperature of the flow at the exit of a dual-mode scramjet combustor in the future. Water vapor absorption measurements in room air are compared to the latest HITRAN spectroscopic data and found to be in good agreement.

Introduction

Wind tunnel testing is an integral part of engine development of hypersonic air breathing propulsion systems such as Supersonic Combustion Ramjets (Scramjets). This testing allows for new designs to be evaluated in a controlled environment to discover where improvements should be made until they are ready for flight. Wind tunnel experiments are not limited to the testing of scramjet designs. They can also be used for comparisons to computational calculations of engine flow. The dual-mode scramjet combustor wind tunnel facility at the University of Virginia has been used to perform experimental studies, using both conventional and state of the art methods to measure flow properties, such as wall pressure distributions, velocity, wall temperature, and species concentrations.

This paper focuses on the experimental design and setup to spatially resolve the two-dimensional water vapor concentration and temperature of the flow at the exit of a dual-mode scramjet combustor using non-intrusive, laser-based techniques. The experimental design is able to accommodate a flat flame burner used for calibration and verification studies, as well as the dual-mode scramjet combustor. A large rotational stage is used to encompass the flat flame burner and short extender of the tunnel for data collection.

The orientation of the infrared laser light can be varied to probe the flow at a variety of angles through which line-of-sight measurements are taken in order to produce tomographic images. One dimensional projections of water concentration are taken at different angles and reconstructed into a two-dimensional water vapor distribution image. The original data is reconstructed through a MATLAB program which employs the techniques of filtered backprojection.

Using computational software, data will be analyzed to determine both the water vapor concentration and the temperature of the flow across the exit of the dual-mode combustor. This will be done for a nonreacting Mach 2 flow with a known water concentration, as well as in a flow with hydrogen combustion in the supersonic dual-mode combustion tunnel. Preliminary line-of-sight measurements have been made in room air and will be presented later in this paper.

Measuring these flow properties will allow determination of the efficiency of the combustion process. The combustion efficiency in a scramjet can be an important part of the analysis of the engine’s performance, such as that occurring with different fuel injector geometries. This direct efficiency measurement is not currently possible and will be very valuable in the optimization of the design of scramjet combustors.

Combustion Efficiency

Combustion efficiency can be determined several ways. It can be determined by the measured enthalpy of the reaction divided by the ideal enthalpy of combustion. This involves introducing probes into the flow to measure a concentration sample or temperature, changing the properties of the flow. Pressure measurements made at different locations along the walls of a tunnel can also be used to analyze combustion efficiency.¹
For this work, it is calculated by determining the fraction of hydrogen that is converted to water during the reaction. First water vapor flux can be determined at the combustor exit by combining the water vapor concentration and velocity field distributions across the same plane. Measurement of the water vapor flux at the combustor exit, combined with the known hydrogen flux injected in the combustor fuel injector, allows the determination of the fraction of the hydrogen fuel that was converted to water during the reaction. This is shown in the equation below, where \( n_{H_2O} \) is the water vapor number density, \( V \) is the velocity normal to the exit plane, and \( n \) is the number density flow rate of the injected hydrogen fuel.

\[
\eta_c = \int_{A_{exit}} n_{H_2O}(y,z) V(y,z) \, dA_{exit}
\]

The velocity field measurements needed to measure the water vapor flux will be performed by a fellow graduate student using a technique called Particle Image Velocimetry (PIV).

**University of Virginia dual-mode scramjet combustor facility**

The scramjet at the University of Virginia is a direct-connect, Mach 2 hydrogen-air combustor, capable of simulating a Mach 5 enthalpy flow. The combustor operates in the mixed ramjet/scramjet, or dual-mode. A single 10 degree, unswept ramp fuel injector produces a highly mixed and combusting flow. \(^2\) Unique to the UVA wind tunnel is the use of electrically heated coils to heat the air to 1200K, which allow the facility to be free of the contaminate gas products generated in combustion-heated facilities. The heater core is contained in an underground flow reservoir (see Figure 1). The multiple measurements required for tomography can be taken on the wind tunnel due to its continuous flow testing ability.

**Review of Literature and Theory**

Reconstructions from projections have been solved mathematically since 1917 when Radon first published the solution in his paper. \(^3\) Since then, scientists have found many applications for this mathematical theory. Physicist Allan Cormack\(^4\) first created cross-sectional images of the human body using a combination of X-rays and tomography in the late 1950s. Godfrey Houndsfield independently invented the first x-ray computed tomographic scanner\(^5\), using iterative algebraic techniques to solve his reconstructions. The first transform-based reconstruction methods were developed by Ramachandran and Lakshminarayanan, and later expanded upon by Shepp and Logan. There are now imaging filters used in reconstruction techniques named after these men. \(^6\)

Among the first to demonstrate the applicability of tunable IR diode lasers to obtain non-intrusive spectroscopic data in combustion gases were Hanson et al\(^7\) in 1977. They are currently measuring water vapor absorption spectra at high pressure and temperature. Since 1980, tomography has been used as a combustion diagnostic technique combined with absorption and other laser based measurement techniques. Bennett et al\(^8\) started conducting absorption experiments using fan beam geometry tomography in 1984 when they mapped iodine vapor using an Argon ion laser and rotating mirror. Quick data collection for fast-reacting flows was researched by Beiting\(^9\), who designed an instrument capable of imaging such flows.

**Theory**

**Infrared Laser Absorption Tomography** is the combination of infrared laser absorption and tomographic image reconstruction. It is used to spatially resolve the two-dimensional water vapor concentration and temperature distribution of the flow across the exit plane of the dual-mode combustor. In the following sections, spectroscopy

---

Snyder 2
theory for the absorption of light by water vapor in the near IR will be discussed as well as measurement collection geometries and methods for tomographic image reconstruction.

Infrared Laser Absorption Spectroscopy

Direct absorption spectroscopy is described by the Beer-Lambert law, which governs the absorption of electromagnetic radiation of water vapor in the near infrared, as shown in equation (2). The transmitted intensity, I(ν), is related to the incident intensity, I_0(ν), by the path length of water vapor, L, and the spectral absorption coefficient, κ(ν).

\[ I(ν) = I_0(ν)e^{-κ(ν)L} \tag{2} \]

The spectral absorption coefficient for water vapor is,

\[ κ(ν) = N \cdot χ_{H_2O} \cdot S(T) \cdot φ(ν) \tag{3} \]

where N is the total number density, \( χ_{H_2O} \) is the water vapor mole fraction, S(T) is the linestrength of the temperature dependent transition, and \( φ(ν) \) is the lineshape function. The linestrength of the transition is dependent on the linestrength at a reference temperature, S(T_0), and the lower state energy, E^", of this transition.

\[ S(T) = S(T_0) \frac{Q(T_0)}{Q(T)} \left( \frac{T_0}{T} \right) ^{\frac{hcE^"}{k \left( \frac{1}{T} - \frac{1}{T_0} \right)}} \times \left[ 1 - \exp\left( \frac{-hcν_0}{kT} \right) \right] ^{-1} \left[ 1 - \exp\left( \frac{-hcν_0}{kT_0} \right) \right] ^{-1} \tag{4} \]

where Q(T) is the partition function of the absorbing molecule, h is Planck’s constant, c is the speed of light, and k is Boltzmann’s constant.

The lineshape function is usually approximated by a Voigt profile, which relates concentration of the absorbing species, temperature, pressure, and location of absorption features in the electromagnetic spectrum through its parameters. The equation for the Voigt profile\(^6\) is shown in equation (5), where \( α_D \) and \( α_L \) are the Doppler and Lorentz half-widths, respectively.

\[ φ(ν) = \frac{1}{α_D} \ln \left( \frac{2}{π} \right) \left[ \frac{\ln 2}{α_D} (ν - ν_0), \frac{α_L}{α_D} \ln 2 \right] \tag{5} \]

The collisional half width \( α_L \) is proportional to the pressures of a binary mixture of air and water vapor in the following relation

\[ α_L = PH_{2O} \cdot γ_{self}(T) + PAir \cdot γ_{Air}(T) \tag{7} \]

where P is the partial pressures of the component gases, \( γ_{self} \) is the self-broadening coefficient of water vapor, and \( γ_{Air} \) is the broadening coefficient due to the collisions between the air and water vapor. The collisional broadening coefficients can be calculated with knowledge of the variation of the broadening coefficient with temperature, n, using the following relation

\[ γ(T) = γ(T_0) \left( \frac{T_0}{T} \right)^n \tag{8} \]

where T_0 is the reference temperature. By fitting a Voigt profile to the experimental data, we are able to use our calculated coefficients to determine the water vapor concentration at the exit of the tunnel. Exhaust temperature is calculated from the ratio of the absorbances by two different spectral lines.

Tomographic Image Reconstruction

Image reconstruction from projections has a wide range of applications, from reconstructing the molecular structures of bacteria to supernova remnants. One of the most common applications is the Computerized Tomography (CT) scanner. Tomographic Image Reconstruction is the process of using a source to probe the interior structure of an object through a variety of angles around the object. In this application, near infrared laser light is the source. Each measurement is a single integrated line-of-sight absorption measurement. By varying the degree of orientation of the laser beam for each measurement, a two-dimensional water vapor distribution image can be reconstructed from these one dimensional projections by a reconstruction algorithm, in relation to the origin of the object.

\[ K(x, y) = \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{\exp(-t^2)}{y^2 + (x - t)^2} dt \tag{6} \]
There are two basic groups of reconstruction methods: transform-based reconstructions and finite series expansion. Transform-based reconstruction methods, such as the inverse Radon transform and filtered backprojection algorithm, are generally used when measurements can be taken in an evenly spaced and symmetric geometry. The central slice theorem is commonly used for transform-based reconstruction algorithms. It states that the one-dimensional Fourier transform of each projection taken in the physical space gives a slice of the distribution, at that same angle, in the frequency space. The original distribution is recovered by taking the two-dimensional inverse Fourier transform of the frequency space, which is filled with all of the one-dimensional Fourier transform projections (See Figure 2). Prior knowledge of the distribution is not required for this type of reconstruction method and the reconstruction algorithms are not as computationally intense as iterative methods.\(^5\) Transform-based reconstructions were chosen for this experiment for its symmetric measurement collection geometry that will be used with the large rotational stage.

Series expansion methods are iterative procedures, where the reconstruction variable converges to a solution after several calculations. These methods are computationally efficient, in that they are simple to implement, although artifacts tend to increase as the concentration distributions become more complex and there is slower convergence. The Algebraic Reconstruction Technique (ART) and Maximum Likelihood-Expectation Maximization (MLEM) are two examples. Finite series expansion reconstruction methods evenly divide the image space into a grid of pixels, where the value of the reconstruction variable is assumed to be uniform throughout the pixel. Using an initial guess, a correction factor is multiplied to the reconstruction variable value based on the difference between the measured value and the expected value, until the correct value is converged upon.\(^\)\(^1\)\(^1\)

Several different absorption beam path geometries are possible for data collection measurements. These include parallel beam and fanbeam geometries, which are shown in Figure 4.

---

**Figure 2:** The 1D Fourier transform of a projection at angle \(\theta\) in the physical space represents a slice of the distribution in the frequency space by the Fourier Slice Theorem.

**Figure 3:** The image space is divided into a grid of pixels in series expansion methods.

**Figure 4:** Absorption laser beam path geometries, (a) parallel beam, (b) fan beam.
In the parallel beam geometry, measurements are taken along parallel paths at a particular angle to the origin. In contrast, fanbeam geometry takes measurements in fans across the object at particular increments around the periphery of the object. The parallel beam geometry was not chosen for this experiment due to the size limitations required for collection equipment, time for data collection, and difficulty of implementation on the wind tunnel. The fanbeam geometry allows for a simpler, more compact assembly, only requiring a fixed distance from the object of interest.

**Experimental Design**

Designing the setup for the supersonic combustion tunnel poses a particular challenge. The measurement equipment must be placed in an area protected from heat and with minimal exposure to humidity in the air, which could adversely affect the data. The absorption emitter and detector must be placed as close as possible to the exit plane (measurement location) in order to reduce humidity effects and avoid shock waves produced from the transition of the sub-atmospheric exhaust to atmospheric pressure just downstream of the combustor exit. In order to find the optimal positioning of the equipment and collection of the data, MATLAB was used to simulate the data collection and reconstructions based on input parameters. This will be discussed more in the following section.

**MATLAB Data Analysis**

MATLAB was used to simulate the data collection process as well as reconstructions based on changing several input parameters. The fanbeam geometry in the Image Processing Toolbox in the MATLAB software package was chosen after examining several algorithms to produce the tomographic reconstructions, including the ML-EM and ART series expansion methods. The fanbeam function allows for many input parameters to be changed and is extremely user friendly. The measurement technique was designed to match the parameters for the fanbeam function in MATLAB.

The fanbeam function computes the projections along paths from a single source, fanning across an image matrix (keeping the same vertex, rotating the laser beam until the image is covered). The function then rotates the source around the center of the image to take projections from different angles. The fan rotation angle, fan sensor spacing, and fanbeam vertex are shown in Figure 5. Each of the projections in this figure is equally angularly spaced from one another. The distance from the center of the object to the position of the laser emitter, D, the fan rotation angle, and fan sensor spacing are all parameters that can be changed using the fanbeam function.

The object to be imaged can be any numerical phantom. Several different phantoms (test reconstruction objects) were used to determine the best parameters to achieve optimal internal structure resolution without requiring excessive data collection time. A four millimeter FWHM Gaussian filter was applied to a diamond phantom to reduce the sharp edge gradients and better simulate tunnel data. A diamond phantom was chosen to replicate the shape of the exit of the combustor. The internal structure of the diamond has three varying levels of absorption. This was done to see if differing levels of absorption affected the reconstructions. Figure 6 shows a study of the original and angular spacing around the periphery of the tunnel of the laser emitter and detector to construct a satisfactory reconstruction, setting the distance between the center of the object and the vertex of each fan to be 1250 units (each unit is equivalent is 0.1mm). Bennett et al recommend that the distance between the center of the object and the vertex of each fan be greater than twice the radius of the object being imaged. The Fan Rotation Angle is the angular spacing between each discrete location around the periphery of the laser path. A fan rotation angle of one implies that the emitter/detector fan over the object every degree around the 360 degree total rotation.

From this study, it was decided that a five degree Fan Rotation Angle was adequate for a reconstruction of the phantom. At this Fan Rotation Angle, the artifacts outside the diamond phantom are minimal with a good internal structure reconstruction. The error of the five degree fan rotation angle in relation to the original phantom is 3.28 percent.

![Figure 5: Fan beam parameters that can be varied by fanbeam function in Matlab software package](image-url)
The relative error of each reconstruction is shown in Table 1. Notice the increase in the error as a function of Fan Rotation Angle. We are able to reduce the data collection time by only taking measurements at each five degree increment and sacrificing very little error. With a five degree rotational increment, the emitter/detector will stop at 72 positions during the experiment.

At each of the 72 positions that the emitter/detector stop at around the periphery of the tunnel, a rotary table allows the emitter/detector to fan the laser beam across the object, using the periphery position as the vertex. The angular spacing between each laser beam in the fan is called Fan Sensor Spacing. This is also a parameter that the fanbeam function from the Matlab software package allows to be changed and examined. A Fan Sensor Spacing of one implies that the laser emitter/detector will fan every one degree until the object has been covered. A study of several Fan Sensor Spacings was conducted, determining that a spacing of one degree will be required to prevent artifacts outside the object and to retain the internal structure of the object.

<table>
<thead>
<tr>
<th>Fan Rotation Angle</th>
<th>1</th>
<th>2</th>
<th>5</th>
<th>8</th>
<th>10</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>% Error from original phantom</td>
<td>3.18</td>
<td>3.19</td>
<td>3.28</td>
<td>7.69</td>
<td>8.99</td>
<td>13.4</td>
</tr>
</tbody>
</table>

Table 1: Relative Error from original phantom of the reconstruction based on varying the Fan Rotation Angle

Rotational Stage

A schematic of the tomography setup around the tunnel is shown in Figure 7.

The cubes which house the laser emitter and detector are shown at the bottom of the figure. They are mounted onto a Velmex B5990TS rotary table, which is the vertex of each fan rotation. Through the use of a half inch plate of aluminum, the rotary table is mounted onto a Newport 240CC rotational stage, which will rotate the entire setup 360 degrees around the tunnel exit on the inner rotational ring. The retroreflector is mounted opposite the cubes, but is not shown in Figure 7 for clarity. With such limited access to the areas around the exit of the tunnel, this small portion of the equipment that is moving makes this type of data collection possible. Through the use of additional lasers and rotary tables mounted on the same aluminum plate, the time required to collect data around tunnel exit will be drastically reduced.
**Optical Setup**

Line-of-sight measurements will be taken to determine the water vapor concentration of absorption features with linecenters of 7161.41 and 7165.82. This is achieved by setting the thermo-electric cooler on an ILX Lightwave 3900 laser controller to two temperatures, 15 degrees Celsius and 28 degrees Celsius. Based on the range of frequencies accessible by Laser Components InFGaAsP diode laser, this pair of absorption lines was chosen for their temperature dependence.

The laser is tuned across the absorption feature of interest by modulating the injection current. In this case, a 10 Hz sawtooth wave is applied to the laser diode while keeping its temperature constant. The laser light is transported to the optical setup on the wind tunnel by a single mode optical fiber. The beam path is bolded in Figure 8 above. The laser light strikes a circular mirror in a right angle kinematic mount, which turns the beam 90 degrees and passes through a beam sampler, picking off a small portion of the beam and sending it to a beam sampler detector. Through the use of a beam sampler detector, accurate real-time background noise can be removed from the collected data. Once through the splitter, the beam passes through a hole in another mirror after which it travels across the flowfield to the retroreflector. The retroreflector directs the diverging beam back along the same path across the flowfield. The return beam strikes the mirror with the hole in it and is turned 90 degrees downward to the signal detector. Both detectors are Thorlabs PDA 400 InGaAs photodiode detectors. Both the emitter and detector cubes and retroreflector are purged with nitrogen, shortening the pathlength (optical path length of 18.68cm) that the laser travels through room air, thus reducing unwanted water absorption.

**Figure 9:** Diagram of the mounting of the optical setup and retroreflector on the tunnel

Figure 9 shows the use of the laser emitter/detector to send the laser beam across the tunnel flow, hitting a retroreflector which returns the beam to the receiving detector. The retroreflector is used to simplify the alignment of the laser and to make the optical setup more compact and easier to rotate in the limited area for the instrumentation around the tunnel. It also doubles the path length, strengthening the absorption signal measurements.
Figure 10 shows the optics mounted on the tunnel above for a line-of-sight measurement. The emitter and detector cubes are located on the right side of the image, where the laser is transmitted across the flow to the retroreflector on the left side of the image, before returning to the detector.

To map the frequency of the laser during tuning, a solid etalon is used. The free spectral range of the etalon is 0.12978 cm\(^{-1}\). This data is usually collected at both of the laser diode operating temperatures to use during analysis.

Results

Due to maintenance on the wind tunnel, only water vapor absorption in room air was used for HITRAN comparisons. Line-of-sight measurements will be taken on the University of Virginia dual-mode scramjet combustor wind tunnel facility at different operating conditions in the near future.

The tunable diode laser technique is demonstrated in Figure 11. The injection current is modulated with a 10 Hz sawtooth wave, shown in Figure 11, scanning the laser through the frequency range of interest. The absorption features are shown below the injection current in this figure. In the calculations for determining the water vapor concentration, the background signal collected using the reference signal was subtracted from the raw data. A Voigt fit with a polynomial baseline was then applied to the data.

Figure 12a shows a Voigt fit of the measured absorbance and is compared to its corresponding HITRAN 2006 absorbance values for the laser operating in spectral region A. The conditions in Figures 12 and 13 are room temperature (300K) and a total pressure of 1.0 atmosphere. The fit in Figure 12b shows good agreement between measurements taken at UVA and HITRAN 2006. Matching the Voigt fit and HITRAN peak at 7161.41 cm\(^{-1}\), the concentration of water vapor is found to be 0.0639 mole fraction.
Once this technique has been demonstrated on the supersonic combustion tunnel at the University of Virginia, it will be applied to wind tunnels at the Hypersonic Airbreathing Propulsion Branch at NASA Langley for the Highly Reliable Reusable Launch Systems (HRRLS) project. Through this direct measurement of the performance of a scramjet combustor, a greater knowledge and understanding of the fundamental physics of high speed combustors will be achieved.

Acknowledgements

This research was supported by grants from NASA Langley Research Center and the Virginia Space Grant Consortium. The author would like to thank Roland Krauss at the University of Virginia and Glenn Diskin at NASA Langley for all of their support and assistance on this project.

References

4Cormack, Allen M., “Early two-dimensional reconstruction and recent topics stemming from it,” Nobel Lecture, 8 December 1979.


